



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:14 AM UTC

PDB ID : 3KBH / pdb_00003kbh
Title : Crystal structure of NL63 respiratory coronavirus receptor-binding domain complexed with its human receptor
Authors : Wu, K.; Li, W.; Peng, G.; Li, F.
Deposited on : 2009-10-20
Resolution : 3.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

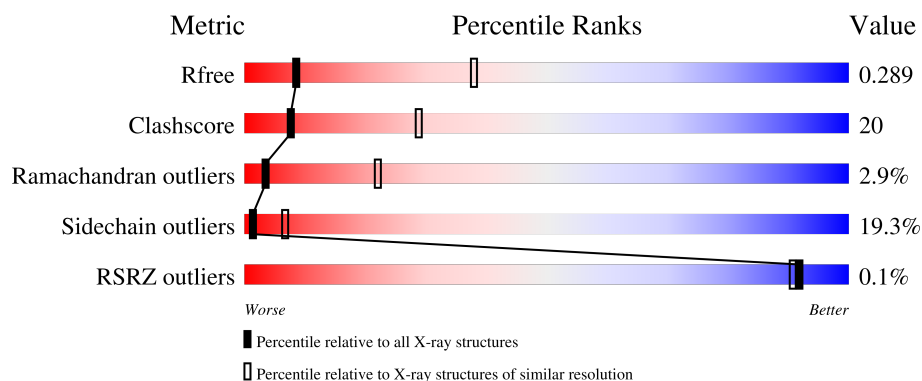
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	597	 53% 36% 9% ..
1	B	597	 56% 34% 9% ..
1	C	597	 54% 36% 9% ..
1	D	597	 53% 36% 9% ..
2	E	136	 39% 24% 14% . 19%

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Mol	Chain	Length	Quality of chain
2	F	136	
2	G	136	
2	H	136	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	801	X	-	-	-
3	NAG	B	801	X	-	-	-
3	NAG	C	801	X	-	-	-
3	NAG	D	801	X	-	-	-
3	NAG	E	1486	X	-	-	-
3	NAG	E	1512	X	-	-	-
3	NAG	F	1486	X	-	-	-
3	NAG	F	1512	X	-	-	-
3	NAG	G	1486	X	-	-	-
3	NAG	G	1512	X	-	-	-
3	NAG	H	1486	X	-	-	-
3	NAG	H	1512	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	B	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	C	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	D	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	F	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	G	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	H	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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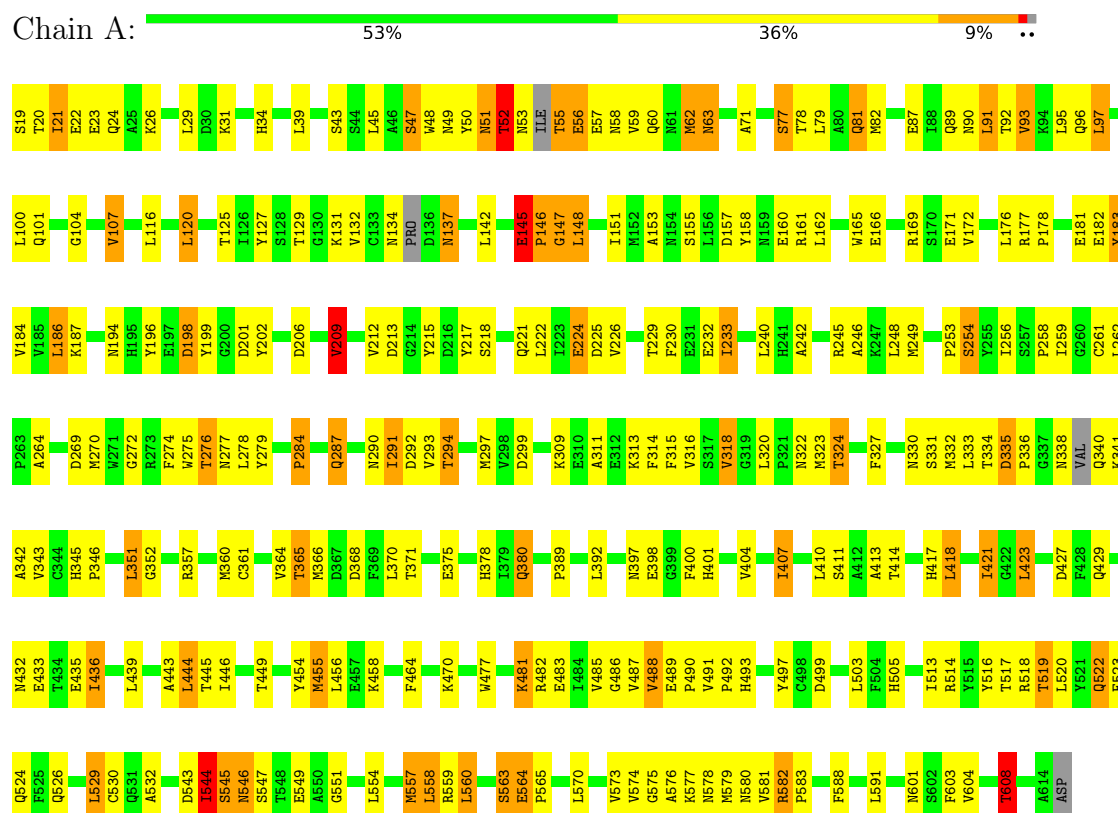
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

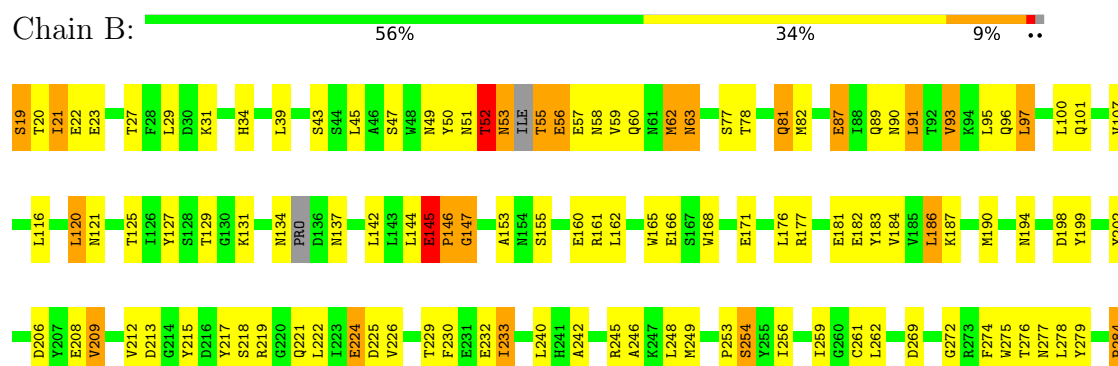
3 Residue-property plots

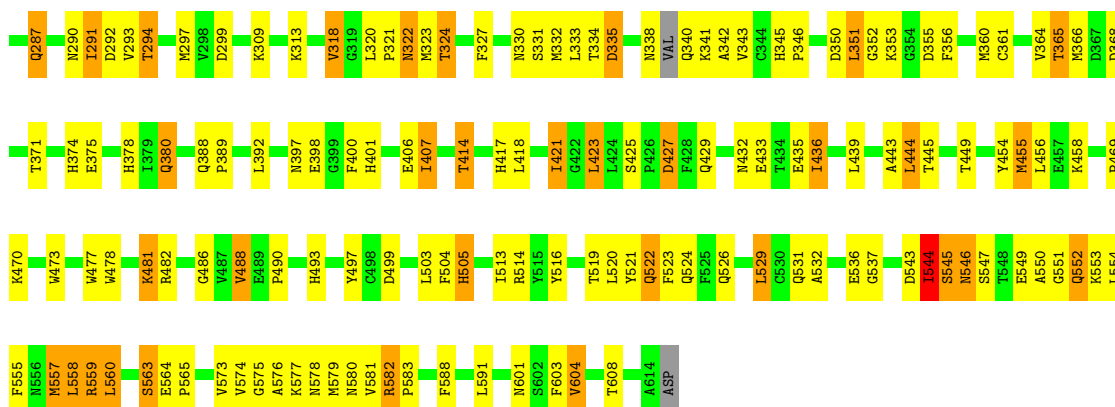
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Angiotensin-converting enzyme 2



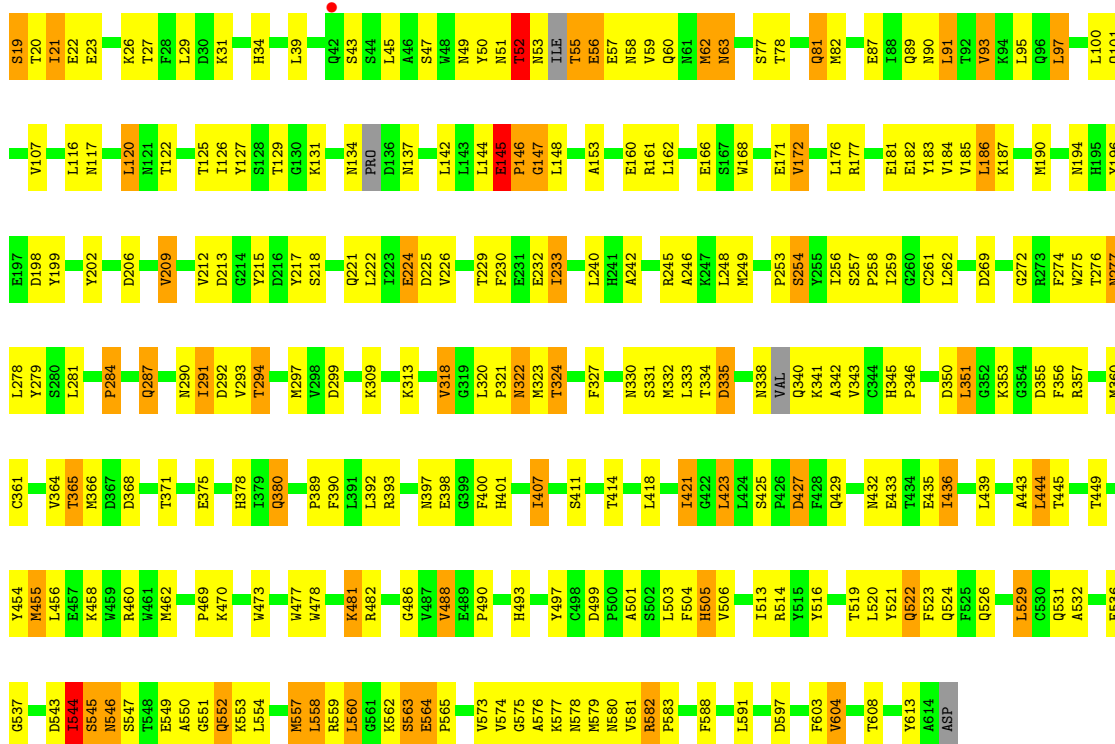
• Molecule 1: Angiotensin-converting enzyme 2





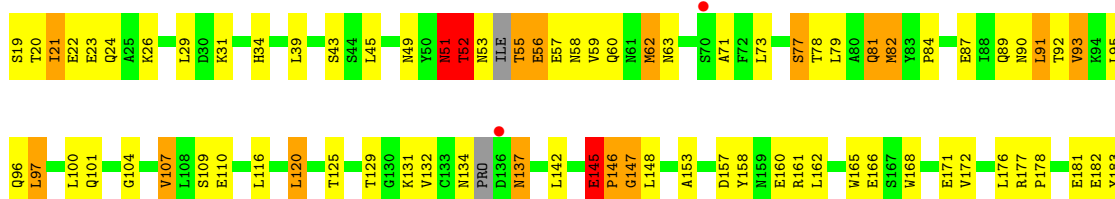
• Molecule 1: Angiotensin-converting enzyme 2

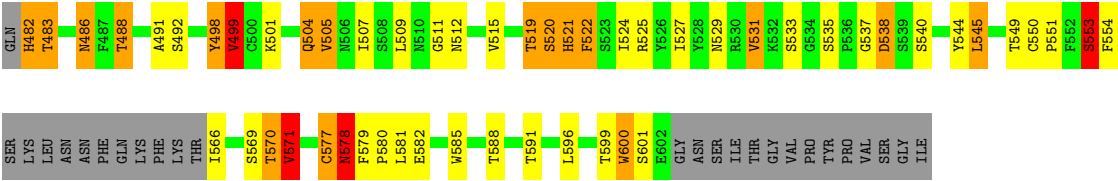
Chain C: 54% 36% 9% ..



• Molecule 1: Angiotensin-converting enzyme 2

Chain D: 53% 36% 9% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.76Å 77.76Å 631.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 3.31 49.01 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.01-3.31) 90.4 (49.01-3.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.268 , 0.300 0.263 , 0.289	Depositor DCC
R_{free} test set	3040 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 127.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	3/4973 (0.1%)	1.05	6/6750 (0.1%)
1	B	0.82	2/4973 (0.0%)	1.06	9/6750 (0.1%)
1	C	0.80	2/4973 (0.0%)	1.04	8/6750 (0.1%)
1	D	0.81	3/4973 (0.1%)	1.04	7/6750 (0.1%)
2	E	1.07	0/888	1.26	9/1212 (0.7%)
2	F	0.97	2/888 (0.2%)	1.22	5/1212 (0.4%)
2	G	0.95	2/888 (0.2%)	1.20	5/1212 (0.4%)
2	H	1.08	0/888	1.27	10/1212 (0.8%)
All	All	0.85	14/23444 (0.1%)	1.08	59/31848 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	1
All	All	0	11

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	VAL	CA-CB	9.35	1.67	1.54
1	C	59	VAL	CA-CB	8.31	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	VAL	CA-CB	7.59	1.65	1.54
1	D	59	VAL	CA-CB	7.58	1.65	1.54
2	G	592	ILE	CA-CB	6.02	1.60	1.53
2	G	499	VAL	CA-CB	5.65	1.62	1.54
1	A	59	VAL	CA-C	5.62	1.60	1.52
1	D	51	ASN	CA-C	5.57	1.59	1.52
1	C	59	VAL	CA-C	5.51	1.60	1.52
2	F	499	VAL	CA-CB	5.40	1.61	1.54
1	B	53	ASN	CA-C	5.34	1.59	1.52
2	F	592	ILE	CA-CB	5.32	1.60	1.54
1	D	59	VAL	CA-C	5.26	1.60	1.52
1	A	209	VAL	CA-CB	5.21	1.61	1.54

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	THR	N-CA-C	10.36	123.54	111.11
1	C	52	THR	N-CA-C	9.58	122.61	111.11
1	D	52	THR	N-CA-C	7.91	124.34	111.37
1	A	52	THR	N-CA-C	7.75	124.08	111.37
2	F	538	ASP	N-CA-C	-6.97	101.30	110.43
2	H	538	ASP	N-CA-C	-6.84	101.47	110.43
2	H	540	SER	N-CA-C	-6.79	104.20	113.30
1	D	345	HIS	CA-C-N	6.73	127.78	119.98
1	D	345	HIS	C-N-CA	6.73	127.78	119.98
2	E	538	ASP	N-CA-C	-6.48	101.94	110.43
2	E	501	LYS	CA-C-N	-6.33	113.26	119.78
2	E	501	LYS	C-N-CA	-6.33	113.26	119.78
1	C	345	HIS	CA-C-N	6.30	127.29	119.98
1	C	345	HIS	C-N-CA	6.30	127.29	119.98
2	E	540	SER	N-CA-C	-6.26	104.92	113.30
2	G	538	ASP	N-CA-C	-6.24	102.26	110.43
2	E	553	SER	N-CA-C	6.11	122.12	113.02
2	F	570	THR	N-CA-C	-6.10	102.43	110.43
2	H	570	THR	N-CA-C	-5.99	102.58	110.43
2	H	501	LYS	CA-C-N	-5.99	113.52	119.92
2	H	501	LYS	C-N-CA	-5.99	113.52	119.92
1	B	345	HIS	CA-C-N	5.90	126.82	119.98
1	B	345	HIS	C-N-CA	5.90	126.82	119.98
1	B	536	GLU	N-CA-C	5.82	120.17	112.72
2	E	570	THR	N-CA-C	-5.81	102.82	110.43
2	F	501	LYS	CA-C-N	-5.78	113.74	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	LYS	C-N-CA	-5.78	113.74	119.92
2	H	521	HIS	N-CA-C	5.75	123.05	110.80
2	E	521	HIS	N-CA-C	5.70	122.94	110.80
2	E	493	PHE	N-CA-C	5.64	118.66	109.24
1	C	537	GLY	CA-C-N	5.63	125.64	119.90
1	C	537	GLY	C-N-CA	5.63	125.64	119.90
1	B	537	GLY	CA-C-N	5.56	125.57	119.90
1	B	537	GLY	C-N-CA	5.56	125.57	119.90
1	A	345	HIS	CA-C-N	5.53	126.39	119.98
1	A	345	HIS	C-N-CA	5.53	126.39	119.98
1	A	564	GLU	N-CA-C	-5.50	103.20	110.40
2	E	549	THR	N-CA-C	5.50	118.78	111.75
2	H	549	THR	N-CA-C	5.29	118.52	111.75
2	F	521	HIS	N-CA-C	5.27	122.03	110.80
1	B	604	VAL	N-CA-C	5.27	115.36	107.51
1	A	564	GLU	CA-C-N	5.26	125.26	119.90
1	A	564	GLU	C-N-CA	5.26	125.26	119.90
1	C	604	VAL	N-CA-C	5.24	115.31	107.51
1	D	351	LEU	N-CA-C	-5.19	104.02	110.41
2	G	521	HIS	N-CA-C	5.18	121.84	110.80
1	B	414	THR	CA-C-N	5.16	124.60	119.24
1	B	414	THR	C-N-CA	5.16	124.60	119.24
2	H	553	SER	N-CA-C	5.15	122.02	113.89
2	G	501	LYS	CA-C-N	-5.12	114.44	119.92
2	G	501	LYS	C-N-CA	-5.12	114.44	119.92
1	D	564	GLU	N-CA-C	-5.12	103.69	110.40
1	D	547	SER	N-CA-C	5.09	117.42	108.56
2	H	571	VAL	N-CA-C	5.07	119.89	109.34
2	H	529	ASN	N-CA-C	5.03	116.82	108.02
1	C	536	GLU	N-CA-C	5.02	119.15	112.72
2	G	570	THR	N-CA-C	-5.01	103.72	110.24
1	C	564	GLU	N-CA-C	-5.01	103.84	110.40
1	D	329	GLU	N-CA-C	5.01	118.65	112.54

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Peptide
1	B	145	GLU	Peptide
1	C	145	GLU	Peptide
1	D	145	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	E	520	SER	Peptide
2	E	569	SER	Peptide
2	F	520	SER	Peptide
2	F	569	SER	Peptide
2	G	520	SER	Peptide
2	G	569	SER	Peptide
2	H	520	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4840	0	4607	183	2
1	B	4840	0	4607	175	0
1	C	4840	0	4607	173	0
1	D	4840	0	4607	184	2
2	E	860	0	797	49	0
2	F	860	0	797	52	2
2	G	860	0	797	47	2
2	H	860	0	797	44	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
3	E	28	0	26	1	0
3	F	28	0	26	1	0
3	G	28	0	26	0	0
3	H	28	0	26	1	0
All	All	23024	0	21824	899	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (899) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:483:THR:HG22	2:G:519:THR:HG23	1.30	1.14
2:E:483:THR:HG22	2:E:519:THR:HG23	1.27	1.13
1:D:51:ASN:HD22	1:D:343:VAL:HG22	1.13	1.10
1:B:145:GLU:OE1	1:B:145:GLU:HA	1.51	1.08
2:F:483:THR:HG22	2:F:519:THR:HG23	1.35	1.07
2:H:483:THR:HG22	2:H:519:THR:HG23	1.28	1.07
1:D:51:ASN:ND2	1:D:343:VAL:HG22	1.70	1.06
1:C:145:GLU:HA	1:C:145:GLU:OE1	1.56	1.06
1:B:53:ASN:O	1:B:55:THR:N	1.89	1.05
2:G:498:TYR:O	2:G:499:VAL:HB	1.55	1.05
1:B:51:ASN:ND2	1:B:343:VAL:HG22	1.75	1.01
2:E:498:TYR:O	2:E:499:VAL:HB	1.56	1.01
2:F:498:TYR:O	2:F:499:VAL:HB	1.57	1.00
2:E:483:THR:HG22	2:E:519:THR:CG2	1.92	0.99
2:H:498:TYR:O	2:H:499:VAL:HB	1.60	0.99
2:H:483:THR:HG22	2:H:519:THR:CG2	1.91	0.98
1:A:51:ASN:HD22	1:A:343:VAL:HG22	1.25	0.98
1:A:145:GLU:HA	1:A:145:GLU:OE1	1.61	0.98
2:G:483:THR:HG22	2:G:519:THR:CG2	1.94	0.98
1:A:51:ASN:ND2	1:A:343:VAL:HG22	1.78	0.97
1:C:51:ASN:ND2	1:C:343:VAL:HG22	1.80	0.97
1:B:81:GLN:HE21	1:B:81:GLN:HA	1.29	0.95
2:F:483:THR:HG22	2:F:519:THR:CG2	1.97	0.95
2:E:578:ASN:H	2:E:578:ASN:HD22	1.14	0.94
1:D:560:LEU:O	1:D:563:SER:HB3	1.68	0.93
2:H:578:ASN:H	2:H:578:ASN:HD22	1.17	0.93
1:D:145:GLU:OE1	1:D:145:GLU:HA	1.67	0.92
1:C:53:ASN:O	1:C:55:THR:N	2.01	0.91
1:C:81:GLN:HE21	1:C:81:GLN:HA	1.31	0.91
1:B:161:ARG:HH12	1:B:278:LEU:HD22	1.34	0.90
1:C:161:ARG:HH12	1:C:278:LEU:HD22	1.36	0.90
1:D:81:GLN:HE21	1:D:81:GLN:HA	1.36	0.89
1:A:81:GLN:HA	1:A:81:GLN:HE21	1.37	0.89
1:A:229:THR:HG23	1:A:516:TYR:OH	1.75	0.87
1:B:51:ASN:HD22	1:B:343:VAL:HG22	1.34	0.87
1:A:560:LEU:O	1:A:563:SER:HB3	1.75	0.86
2:G:578:ASN:HD22	2:G:578:ASN:H	1.22	0.85
1:C:560:LEU:O	1:C:563:SER:HB3	1.76	0.85
2:F:553:SER:O	2:F:554:PHE:HB2	1.77	0.85
1:A:161:ARG:HH12	1:A:278:LEU:HD22	1.40	0.84
1:D:53:ASN:O	1:D:55:THR:N	2.10	0.84
2:H:483:THR:CG2	2:H:519:THR:HG23	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:483:THR:CG2	2:E:519:THR:HG23	2.07	0.84
1:B:153:ALA:HA	1:B:277:ASN:OD1	1.78	0.83
2:F:578:ASN:HD22	2:F:578:ASN:H	1.23	0.83
1:C:51:ASN:HD22	1:C:343:VAL:HG22	1.38	0.83
1:C:153:ALA:HA	1:C:277:ASN:OD1	1.78	0.83
1:C:21:ILE:HD13	1:C:21:ILE:H	1.43	0.82
2:G:553:SER:O	2:G:554:PHE:HB2	1.78	0.82
1:D:327:PHE:O	1:D:331:SER:HB2	1.80	0.82
1:A:53:ASN:O	1:A:55:THR:N	2.12	0.82
1:D:229:THR:HG23	1:D:516:TYR:OH	1.80	0.81
2:G:483:THR:CG2	2:G:519:THR:HG23	2.10	0.81
1:C:327:PHE:O	1:C:331:SER:HB2	1.80	0.81
1:B:560:LEU:O	1:B:563:SER:HB3	1.80	0.81
1:B:97:LEU:O	1:B:101:GLN:HG2	1.80	0.81
1:D:21:ILE:HD13	1:D:21:ILE:H	1.45	0.80
1:A:327:PHE:O	1:A:331:SER:HB2	1.82	0.80
1:A:153:ALA:HA	1:A:277:ASN:OD1	1.82	0.80
1:A:183:TYR:O	1:A:187:LYS:HB2	1.82	0.79
1:B:21:ILE:HD13	1:B:21:ILE:H	1.45	0.79
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.65	0.79
1:A:21:ILE:H	1:A:21:ILE:HD13	1.45	0.79
1:C:183:TYR:O	1:C:187:LYS:HB2	1.82	0.79
2:E:553:SER:O	2:E:554:PHE:HB2	1.80	0.79
1:B:217:TYR:HE1	1:B:578:ASN:ND2	1.81	0.79
2:G:566:ILE:HG12	2:G:600:TRP:HA	1.65	0.79
1:D:153:ALA:HA	1:D:277:ASN:OD1	1.82	0.79
1:A:97:LEU:O	1:A:101:GLN:HG2	1.83	0.78
1:B:183:TYR:O	1:B:187:LYS:HB2	1.83	0.78
1:C:97:LEU:O	1:C:101:GLN:HG2	1.82	0.77
1:D:183:TYR:O	1:D:187:LYS:HB2	1.85	0.77
2:F:566:ILE:HG12	2:F:600:TRP:HA	1.66	0.77
1:C:323:MET:HE1	1:C:380:GLN:HE22	1.50	0.77
1:D:161:ARG:HH12	1:D:278:LEU:HD22	1.49	0.77
1:D:62:MET:HG3	1:D:63:ASN:N	2.00	0.76
1:D:97:LEU:O	1:D:101:GLN:HG2	1.84	0.76
1:B:327:PHE:O	1:B:331:SER:HB2	1.86	0.75
2:H:553:SER:O	2:H:554:PHE:HB2	1.85	0.75
1:A:493:HIS:CD2	1:A:499:ASP:OD1	2.40	0.74
1:D:493:HIS:HD2	1:D:499:ASP:OD1	1.68	0.74
1:D:323:MET:HE1	1:D:380:GLN:HE22	1.53	0.74
2:E:566:ILE:HG12	2:E:600:TRP:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLN:NE2	1:A:580:ASN:H	1.86	0.73
1:C:544:ILE:O	1:C:547:SER:HB2	1.87	0.73
1:D:407:ILE:HD11	1:D:529:LEU:HD22	1.70	0.73
1:A:323:MET:HE1	1:A:380:GLN:HE22	1.54	0.73
1:C:162:LEU:CD1	1:C:490:PRO:HB2	2.18	0.73
2:H:486:ASN:HB3	2:H:527:ILE:HD12	1.70	0.73
2:E:486:ASN:HB3	2:E:527:ILE:HD12	1.70	0.73
2:F:483:THR:CG2	2:F:519:THR:HG23	2.16	0.73
1:A:62:MET:HG3	1:A:63:ASN:N	2.03	0.72
2:G:491:ALA:O	2:G:531:VAL:HG22	1.89	0.72
1:B:218:SER:HB3	1:B:221:GLN:HB2	1.71	0.72
1:D:524:GLN:NE2	1:D:580:ASN:H	1.87	0.72
1:B:162:LEU:CD1	1:B:490:PRO:HB2	2.19	0.72
1:A:182:GLU:O	1:A:186:LEU:HD12	1.90	0.72
1:B:323:MET:HE1	1:B:380:GLN:HE22	1.55	0.72
1:C:217:TYR:HE1	1:C:578:ASN:ND2	1.86	0.71
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.70	0.71
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.73	0.71
1:B:545:SER:O	1:B:546:ASN:HB2	1.90	0.71
1:C:245:ARG:HB3	1:C:262:LEU:HD21	1.72	0.71
1:B:229:THR:HG23	1:B:516:TYR:OH	1.90	0.71
1:B:245:ARG:HB3	1:B:262:LEU:HD21	1.70	0.71
2:H:566:ILE:HG12	2:H:600:TRP:HA	1.72	0.71
1:A:245:ARG:HB3	1:A:262:LEU:HD21	1.72	0.71
1:D:574:VAL:HG23	1:D:576:ALA:H	1.56	0.70
1:A:233:ILE:HD13	1:A:233:ILE:O	1.92	0.70
1:C:229:THR:HG23	1:C:516:TYR:OH	1.91	0.70
1:D:524:GLN:HG2	1:D:583:PRO:HG2	1.74	0.70
1:A:574:VAL:HG23	1:A:576:ALA:H	1.54	0.70
1:A:162:LEU:CD1	1:A:490:PRO:HB2	2.22	0.70
1:C:524:GLN:HG2	1:C:583:PRO:HG2	1.72	0.70
1:D:493:HIS:CD2	1:D:499:ASP:OD1	2.44	0.70
2:G:488:THR:HG22	2:G:527:ILE:HB	1.72	0.70
2:E:488:THR:HG22	2:E:527:ILE:HB	1.72	0.70
1:C:493:HIS:HD2	1:C:499:ASP:OD1	1.74	0.70
1:C:218:SER:HB3	1:C:221:GLN:HB2	1.74	0.70
2:F:491:ALA:O	2:F:531:VAL:HG22	1.92	0.69
1:B:62:MET:HG3	1:B:63:ASN:N	2.06	0.69
1:A:601:ASN:ND2	1:C:254:SER:O	2.26	0.69
1:B:134:ASN:HB2	1:B:137:ASN:HB3	1.75	0.69
1:B:493:HIS:CD2	1:B:499:ASP:OD1	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLU:O	1:D:186:LEU:HD12	1.92	0.69
1:B:224:GLU:HG3	1:B:225:ASP:N	2.08	0.69
1:C:574:VAL:HG23	1:C:576:ALA:H	1.58	0.69
2:G:486:ASN:HB3	2:G:527:ILE:HD12	1.75	0.69
1:D:545:SER:O	1:D:546:ASN:HB2	1.93	0.69
1:B:161:ARG:NH1	1:B:278:LEU:HD22	2.08	0.68
1:C:134:ASN:HB2	1:C:137:ASN:HB3	1.76	0.68
1:D:245:ARG:HB3	1:D:262:LEU:HD21	1.75	0.68
1:B:544:ILE:O	1:B:547:SER:HB2	1.93	0.68
1:C:545:SER:O	1:C:546:ASN:HB2	1.92	0.68
1:A:261:CYS:HB3	1:A:486:GLY:C	2.18	0.68
1:B:261:CYS:HB3	1:B:486:GLY:C	2.19	0.68
1:B:297:MET:HG3	1:B:423:LEU:HD21	1.76	0.68
1:B:414:THR:HG21	1:B:543:ASP:HB2	1.76	0.68
1:B:574:VAL:HG23	1:B:576:ALA:H	1.59	0.67
1:D:290:ASN:ND2	1:D:292:ASP:HB2	2.09	0.67
1:A:545:SER:O	1:A:546:ASN:HB2	1.94	0.67
1:C:224:GLU:HG3	1:C:225:ASP:N	2.10	0.67
1:D:162:LEU:CD1	1:D:490:PRO:HB2	2.24	0.67
1:B:125:THR:O	1:B:129:THR:HG22	1.94	0.67
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.77	0.67
2:F:488:THR:HG22	2:F:527:ILE:HB	1.75	0.67
1:C:125:THR:O	1:C:129:THR:HG22	1.94	0.67
1:A:218:SER:HB3	1:A:221:GLN:HB2	1.76	0.67
1:A:293:VAL:HB	1:A:423:LEU:HD22	1.75	0.66
1:B:81:GLN:HE21	1:B:81:GLN:CA	2.02	0.66
1:D:217:TYR:HE1	1:D:578:ASN:ND2	1.93	0.66
1:D:134:ASN:HB2	1:D:137:ASN:HB3	1.77	0.66
1:C:297:MET:HG3	1:C:423:LEU:HD21	1.76	0.66
2:H:488:THR:HG22	2:H:527:ILE:HB	1.78	0.66
1:C:62:MET:HG3	1:C:63:ASN:N	2.09	0.66
1:A:60:GLN:HA	1:A:63:ASN:HD21	1.60	0.66
1:A:269:ASP:OD2	1:A:272:GLY:N	2.26	0.66
1:C:493:HIS:CD2	1:C:499:ASP:OD1	2.49	0.66
1:D:81:GLN:HE21	1:D:81:GLN:CA	2.08	0.66
1:C:375:GLU:O	1:C:378:HIS:HB2	1.97	0.65
2:F:486:ASN:HB3	2:F:527:ILE:HD12	1.77	0.65
1:B:233:ILE:HD13	1:B:233:ILE:O	1.96	0.65
1:C:91:LEU:HD12	1:C:91:LEU:H	1.61	0.65
1:D:297:MET:HG3	1:D:423:LEU:HD21	1.79	0.65
1:A:107:VAL:HG11	1:A:194:ASN:OD1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HD11	1:A:529:LEU:HD22	1.77	0.65
1:B:290:ASN:ND2	1:B:292:ASP:HB2	2.11	0.65
1:A:505:HIS:CD2	1:A:505:HIS:H	2.12	0.65
1:C:81:GLN:HE21	1:C:81:GLN:CA	2.02	0.65
1:A:290:ASN:ND2	1:A:292:ASP:HB2	2.12	0.65
2:E:578:ASN:HD22	2:E:578:ASN:N	1.90	0.65
1:D:107:VAL:HG11	1:D:194:ASN:OD1	1.96	0.65
1:D:293:VAL:HB	1:D:423:LEU:HD22	1.79	0.65
1:D:212:VAL:HG12	1:D:215:TYR:HB2	1.79	0.64
2:H:499:VAL:HG22	2:H:585:TRP:CD2	2.32	0.64
1:D:49:ASN:HB3	1:D:58:ASN:HD22	1.63	0.64
1:C:212:VAL:HG12	1:C:215:TYR:HB2	1.80	0.64
1:C:246:ALA:HA	1:C:249:MET:HE2	1.79	0.64
1:A:134:ASN:HB2	1:A:137:ASN:HB3	1.80	0.64
1:D:261:CYS:HB3	1:D:486:GLY:C	2.21	0.64
1:B:246:ALA:HA	1:B:249:MET:HE2	1.80	0.64
1:C:49:ASN:HB3	1:C:58:ASN:HD22	1.63	0.64
2:G:553:SER:O	2:G:554:PHE:CB	2.45	0.64
1:A:212:VAL:HG12	1:A:215:TYR:HB2	1.79	0.64
2:F:553:SER:O	2:F:554:PHE:CB	2.45	0.64
1:C:161:ARG:NH1	1:C:278:LEU:HD22	2.09	0.64
2:E:499:VAL:HG22	2:E:585:TRP:CD2	2.33	0.64
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.79	0.64
1:D:218:SER:HB3	1:D:221:GLN:HB2	1.79	0.64
1:A:81:GLN:HE21	1:A:81:GLN:CA	2.08	0.63
2:F:499:VAL:HG22	2:F:585:TRP:CD2	2.34	0.63
1:A:297:MET:HG3	1:A:423:LEU:HD21	1.79	0.63
1:C:414:THR:HG21	1:C:543:ASP:HB2	1.80	0.63
1:D:505:HIS:H	1:D:505:HIS:CD2	2.17	0.63
2:E:545:LEU:HB3	2:E:581:LEU:HD12	1.81	0.63
2:H:545:LEU:HB3	2:H:581:LEU:HD12	1.81	0.63
1:A:60:GLN:O	1:A:63:ASN:OD1	2.17	0.63
1:C:334:THR:O	1:C:335:ASP:HB3	1.99	0.62
1:B:505:HIS:H	1:B:505:HIS:CD2	2.17	0.62
2:F:578:ASN:H	2:F:578:ASN:ND2	1.96	0.62
1:C:290:ASN:ND2	1:C:292:ASP:HB2	2.14	0.62
1:D:375:GLU:O	1:D:378:HIS:HB2	1.99	0.62
1:B:439:LEU:HD23	1:B:591:LEU:HB2	1.81	0.62
1:C:60:GLN:HA	1:C:63:ASN:HD21	1.64	0.62
2:G:499:VAL:HG22	2:G:585:TRP:CD2	2.34	0.62
1:B:142:LEU:HD22	1:B:147:GLY:HA2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:492:SER:HA	2:F:531:VAL:HG23	1.79	0.62
1:D:400:PHE:O	1:D:404:VAL:HG23	2.00	0.62
2:H:553:SER:O	2:H:554:PHE:CB	2.48	0.62
1:A:177:ARG:NH1	1:A:470:LYS:O	2.30	0.62
1:A:544:ILE:O	1:A:547:SER:HB2	1.98	0.62
1:B:212:VAL:HG12	1:B:215:TYR:HB2	1.79	0.62
1:A:125:THR:O	1:A:129:THR:HG22	1.99	0.62
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.80	0.62
1:D:230:PHE:HA	1:D:233:ILE:HG22	1.81	0.62
1:A:161:ARG:NH1	1:A:278:LEU:HD22	2.14	0.62
2:F:545:LEU:HB3	2:F:581:LEU:HD12	1.80	0.62
1:C:142:LEU:HD22	1:C:147:GLY:HA2	1.82	0.61
1:C:505:HIS:CD2	1:C:505:HIS:H	2.16	0.61
1:C:439:LEU:HD23	1:C:591:LEU:HB2	1.81	0.61
2:E:491:ALA:O	2:E:531:VAL:HG22	2.00	0.61
1:C:182:GLU:O	1:C:186:LEU:HD12	2.01	0.61
1:C:293:VAL:HB	1:C:423:LEU:HD22	1.82	0.61
2:G:492:SER:HA	2:G:531:VAL:HG23	1.81	0.61
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.82	0.61
2:G:545:LEU:HB3	2:G:581:LEU:HD12	1.81	0.61
1:D:233:ILE:HD13	1:D:233:ILE:O	2.00	0.61
1:C:261:CYS:HB3	1:C:486:GLY:C	2.25	0.61
1:D:60:GLN:HA	1:D:63:ASN:HD21	1.65	0.60
1:D:91:LEU:HD12	1:D:91:LEU:H	1.66	0.60
2:E:553:SER:O	2:E:554:PHE:CB	2.46	0.60
2:G:578:ASN:H	2:G:578:ASN:ND2	1.97	0.60
2:E:492:SER:HA	2:E:531:VAL:HG23	1.83	0.60
1:B:293:VAL:HB	1:B:423:LEU:HD22	1.82	0.60
1:D:125:THR:O	1:D:129:THR:HG22	2.01	0.60
1:D:334:THR:O	1:D:335:ASP:HB3	2.01	0.60
1:B:245:ARG:O	1:B:249:MET:HG3	2.02	0.60
1:A:334:THR:O	1:A:335:ASP:HB3	2.02	0.60
2:E:482:HIS:CD2	2:E:483:THR:N	2.70	0.60
1:A:246:ALA:HA	1:A:249:MET:HE2	1.83	0.60
1:C:222:LEU:O	1:C:226:VAL:HG23	2.02	0.60
1:B:91:LEU:HD12	1:B:91:LEU:H	1.66	0.59
1:B:107:VAL:HG11	1:B:194:ASN:OD1	2.02	0.59
1:C:327:PHE:O	1:C:331:SER:CB	2.50	0.59
1:D:60:GLN:O	1:D:63:ASN:OD1	2.20	0.59
1:B:334:THR:O	1:B:335:ASP:HB3	2.01	0.59
2:H:491:ALA:O	2:H:531:VAL:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:ND2	1:D:343:VAL:CG2	2.57	0.59
1:A:166:GLU:OE2	1:A:497:TYR:OH	2.17	0.59
1:C:233:ILE:HD13	1:C:233:ILE:O	2.03	0.59
1:C:407:ILE:HD11	1:C:529:LEU:HD22	1.85	0.58
1:C:524:GLN:NE2	1:C:580:ASN:H	2.01	0.58
1:B:557:MET:HE3	1:B:558:LEU:HD12	1.84	0.58
1:A:276:THR:HG23	1:A:445:THR:OG1	2.02	0.58
1:A:327:PHE:O	1:A:331:SER:CB	2.52	0.58
2:F:553:SER:HA	2:F:579:PHE:HE1	1.67	0.58
1:A:414:THR:HG21	1:A:543:ASP:HB2	1.85	0.58
1:C:177:ARG:NH1	1:C:470:LYS:O	2.37	0.58
1:A:224:GLU:HG3	1:A:225:ASP:N	2.18	0.58
1:C:397:ASN:OD1	1:C:400:PHE:HD1	1.87	0.58
2:G:578:ASN:O	2:G:580:PRO:HD3	2.03	0.58
1:D:327:PHE:O	1:D:331:SER:CB	2.50	0.58
1:A:217:TYR:HE1	1:A:578:ASN:ND2	2.02	0.57
2:G:553:SER:HA	2:G:579:PHE:HE1	1.68	0.57
1:B:226:VAL:HA	1:B:229:THR:HG22	1.86	0.57
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.85	0.57
1:B:375:GLU:O	1:B:378:HIS:HB2	2.04	0.57
1:D:544:ILE:O	1:D:547:SER:HB2	2.04	0.57
2:H:578:ASN:O	2:H:580:PRO:HD3	2.05	0.57
1:B:60:GLN:HA	1:B:63:ASN:HD21	1.70	0.57
1:C:107:VAL:HG11	1:C:194:ASN:OD1	2.05	0.57
1:C:162:LEU:HD13	1:C:490:PRO:HB2	1.87	0.57
1:C:335:ASP:HB2	1:C:361:CYS:SG	2.44	0.57
1:A:400:PHE:O	1:A:404:VAL:HG23	2.04	0.57
1:A:418:LEU:O	1:A:421:ILE:HG22	2.05	0.57
1:A:456:LEU:HD23	1:A:477:TRP:HH2	1.69	0.57
2:G:491:ALA:O	2:G:531:VAL:CG2	2.52	0.57
2:G:578:ASN:HD22	2:G:578:ASN:N	1.95	0.56
1:D:161:ARG:NH1	1:D:278:LEU:HD22	2.19	0.56
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.86	0.56
1:A:248:LEU:HB3	1:A:256:ILE:HD13	1.87	0.56
1:B:182:GLU:O	1:B:186:LEU:HD12	2.04	0.56
1:D:418:LEU:O	1:D:421:ILE:HG22	2.05	0.56
1:A:49:ASN:HB3	1:A:58:ASN:HD22	1.71	0.56
1:D:248:LEU:HB3	1:D:256:ILE:HD13	1.87	0.56
1:D:245:ARG:O	1:D:249:MET:HG3	2.05	0.56
2:E:553:SER:HA	2:E:579:PHE:HE1	1.71	0.56
1:B:162:LEU:HD13	1:B:490:PRO:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:535:SER:C	2:F:537:GLY:H	2.14	0.56
1:D:246:ALA:HA	1:D:249:MET:HE2	1.87	0.56
1:C:226:VAL:HA	1:C:229:THR:HG22	1.86	0.56
1:D:582:ARG:O	1:D:583:PRO:C	2.48	0.56
1:A:226:VAL:HA	1:A:229:THR:HG22	1.86	0.56
1:B:217:TYR:CE1	1:B:578:ASN:ND2	2.70	0.56
1:D:389:PRO:HG2	1:D:392:LEU:HD22	1.87	0.56
2:H:482:HIS:CD2	2:H:483:THR:N	2.74	0.56
2:H:483:THR:CG2	2:H:519:THR:CG2	2.73	0.56
2:E:483:THR:CG2	2:E:519:THR:CG2	2.75	0.55
1:C:320:LEU:HD13	1:C:380:GLN:HG2	1.87	0.55
1:D:226:VAL:HA	1:D:229:THR:HG22	1.88	0.55
1:B:60:GLN:O	1:B:63:ASN:OD1	2.25	0.55
1:D:324:THR:O	1:D:327:PHE:HB3	2.06	0.55
1:A:187:LYS:HE3	1:A:199:TYR:CZ	2.42	0.55
2:E:550:CYS:HB2	2:E:551:PRO:CD	2.36	0.55
1:B:327:PHE:O	1:B:331:SER:CB	2.55	0.55
1:B:455:MET:SD	1:B:481:LYS:HG2	2.46	0.55
1:D:181:GLU:O	1:D:184:VAL:HG22	2.06	0.55
1:A:582:ARG:O	1:A:583:PRO:C	2.48	0.55
1:A:324:THR:O	1:A:327:PHE:HB3	2.06	0.55
1:A:275:TRP:O	1:A:276:THR:C	2.49	0.55
2:E:482:HIS:CD2	2:E:522:PHE:HA	2.42	0.55
1:C:90:ASN:HB3	1:C:93:VAL:HG13	1.88	0.55
1:C:324:THR:O	1:C:327:PHE:HB3	2.07	0.55
1:C:454:TYR:OH	1:C:458:LYS:HD3	2.07	0.55
2:G:483:THR:CG2	2:G:519:THR:CG2	2.77	0.55
1:D:224:GLU:HG3	1:D:225:ASP:N	2.21	0.55
1:A:253:PRO:O	1:A:254:SER:HB2	2.06	0.55
1:A:580:ASN:HD21	1:A:582:ARG:HH12	1.52	0.55
1:D:177:ARG:NH1	1:D:470:LYS:O	2.37	0.55
1:D:414:THR:HG21	1:D:543:ASP:HB2	1.89	0.55
1:D:455:MET:SD	1:D:481:LYS:HG2	2.46	0.55
2:H:553:SER:HA	2:H:579:PHE:HE1	1.72	0.55
1:A:51:ASN:HB3	1:A:342:ALA:HB1	1.89	0.54
2:G:504:GLN:HG2	2:G:505:VAL:N	2.22	0.54
1:A:397:ASN:OD1	1:A:400:PHE:HD1	1.90	0.54
1:B:318:VAL:O	1:B:551:GLY:HA3	2.08	0.54
1:C:580:ASN:HD21	1:C:582:ARG:HH12	1.56	0.54
2:E:577:CYS:O	2:E:578:ASN:C	2.51	0.54
2:F:566:ILE:HA	2:F:599:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:482:HIS:HD2	2:G:522:PHE:HA	1.73	0.54
2:H:550:CYS:HB2	2:H:551:PRO:CD	2.38	0.54
1:A:181:GLU:O	1:A:184:VAL:HG22	2.08	0.54
1:B:524:GLN:NE2	1:B:580:ASN:H	2.06	0.54
1:C:353:LYS:HA	2:G:498:TYR:CD2	2.42	0.54
1:D:187:LYS:HE3	1:D:199:TYR:CZ	2.43	0.54
1:B:177:ARG:NH1	1:B:470:LYS:O	2.38	0.54
1:A:162:LEU:HD11	1:A:490:PRO:HB2	1.90	0.54
1:A:351:LEU:HD12	1:A:351:LEU:H	1.72	0.54
2:F:553:SER:HA	2:F:579:PHE:CE1	2.43	0.54
1:C:269:ASP:OD2	1:C:272:GLY:N	2.35	0.54
2:H:578:ASN:H	2:H:578:ASN:ND2	1.97	0.54
2:H:492:SER:HA	2:H:531:VAL:HG23	1.90	0.53
2:E:535:SER:C	2:E:537:GLY:H	2.15	0.53
1:B:116:LEU:O	1:B:120:LEU:HD12	2.08	0.53
1:C:245:ARG:O	1:C:249:MET:HG3	2.08	0.53
1:B:90:ASN:HB3	1:B:93:VAL:HG13	1.90	0.53
1:B:580:ASN:HD21	1:B:582:ARG:HH12	1.56	0.53
1:B:397:ASN:OD1	1:B:400:PHE:HD1	1.90	0.53
1:C:60:GLN:O	1:C:63:ASN:OD1	2.27	0.53
2:G:566:ILE:HA	2:G:599:THR:O	2.09	0.53
1:A:455:MET:SD	1:A:481:LYS:HG2	2.49	0.53
2:E:600:TRP:HE3	2:E:600:TRP:O	1.92	0.53
2:H:535:SER:C	2:H:537:GLY:H	2.16	0.53
1:B:276:THR:HG23	1:B:445:THR:OG1	2.08	0.53
1:B:335:ASP:HB2	1:B:361:CYS:SG	2.48	0.53
1:A:116:LEU:O	1:A:120:LEU:HD12	2.09	0.53
2:E:522:PHE:CD1	2:E:522:PHE:C	2.86	0.53
1:C:389:PRO:HG2	1:C:392:LEU:HD22	1.90	0.53
2:H:577:CYS:O	2:H:578:ASN:C	2.52	0.53
1:A:365:THR:HB	1:A:368:ASP:H	1.73	0.53
1:C:162:LEU:HD11	1:C:490:PRO:HB2	1.90	0.53
1:C:455:MET:SD	1:C:481:LYS:HG2	2.49	0.53
2:E:578:ASN:O	2:E:580:PRO:HD3	2.08	0.53
1:D:51:ASN:HB3	1:D:342:ALA:HB1	1.90	0.53
1:D:96:GLN:HG2	1:D:392:LEU:HD11	1.91	0.53
1:D:253:PRO:O	1:D:254:SER:HB2	2.09	0.53
2:G:553:SER:HA	2:G:579:PHE:CE1	2.44	0.52
1:C:116:LEU:O	1:C:120:LEU:HD12	2.09	0.52
1:C:418:LEU:O	1:C:421:ILE:HG22	2.09	0.52
1:C:456:LEU:HD23	1:C:477:TRP:HH2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD22	1:A:147:GLY:HA2	1.90	0.52
1:B:407:ILE:HD11	1:B:529:LEU:HD22	1.91	0.52
1:D:275:TRP:O	1:D:276:THR:C	2.50	0.52
1:A:249:MET:HG2	1:A:256:ILE:HB	1.90	0.52
1:B:52:THR:CG2	1:B:53:ASN:N	2.72	0.52
2:F:578:ASN:O	2:F:580:PRO:HD3	2.08	0.52
1:D:104:GLY:O	1:D:107:VAL:HG12	2.09	0.52
1:D:242:ALA:HA	1:D:245:ARG:HG2	1.91	0.52
1:A:104:GLY:O	1:A:107:VAL:HG12	2.10	0.52
1:A:284:PRO:HG3	1:A:436:ILE:HG22	1.92	0.52
1:C:350:ASP:OD2	1:C:356:PHE:CE2	2.63	0.52
2:G:600:TRP:HE3	2:G:600:TRP:O	1.91	0.52
1:D:456:LEU:HD23	1:D:477:TRP:HH2	1.74	0.52
2:H:498:TYR:O	2:H:499:VAL:CB	2.41	0.52
1:B:249:MET:HG2	1:B:256:ILE:HB	1.91	0.52
1:B:350:ASP:OD2	1:B:356:PHE:CE2	2.62	0.52
2:F:550:CYS:HB2	2:F:551:PRO:CD	2.40	0.52
1:D:90:ASN:HB3	1:D:93:VAL:HG13	1.92	0.52
1:D:397:ASN:OD1	1:D:400:PHE:HD1	1.93	0.52
2:H:482:HIS:HD2	2:H:522:PHE:HA	1.74	0.52
2:E:482:HIS:HD2	2:E:522:PHE:HA	1.73	0.52
1:D:365:THR:HB	1:D:368:ASP:H	1.74	0.52
1:D:432:ASN:O	1:D:435:GLU:HB3	2.09	0.52
2:H:482:HIS:CD2	2:H:522:PHE:HA	2.44	0.52
1:A:222:LEU:O	1:A:226:VAL:HG23	2.09	0.52
1:A:493:HIS:CE1	1:A:497:TYR:CE1	2.97	0.52
1:B:456:LEU:HD23	1:B:477:TRP:HH2	1.74	0.52
2:E:566:ILE:HA	2:E:599:THR:O	2.10	0.52
1:B:162:LEU:HD11	1:B:490:PRO:HB2	1.91	0.52
1:B:222:LEU:O	1:B:226:VAL:HG23	2.10	0.52
1:B:242:ALA:HA	1:B:245:ARG:HG2	1.92	0.52
1:D:580:ASN:HD21	1:D:582:ARG:HH12	1.56	0.52
1:A:397:ASN:OD1	1:A:400:PHE:CD1	2.63	0.51
1:D:206:ASP:OD1	1:D:398:GLU:HG2	2.10	0.51
1:D:249:MET:HG2	1:D:256:ILE:HB	1.92	0.51
1:D:276:THR:HG23	1:D:445:THR:OG1	2.09	0.51
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.75	0.51
1:A:578:ASN:OD1	1:A:579:MET:N	2.43	0.51
1:D:290:ASN:HD21	1:D:292:ASP:HB2	1.74	0.51
2:H:522:PHE:CD1	2:H:522:PHE:C	2.86	0.51
1:B:209:VAL:HG21	1:B:565:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:PRO:O	1:B:473:TRP:CD1	2.64	0.51
2:F:483:THR:CG2	2:F:519:THR:CG2	2.80	0.51
1:A:245:ARG:O	1:A:249:MET:HG3	2.10	0.51
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.93	0.51
2:G:535:SER:C	2:G:537:GLY:H	2.18	0.51
1:A:90:ASN:HB3	1:A:93:VAL:HG13	1.92	0.51
1:C:276:THR:OG1	1:C:445:THR:HG23	2.10	0.51
2:E:498:TYR:O	2:E:499:VAL:CB	2.37	0.51
2:F:482:HIS:CD2	2:F:483:THR:N	2.79	0.51
2:F:482:HIS:HD2	2:F:522:PHE:HA	1.75	0.51
2:F:600:TRP:HE3	2:F:600:TRP:O	1.94	0.51
1:A:287:GLN:H	1:A:287:GLN:HE21	1.57	0.51
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.91	0.51
2:F:522:PHE:C	2:F:522:PHE:CD1	2.89	0.51
2:F:544:TYR:CE1	2:F:582:GLU:HB3	2.45	0.51
1:B:20:THR:HB	1:B:23:GLU:HB2	1.94	0.51
1:B:320:LEU:HB3	1:B:321:PRO:CD	2.41	0.51
1:D:116:LEU:O	1:D:120:LEU:HD12	2.10	0.51
1:D:142:LEU:HD22	1:D:147:GLY:HA2	1.93	0.51
1:D:276:THR:OG1	1:D:445:THR:HG23	2.10	0.51
1:B:49:ASN:HB3	1:B:58:ASN:HD22	1.76	0.50
2:E:550:CYS:HB2	2:E:551:PRO:HD2	1.93	0.50
1:C:217:TYR:CE1	1:C:578:ASN:ND2	2.74	0.50
1:D:543:ASP:O	1:D:545:SER:N	2.44	0.50
1:A:91:LEU:H	1:A:91:LEU:HD12	1.75	0.50
1:B:146:PRO:O	1:B:147:GLY:C	2.55	0.50
1:B:454:TYR:OH	1:B:458:LYS:HD3	2.10	0.50
1:C:249:MET:HG2	1:C:256:ILE:HB	1.94	0.50
1:D:327:PHE:CD1	1:D:327:PHE:C	2.89	0.50
1:C:146:PRO:O	1:C:147:GLY:C	2.54	0.50
1:C:390:PHE:HA	1:C:393:ARG:HD2	1.94	0.50
1:D:107:VAL:HG22	1:D:107:VAL:O	2.10	0.50
1:D:209:VAL:HG21	1:D:565:PRO:HB3	1.93	0.50
1:B:290:ASN:HD21	1:B:292:ASP:HB2	1.76	0.50
2:F:504:GLN:HG2	2:F:505:VAL:N	2.26	0.50
1:C:290:ASN:HD21	1:C:292:ASP:HB2	1.77	0.50
2:G:522:PHE:CD1	2:G:522:PHE:C	2.87	0.50
1:A:107:VAL:HG22	1:A:107:VAL:O	2.12	0.50
1:A:574:VAL:HG23	1:A:575:GLY:N	2.26	0.50
1:C:397:ASN:OD1	1:C:400:PHE:CD1	2.65	0.50
1:C:557:MET:HE3	1:C:558:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:GLN:HE21	1:D:526:GLN:HA	1.76	0.50
1:B:332:MET:O	1:B:332:MET:HG2	2.10	0.49
1:B:601:ASN:ND2	1:D:254:SER:O	2.44	0.49
2:G:570:THR:O	2:G:571:VAL:HG12	2.12	0.49
1:C:578:ASN:OD1	1:C:579:MET:N	2.46	0.49
1:D:177:ARG:HB3	1:D:178:PRO:HD3	1.94	0.49
1:B:226:VAL:O	1:B:229:THR:HG22	2.12	0.49
1:B:522:GLN:NE2	1:B:523:PHE:CE2	2.80	0.49
1:D:222:LEU:O	1:D:226:VAL:HG23	2.13	0.49
1:D:269:ASP:C	1:D:269:ASP:OD2	2.55	0.49
1:B:284:PRO:HG3	1:B:436:ILE:HG22	1.95	0.49
1:B:418:LEU:O	1:B:421:ILE:HG22	2.13	0.49
1:B:523:PHE:O	1:B:524:GLN:C	2.55	0.49
1:D:92:THR:O	1:D:96:GLN:HG3	2.13	0.49
1:D:414:THR:HG23	1:D:417:HIS:H	1.77	0.49
2:H:553:SER:O	2:H:554:PHE:CD2	2.65	0.49
1:A:543:ASP:O	1:A:545:SER:N	2.45	0.49
1:B:574:VAL:HG23	1:B:575:GLY:N	2.28	0.49
1:C:242:ALA:HA	1:C:245:ARG:HG2	1.94	0.49
1:C:293:VAL:CG2	1:C:366:MET:HG3	2.43	0.49
2:G:575:GLY:O	2:G:600:TRP:CH2	2.66	0.49
1:D:287:GLN:H	1:D:287:GLN:HE21	1.59	0.49
1:A:414:THR:HG23	1:A:417:HIS:H	1.76	0.49
1:D:279:TYR:HB2	1:D:444:LEU:HD23	1.95	0.49
1:A:520:LEU:HD22	1:A:581:VAL:HA	1.95	0.49
1:B:199:TYR:O	1:B:202:TYR:HB3	2.13	0.49
1:D:284:PRO:HG3	1:D:436:ILE:HG22	1.94	0.49
1:A:187:LYS:HE3	1:A:199:TYR:CE1	2.48	0.49
1:A:318:VAL:HG12	1:A:551:GLY:HA3	1.94	0.49
1:B:226:VAL:CA	1:B:229:THR:HG22	2.42	0.49
1:B:560:LEU:HD21	1:B:564:GLU:HB2	1.95	0.49
1:C:275:TRP:O	1:C:276:THR:C	2.56	0.49
2:G:482:HIS:CD2	2:G:522:PHE:HA	2.48	0.49
1:D:146:PRO:O	1:D:147:GLY:C	2.56	0.49
2:F:482:HIS:CD2	2:F:522:PHE:HA	2.48	0.48
1:C:318:VAL:O	1:C:551:GLY:HA3	2.12	0.48
1:C:365:THR:HB	1:C:368:ASP:H	1.78	0.48
1:C:469:PRO:O	1:C:473:TRP:CD1	2.66	0.48
1:A:20:THR:HB	1:A:23:GLU:HB2	1.95	0.48
1:A:338:ASN:O	1:A:340:GLN:N	2.46	0.48
1:B:287:GLN:HE21	1:B:287:GLN:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ASN:O	1:B:435:GLU:HB3	2.13	0.48
1:C:253:PRO:O	1:C:254:SER:HB2	2.13	0.48
1:D:397:ASN:OD1	1:D:400:PHE:CD1	2.66	0.48
2:H:600:TRP:HE3	2:H:600:TRP:O	1.96	0.48
1:A:209:VAL:HG21	1:A:565:PRO:HB3	1.95	0.48
1:C:529:LEU:HD11	1:C:554:LEU:HB2	1.94	0.48
1:D:162:LEU:HD11	1:D:490:PRO:HB2	1.94	0.48
1:B:19:SER:O	1:B:20:THR:C	2.56	0.48
2:F:577:CYS:O	2:F:578:ASN:C	2.57	0.48
1:C:52:THR:CG2	1:C:53:ASN:N	2.75	0.48
1:D:34:HIS:C	1:D:34:HIS:CD2	2.91	0.48
1:A:92:THR:O	1:A:96:GLN:HG3	2.13	0.48
1:A:261:CYS:HB3	1:A:487:VAL:N	2.28	0.48
1:B:543:ASP:O	1:B:545:SER:N	2.46	0.48
1:C:276:THR:HG23	1:C:445:THR:OG1	2.13	0.48
2:G:550:CYS:HB2	2:G:551:PRO:CD	2.43	0.48
1:C:322:ASN:O	2:G:586:HIS:HE1	1.96	0.48
2:E:578:ASN:H	2:E:578:ASN:ND2	1.95	0.48
1:C:284:PRO:HG3	1:C:436:ILE:HG22	1.95	0.48
1:B:324:THR:O	1:B:327:PHE:HB3	2.14	0.48
1:D:166:GLU:OE2	1:D:497:TYR:OH	2.19	0.48
1:A:146:PRO:O	1:A:147:GLY:C	2.57	0.48
1:A:443:ALA:HB2	1:A:588:PHE:CE2	2.49	0.48
2:E:581:LEU:HD23	2:E:593:VAL:HG23	1.95	0.48
1:B:254:SER:O	1:D:601:ASN:ND2	2.47	0.48
1:D:493:HIS:CE1	1:D:497:TYR:CE1	3.02	0.48
1:A:432:ASN:O	1:A:435:GLU:HB3	2.13	0.48
1:B:353:LYS:HA	2:F:498:TYR:CD2	2.48	0.48
1:B:414:THR:HG23	1:B:417:HIS:H	1.77	0.48
1:C:320:LEU:HB3	1:C:321:PRO:CD	2.44	0.48
1:C:327:PHE:CD1	1:C:327:PHE:C	2.92	0.48
1:B:293:VAL:CG2	1:B:366:MET:HG3	2.44	0.47
2:F:491:ALA:O	2:F:531:VAL:CG2	2.59	0.47
1:A:279:TYR:HB2	1:A:444:LEU:HD23	1.96	0.47
1:C:248:LEU:HB3	1:C:256:ILE:HD13	1.97	0.47
2:H:566:ILE:HA	2:H:599:THR:O	2.14	0.47
1:B:274:PHE:CD2	1:B:449:THR:HB	2.49	0.47
1:C:226:VAL:O	1:C:229:THR:HG22	2.14	0.47
1:A:242:ALA:HA	1:A:245:ARG:HG2	1.95	0.47
1:B:269:ASP:OD2	1:B:272:GLY:N	2.34	0.47
2:H:578:ASN:HD22	2:H:578:ASN:N	1.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLN:H	1:C:287:GLN:HE21	1.62	0.47
1:A:332:MET:HE1	1:A:336:PRO:HG3	1.96	0.47
1:B:187:LYS:HE3	1:B:199:TYR:CZ	2.49	0.47
2:G:482:HIS:CD2	2:G:483:THR:N	2.83	0.47
1:D:269:ASP:OD2	1:D:272:GLY:N	2.34	0.47
1:D:560:LEU:HD21	1:D:564:GLU:HB2	1.96	0.47
1:A:34:HIS:C	1:A:34:HIS:CD2	2.91	0.47
1:A:162:LEU:HD13	1:A:490:PRO:HB2	1.95	0.47
1:B:529:LEU:HG	1:B:550:ALA:HB1	1.96	0.47
1:B:532:ALA:O	1:B:549:GLU:HG2	2.14	0.47
1:C:91:LEU:H	1:C:91:LEU:CD1	2.27	0.47
1:C:226:VAL:CA	1:C:229:THR:HG22	2.44	0.47
1:C:522:GLN:NE2	1:C:523:PHE:CE2	2.83	0.47
1:D:20:THR:HB	1:D:23:GLU:HB2	1.96	0.47
1:D:483:GLU:HG2	1:D:608:THR:HG21	1.97	0.47
1:D:557:MET:HE3	1:D:558:LEU:HD12	1.95	0.47
1:A:483:GLU:HG2	1:A:608:THR:HG21	1.95	0.47
2:F:498:TYR:CD1	2:F:498:TYR:C	2.93	0.47
1:C:338:ASN:O	1:C:340:GLN:N	2.47	0.47
1:D:338:ASN:O	1:D:340:GLN:N	2.47	0.47
1:A:398:GLU:OE2	1:A:514:ARG:HB3	2.15	0.47
1:A:489:GLU:O	1:A:489:GLU:HG2	2.14	0.47
2:E:535:SER:C	2:E:537:GLY:N	2.73	0.47
1:B:275:TRP:O	1:B:276:THR:C	2.57	0.47
1:C:432:ASN:O	1:C:435:GLU:HB3	2.14	0.47
1:B:545:SER:O	1:B:546:ASN:CB	2.61	0.47
1:C:34:HIS:C	1:C:34:HIS:CD2	2.93	0.47
1:A:96:GLN:HG2	1:A:392:LEU:HD11	1.98	0.46
1:A:226:VAL:O	1:A:229:THR:HG22	2.15	0.46
2:F:570:THR:O	2:F:571:VAL:HG12	2.14	0.46
1:C:526:GLN:HE21	1:C:526:GLN:HA	1.80	0.46
1:A:127:TYR:CD1	1:A:127:TYR:C	2.93	0.46
1:A:274:PHE:CD2	1:A:449:THR:HB	2.51	0.46
1:B:81:GLN:NE2	1:B:101:GLN:HB2	2.30	0.46
1:B:327:PHE:CD1	1:B:327:PHE:C	2.92	0.46
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.79	0.46
1:C:81:GLN:NE2	1:C:101:GLN:HB2	2.30	0.46
1:D:532:ALA:O	1:D:549:GLU:HG2	2.14	0.46
1:A:327:PHE:CD1	1:A:327:PHE:C	2.93	0.46
1:A:375:GLU:O	1:A:378:HIS:HB2	2.16	0.46
1:C:524:GLN:CD	1:C:580:ASN:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:CYS:HB3	1:D:487:VAL:N	2.30	0.46
1:D:578:ASN:OD1	1:D:579:MET:N	2.48	0.46
1:A:332:MET:O	1:A:332:MET:HG2	2.14	0.46
1:B:51:ASN:ND2	1:B:343:VAL:CG2	2.64	0.46
1:B:81:GLN:CA	1:B:81:GLN:NE2	2.75	0.46
1:B:261:CYS:HB3	1:B:486:GLY:O	2.15	0.46
1:B:269:ASP:OD2	1:B:269:ASP:C	2.58	0.46
1:C:51:ASN:HB3	1:C:342:ALA:HB1	1.97	0.46
1:C:209:VAL:HG21	1:C:565:PRO:HB3	1.97	0.46
1:D:162:LEU:HD13	1:D:490:PRO:HB2	1.94	0.46
1:D:226:VAL:CA	1:D:229:THR:HG22	2.46	0.46
2:F:550:CYS:HB2	2:F:551:PRO:HD2	1.97	0.46
1:C:521:TYR:O	1:C:524:GLN:N	2.49	0.46
1:B:253:PRO:O	1:B:254:SER:HB2	2.16	0.46
1:B:398:GLU:OE2	1:B:514:ARG:HB3	2.15	0.46
1:A:318:VAL:O	1:A:551:GLY:HA3	2.15	0.46
2:E:528:TYR:HE1	2:E:543:ILE:HD12	1.81	0.46
1:B:248:LEU:HB3	1:B:256:ILE:HD13	1.96	0.46
1:D:166:GLU:OE1	1:D:493:HIS:HE1	1.99	0.46
1:D:249:MET:SD	1:D:258:PRO:HG3	2.56	0.46
1:A:335:ASP:HB2	1:A:361:CYS:SG	2.56	0.46
1:B:529:LEU:HD11	1:B:554:LEU:HB2	1.98	0.46
1:C:199:TYR:O	1:C:202:TYR:HB3	2.16	0.46
1:C:355:ASP:OD2	1:C:357:ARG:NH1	2.39	0.46
1:D:22:GLU:O	1:D:26:LYS:HG3	2.15	0.46
1:A:259:ILE:HA	1:A:603:PHE:CD1	2.51	0.46
2:F:531:VAL:O	2:F:532:LYS:C	2.58	0.46
1:C:269:ASP:OD2	1:C:269:ASP:C	2.58	0.46
2:H:498:TYR:HD1	2:H:499:VAL:N	2.13	0.46
2:H:499:VAL:HG22	2:H:585:TRP:CG	2.51	0.46
1:A:226:VAL:CA	1:A:229:THR:HG22	2.46	0.45
2:E:528:TYR:CE1	2:E:543:ILE:HB	2.51	0.45
1:B:51:ASN:HB3	1:B:342:ALA:HB1	1.98	0.45
1:B:374:HIS:CE1	1:B:406:GLU:HG2	2.51	0.45
2:F:498:TYR:O	2:F:499:VAL:CB	2.40	0.45
1:C:274:PHE:CD2	1:C:449:THR:HB	2.51	0.45
1:D:482:ARG:HE	1:D:488:VAL:HG12	1.81	0.45
1:A:253:PRO:O	1:A:254:SER:CB	2.65	0.45
1:A:557:MET:HE3	1:A:558:LEU:HD12	1.98	0.45
1:C:144:LEU:HB2	1:C:168:TRP:CH2	2.51	0.45
2:E:538:ASP:O	2:E:539:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:HIS:C	1:B:34:HIS:CD2	2.94	0.45
1:C:411:SER:O	1:C:414:THR:HG22	2.17	0.45
1:D:351:LEU:HD12	1:D:351:LEU:H	1.79	0.45
1:D:411:SER:O	1:D:414:THR:HG22	2.16	0.45
1:D:520:LEU:HD22	1:D:581:VAL:HA	1.98	0.45
2:F:595:ALA:HB3	2:F:597:TYR:CE2	2.51	0.45
1:C:322:ASN:O	2:G:586:HIS:CE1	2.69	0.45
2:E:600:TRP:CE3	2:E:600:TRP:N	2.84	0.45
2:G:544:TYR:CE1	2:G:582:GLU:HB3	2.51	0.45
1:D:53:ASN:CG	1:D:55:THR:HG1	2.22	0.45
1:A:259:ILE:HA	1:A:603:PHE:HD1	1.81	0.45
2:F:578:ASN:HD22	2:F:578:ASN:N	1.96	0.45
1:C:478:TRP:HA	1:C:481:LYS:HB2	1.99	0.45
1:D:225:ASP:O	1:D:229:THR:HG22	2.17	0.45
1:A:524:GLN:CD	1:A:580:ASN:H	2.23	0.45
1:B:338:ASN:O	1:B:340:GLN:N	2.50	0.45
1:C:20:THR:HB	1:C:23:GLU:HB2	1.99	0.45
1:A:290:ASN:HD21	1:A:292:ASP:HB2	1.78	0.45
1:B:397:ASN:OD1	1:B:400:PHE:CD1	2.68	0.45
2:F:528:TYR:HE1	2:F:543:ILE:HD12	1.82	0.45
1:C:19:SER:O	1:C:20:THR:C	2.59	0.45
1:C:162:LEU:HD13	1:C:490:PRO:CB	2.46	0.45
2:G:577:CYS:O	2:G:578:ASN:C	2.59	0.45
1:A:22:GLU:O	1:A:26:LYS:HG3	2.16	0.45
1:A:165:TRP:CZ3	1:A:490:PRO:HD2	2.52	0.45
1:A:166:GLU:OE1	1:A:493:HIS:HE1	2.00	0.45
1:B:22:GLU:OE2	1:B:90:ASN:HB2	2.17	0.45
1:B:425:SER:OG	1:B:427:ASP:HB2	2.17	0.45
1:B:521:TYR:O	1:B:524:GLN:N	2.50	0.45
1:A:370:LEU:HD21	1:A:413:ALA:HB2	2.00	0.44
1:A:454:TYR:OH	1:A:458:LYS:HD3	2.17	0.44
1:A:560:LEU:HD21	1:A:564:GLU:HB2	1.99	0.44
2:E:570:THR:O	2:E:571:VAL:HG12	2.16	0.44
1:B:346:PRO:HB3	1:B:360:MET:HE2	1.98	0.44
1:B:493:HIS:CE1	1:B:497:TYR:CE1	3.06	0.44
2:F:535:SER:C	2:F:537:GLY:N	2.75	0.44
2:G:600:TRP:CE3	2:G:600:TRP:N	2.85	0.44
1:D:187:LYS:HE3	1:D:199:TYR:CE1	2.52	0.44
1:B:206:ASP:OD1	1:B:398:GLU:HG2	2.18	0.44
1:B:578:ASN:OD1	1:B:579:MET:N	2.51	0.44
1:C:532:ALA:O	1:C:549:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:VAL:HG23	1:D:575:GLY:N	2.33	0.44
1:A:155:SER:O	1:A:161:ARG:HD2	2.18	0.44
1:C:127:TYR:CD1	1:C:127:TYR:C	2.95	0.44
1:D:318:VAL:HG12	1:D:551:GLY:HA3	2.00	0.44
1:D:543:ASP:OD1	1:D:545:SER:OG	2.36	0.44
2:H:535:SER:C	2:H:537:GLY:N	2.75	0.44
2:E:553:SER:O	2:E:554:PHE:CD2	2.71	0.44
1:C:259:ILE:HA	1:C:603:PHE:CD1	2.53	0.44
2:H:498:TYR:CD1	2:H:498:TYR:C	2.95	0.44
2:H:504:GLN:HG2	2:H:505:VAL:N	2.33	0.44
1:A:96:GLN:NE2	1:A:389:PRO:HB2	2.33	0.44
1:C:529:LEU:HG	1:C:550:ALA:HB1	1.99	0.44
1:C:560:LEU:HD21	1:C:564:GLU:HB2	2.00	0.44
1:C:574:VAL:HG23	1:C:575:GLY:N	2.32	0.44
1:D:274:PHE:CD2	1:D:449:THR:HB	2.53	0.44
1:B:166:GLU:OE1	1:B:493:HIS:HE1	2.00	0.44
1:B:455:MET:HE2	1:B:455:MET:HB3	1.73	0.44
1:B:469:PRO:O	1:B:473:TRP:HD1	2.01	0.44
1:D:52:THR:CG2	1:D:53:ASN:N	2.81	0.44
1:D:168:TRP:O	1:D:172:VAL:HG22	2.18	0.44
1:D:293:VAL:CG2	1:D:366:MET:HG3	2.48	0.44
1:D:332:MET:HE1	1:D:336:PRO:HG3	2.00	0.44
1:D:469:PRO:O	1:D:473:TRP:CD1	2.71	0.44
1:A:482:ARG:HE	1:A:488:VAL:HG12	1.83	0.44
1:C:346:PRO:HB3	1:C:360:MET:HE2	2.00	0.44
1:C:351:LEU:H	1:C:351:LEU:HD12	1.82	0.44
1:C:523:PHE:O	1:C:524:GLN:C	2.60	0.44
1:D:225:ASP:O	1:D:229:THR:CG2	2.65	0.44
1:A:51:ASN:ND2	1:A:343:VAL:CG2	2.65	0.44
1:A:274:PHE:HD2	1:A:449:THR:HB	1.83	0.44
1:A:491:VAL:HG13	1:A:492:PRO:HD2	1.99	0.44
1:B:276:THR:OG1	1:B:445:THR:HG23	2.17	0.44
2:F:499:VAL:HG22	2:F:585:TRP:CG	2.53	0.44
1:D:320:LEU:HD13	1:D:380:GLN:HG2	2.00	0.44
1:D:489:GLU:HG3	1:D:491:VAL:O	2.18	0.44
1:A:199:TYR:O	1:A:202:TYR:HB3	2.18	0.43
1:A:529:LEU:HD11	1:A:554:LEU:HB2	2.00	0.43
2:E:498:TYR:CD1	2:E:498:TYR:C	2.96	0.43
2:E:499:VAL:HG22	2:E:585:TRP:CG	2.52	0.43
1:B:478:TRP:HA	1:B:481:LYS:HB2	2.00	0.43
1:D:259:ILE:HA	1:D:603:PHE:HD1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:PHE:HD2	1:B:449:THR:HB	1.82	0.43
1:B:482:ARG:HE	1:B:488:VAL:HG12	1.82	0.43
1:C:482:ARG:HE	1:C:488:VAL:HG12	1.82	0.43
1:A:505:HIS:CD2	1:A:505:HIS:N	2.85	0.43
2:E:511:GLY:HA3	3:E:1512:NAG:H3	2.01	0.43
1:B:521:TYR:O	1:B:523:PHE:N	2.51	0.43
1:A:177:ARG:HB3	1:A:178:PRO:HD3	2.00	0.43
1:A:311:ALA:O	1:A:314:PHE:HB3	2.18	0.43
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.86	0.43
1:C:582:ARG:O	1:C:583:PRO:C	2.59	0.43
2:G:550:CYS:HB2	2:G:551:PRO:HD2	2.01	0.43
1:A:491:VAL:CG1	1:A:492:PRO:HD2	2.49	0.43
1:C:122:THR:O	1:C:126:ILE:HG13	2.18	0.43
1:C:187:LYS:HE3	1:C:199:TYR:CZ	2.53	0.43
1:A:446:ILE:HG23	1:A:519:THR:HG21	2.00	0.43
1:B:53:ASN:CG	1:B:55:THR:HG1	2.23	0.43
1:B:166:GLU:OE1	1:B:493:HIS:CE1	2.72	0.43
2:F:498:TYR:HD1	2:F:499:VAL:N	2.16	0.43
1:C:181:GLU:O	1:C:184:VAL:HG22	2.18	0.43
1:C:501:ALA:HA	1:C:506:VAL:CG1	2.49	0.43
1:D:81:GLN:CA	1:D:81:GLN:NE2	2.80	0.43
1:D:318:VAL:O	1:D:551:GLY:HA3	2.18	0.43
2:H:553:SER:O	2:H:554:PHE:HD2	2.02	0.43
1:A:276:THR:OG1	1:A:445:THR:HG23	2.19	0.43
1:B:91:LEU:H	1:B:91:LEU:CD1	2.30	0.43
1:B:181:GLU:O	1:B:184:VAL:HG22	2.18	0.43
2:F:543:ILE:HG12	2:F:583:ALA:CB	2.47	0.43
2:G:543:ILE:HG12	2:G:583:ALA:CB	2.49	0.43
1:A:411:SER:O	1:A:414:THR:HG22	2.18	0.43
1:A:580:ASN:HD21	1:A:582:ARG:NH1	2.15	0.43
2:E:504:GLN:HG2	2:E:505:VAL:N	2.32	0.43
1:B:47:SER:O	1:B:50:TYR:HB3	2.18	0.43
1:B:351:LEU:HD12	1:B:351:LEU:H	1.84	0.43
1:C:206:ASP:OD1	1:C:398:GLU:HG2	2.19	0.43
1:C:279:TYR:HB2	1:C:444:LEU:HD23	2.00	0.43
1:D:259:ILE:HA	1:D:603:PHE:CD1	2.53	0.43
1:C:81:GLN:CA	1:C:81:GLN:NE2	2.75	0.43
1:C:166:GLU:OE1	1:C:493:HIS:CE1	2.72	0.43
1:D:257:SER:HA	1:D:258:PRO:HD3	1.88	0.43
2:H:544:TYR:CE1	2:H:582:GLU:HB3	2.53	0.43
1:B:388:GLN:O	1:B:389:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:GLN:HG3	1:D:101:GLN:O	2.19	0.43
1:D:501:ALA:HA	1:D:506:VAL:CG1	2.48	0.43
1:A:53:ASN:CG	1:A:55:THR:HG1	2.24	0.42
1:B:552:GLN:O	1:B:553:LYS:C	2.61	0.42
1:D:77:SER:C	1:D:79:LEU:H	2.27	0.42
1:D:162:LEU:HD13	1:D:490:PRO:CB	2.49	0.42
1:D:165:TRP:CZ3	1:D:490:PRO:HD2	2.54	0.42
1:D:335:ASP:HB2	1:D:361:CYS:SG	2.59	0.42
1:B:155:SER:O	1:B:161:ARG:HD2	2.19	0.42
1:B:351:LEU:HD13	1:B:355:ASP:OD2	2.18	0.42
1:D:229:THR:OG1	1:D:581:VAL:HB	2.19	0.42
1:A:52:THR:CG2	1:A:53:ASN:N	2.81	0.42
1:A:184:VAL:HG12	1:A:464:PHE:HE2	1.84	0.42
1:A:249:MET:SD	1:A:258:PRO:HG3	2.58	0.42
2:E:498:TYR:HD1	2:E:499:VAL:N	2.17	0.42
1:B:365:THR:HB	1:B:368:ASP:H	1.84	0.42
1:C:552:GLN:O	1:C:553:LYS:C	2.61	0.42
2:G:568:PHE:HD1	2:G:596:LEU:HD11	1.85	0.42
1:A:48:TRP:NE1	1:A:52:THR:OG1	2.52	0.42
1:B:53:ASN:C	1:B:55:THR:N	2.70	0.42
1:C:51:ASN:ND2	1:C:343:VAL:CG2	2.68	0.42
2:G:531:VAL:O	2:G:532:LYS:C	2.61	0.42
2:F:575:GLY:O	2:F:600:TRP:CH2	2.72	0.42
2:F:581:LEU:HD23	2:F:593:VAL:HG23	2.01	0.42
1:C:166:GLU:OE1	1:C:493:HIS:HE1	2.02	0.42
1:C:398:GLU:OE2	1:C:514:ARG:HB3	2.19	0.42
1:D:456:LEU:HD13	1:D:460:ARG:HD2	2.02	0.42
2:F:568:PHE:HD1	2:F:596:LEU:HD11	1.84	0.42
1:D:96:GLN:HG2	1:D:392:LEU:CD1	2.49	0.42
1:D:253:PRO:O	1:D:254:SER:CB	2.68	0.42
1:D:454:TYR:OH	1:D:458:LYS:HD3	2.19	0.42
2:H:525:ARG:HE	2:H:525:ARG:HB3	1.60	0.42
1:A:162:LEU:HD13	1:A:490:PRO:CB	2.49	0.42
1:B:127:TYR:CD1	1:B:127:TYR:C	2.97	0.42
1:B:322:ASN:O	2:F:586:HIS:CE1	2.71	0.42
1:C:257:SER:HA	1:C:258:PRO:HD3	1.84	0.42
1:C:493:HIS:CE1	1:C:497:TYR:CE1	3.07	0.42
1:D:278:LEU:HD12	1:D:278:LEU:HA	1.97	0.42
1:C:259:ILE:HA	1:C:603:PHE:HD1	1.83	0.42
1:C:443:ALA:HB2	1:C:588:PHE:CE2	2.55	0.42
1:D:443:ALA:HB2	1:D:588:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ILE:HG23	1:D:519:THR:HG21	2.00	0.42
1:A:169:ARG:NH2	1:A:270:MET:O	2.52	0.42
1:B:162:LEU:HD13	1:B:490:PRO:CB	2.49	0.42
1:C:332:MET:O	1:C:332:MET:HG2	2.20	0.42
1:D:166:GLU:OE1	1:D:493:HIS:CE1	2.72	0.42
2:H:498:TYR:CD1	2:H:499:VAL:N	2.88	0.42
2:H:600:TRP:CE3	2:H:600:TRP:N	2.88	0.42
1:A:48:TRP:CE2	1:A:357:ARG:HD2	2.55	0.42
1:A:198:ASP:H	1:A:201:ASP:HB3	1.85	0.42
1:A:407:ILE:HA	1:A:410:LEU:HD12	2.01	0.42
1:B:121:ASN:O	1:B:125:THR:HG23	2.20	0.42
1:B:225:ASP:O	1:B:229:THR:CG2	2.68	0.42
1:D:184:VAL:HG12	1:D:464:PHE:HE2	1.85	0.42
1:D:360:MET:HE3	1:D:375:GLU:HG3	2.02	0.42
1:D:499:ASP:N	1:D:500:PRO:HD2	2.35	0.42
1:A:157:ASP:O	1:A:158:TYR:C	2.63	0.41
1:B:524:GLN:CD	1:B:580:ASN:H	2.28	0.41
2:F:538:ASP:O	2:F:539:SER:OG	2.36	0.41
2:G:522:PHE:C	2:G:522:PHE:HD1	2.27	0.41
2:H:550:CYS:HB2	2:H:551:PRO:HD2	2.00	0.41
1:B:52:THR:HG22	1:B:53:ASN:N	2.35	0.41
2:F:511:GLY:HA3	3:F:1512:NAG:H3	2.02	0.41
1:B:520:LEU:HD22	1:B:581:VAL:HA	2.03	0.41
1:C:168:TRP:O	1:C:172:VAL:HG22	2.20	0.41
1:D:198:ASP:HB2	1:D:464:PHE:O	2.21	0.41
1:A:77:SER:C	1:A:79:LEU:H	2.28	0.41
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.73	0.41
1:B:559:ARG:HH11	1:B:559:ARG:HB2	1.85	0.41
1:D:365:THR:HG22	1:D:367:ASP:H	1.86	0.41
2:F:600:TRP:CE3	2:F:600:TRP:N	2.87	0.41
1:C:324:THR:HG23	1:C:327:PHE:HB2	2.02	0.41
1:D:439:LEU:HD23	1:D:591:LEU:HB2	2.03	0.41
1:A:206:ASP:OD1	1:A:398:GLU:HG2	2.20	0.41
2:F:498:TYR:C	2:F:498:TYR:HD1	2.28	0.41
1:C:225:ASP:O	1:C:229:THR:HG22	2.21	0.41
1:C:456:LEU:HD13	1:C:460:ARG:HD2	2.03	0.41
1:D:198:ASP:H	1:D:201:ASP:HB3	1.85	0.41
1:D:489:GLU:O	1:D:489:GLU:HG2	2.19	0.41
1:B:443:ALA:HB2	1:B:588:PHE:CE2	2.56	0.41
1:C:22:GLU:O	1:C:26:LYS:HG3	2.19	0.41
1:C:505:HIS:CD2	1:C:505:HIS:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:VAL:O	1:D:229:THR:HG22	2.20	0.41
1:D:418:LEU:HA	1:D:421:ILE:HG22	2.02	0.41
2:H:511:GLY:HA3	3:H:1512:NAG:H3	2.02	0.41
2:H:570:THR:O	2:H:571:VAL:HG12	2.20	0.41
1:A:101:GLN:HG3	1:A:101:GLN:O	2.21	0.41
1:C:47:SER:O	1:C:50:TYR:HB3	2.21	0.41
1:C:425:SER:OG	1:C:427:ASP:HB2	2.20	0.41
1:C:469:PRO:O	1:C:473:TRP:HD1	2.04	0.41
1:D:96:GLN:NE2	1:D:389:PRO:HB2	2.35	0.41
1:D:461:TRP:CH2	1:D:513:ILE:HG13	2.55	0.41
1:A:229:THR:OG1	1:A:581:VAL:HB	2.21	0.41
1:A:293:VAL:CG2	1:A:366:MET:HG3	2.50	0.41
1:A:315:PHE:O	1:A:316:VAL:C	2.63	0.41
1:A:346:PRO:HB3	1:A:360:MET:HE2	2.03	0.41
1:A:418:LEU:HA	1:A:421:ILE:HG22	2.03	0.41
1:A:526:GLN:O	1:A:530:CYS:SG	2.79	0.41
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.91	0.41
2:E:504:GLN:HE21	2:E:504:GLN:HB3	1.68	0.41
2:E:544:TYR:CE1	2:E:582:GLU:HB3	2.55	0.41
2:E:553:SER:HA	2:E:579:PHE:CE1	2.53	0.41
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.54	0.41
1:B:165:TRP:CZ3	1:B:490:PRO:HD2	2.55	0.41
1:B:225:ASP:O	1:B:229:THR:HG22	2.21	0.41
1:B:259:ILE:HA	1:B:603:PHE:CD1	2.55	0.41
1:B:521:TYR:O	1:B:522:GLN:C	2.63	0.41
1:C:520:LEU:HD22	1:C:581:VAL:HA	2.03	0.41
2:G:595:ALA:HB3	2:G:597:TYR:CE2	2.56	0.41
1:D:535:HIS:CD2	1:D:536:GLU:N	2.89	0.41
1:A:493:HIS:CE1	1:A:497:TYR:CZ	3.08	0.41
2:E:491:ALA:O	2:E:531:VAL:CG2	2.66	0.41
1:B:134:ASN:C	1:B:137:ASN:H	2.28	0.41
1:C:22:GLU:OE2	1:C:90:ASN:HB2	2.21	0.41
1:C:196:TYR:CD1	1:C:202:TYR:HA	2.55	0.41
1:D:73:LEU:HD12	1:D:73:LEU:HA	1.90	0.41
1:D:82:MET:O	1:D:84:PRO:HD3	2.21	0.41
1:D:332:MET:O	1:D:332:MET:HG2	2.22	0.41
1:A:148:LEU:O	1:A:151:ILE:N	2.53	0.40
1:A:574:VAL:CG2	1:A:575:GLY:N	2.84	0.40
1:D:252:TYR:CE1	1:D:266:LEU:HD22	2.56	0.40
1:D:398:GLU:OE2	1:D:514:ARG:HB3	2.20	0.40
1:A:217:TYR:CE1	1:A:578:ASN:ND2	2.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:HD23	1:A:591:LEU:HB2	2.04	0.40
1:A:522:GLN:NE2	1:A:523:PHE:CE2	2.89	0.40
1:B:279:TYR:HB2	1:B:444:LEU:HD23	2.03	0.40
1:D:104:GLY:O	1:D:107:VAL:CG1	2.68	0.40
1:D:157:ASP:O	1:D:158:TYR:C	2.64	0.40
1:A:278:LEU:HD12	1:A:278:LEU:HA	1.97	0.40
1:A:517:THR:O	1:A:518:ARG:C	2.65	0.40
1:A:532:ALA:O	1:A:549:GLU:HG2	2.20	0.40
2:E:522:PHE:C	2:E:522:PHE:HD1	2.30	0.40
1:C:458:LYS:HE3	1:C:462:MET:HE3	2.03	0.40
1:C:562:LYS:O	1:C:562:LYS:CG	2.69	0.40
1:D:363:LYS:HE3	1:D:363:LYS:HB2	1.90	0.40
1:D:529:LEU:HD11	1:D:554:LEU:HB2	2.03	0.40
1:A:47:SER:O	1:A:50:TYR:HB3	2.22	0.40
1:A:196:TYR:CD1	1:A:202:TYR:HA	2.56	0.40
1:A:524:GLN:CG	1:A:583:PRO:HG2	2.47	0.40
2:E:543:ILE:HG12	2:E:583:ALA:CB	2.51	0.40
1:B:208:GLU:CD	1:B:219:ARG:HG3	2.46	0.40
1:B:259:ILE:HA	1:B:603:PHE:HD1	1.85	0.40
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.98	0.40
1:C:274:PHE:HD2	1:C:449:THR:HB	1.85	0.40
1:C:580:ASN:ND2	1:C:581:VAL:H	2.20	0.40
1:C:613:TYR:CD1	1:C:613:TYR:O	2.74	0.40
2:G:504:GLN:HE21	2:G:504:GLN:HB3	1.73	0.40
2:G:535:SER:C	2:G:537:GLY:N	2.79	0.40
1:D:217:TYR:CE1	1:D:578:ASN:ND2	2.82	0.40
1:D:517:THR:O	1:D:518:ARG:C	2.64	0.40
1:D:521:TYR:O	1:D:522:GLN:C	2.65	0.40
2:H:553:SER:HA	2:H:579:PHE:CE1	2.54	0.40
1:B:21:ILE:CG1	1:B:87:GLU:HG2	2.51	0.40
1:B:96:GLN:HG2	1:B:392:LEU:HD11	2.03	0.40
1:B:555:PHE:O	1:B:559:ARG:HG2	2.22	0.40
1:C:225:ASP:O	1:C:229:THR:CG2	2.70	0.40
1:C:279:TYR:C	1:C:281:LEU:N	2.78	0.40
2:G:581:LEU:HD23	2:G:593:VAL:HG23	2.03	0.40
1:D:109:SER:O	1:D:110:GLU:C	2.64	0.40
1:D:526:GLN:O	1:D:530:CYS:SG	2.80	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:O	2:G:518:ARG:NH2[3_554]	1.69	0.51
2:F:518:ARG:NH2	1:D:71:ALA:O[3_454]	2.04	0.16
2:F:572:GLU:OE2	1:D:24:GLN:OE1[3_454]	2.09	0.11
1:A:24:GLN:OE1	2:G:572:GLU:OE2[3_554]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/597 (98%)	516 (88%)	55 (9%)	14 (2%)	4	25
1	B	585/597 (98%)	515 (88%)	57 (10%)	13 (2%)	5	27
1	C	585/597 (98%)	514 (88%)	57 (10%)	14 (2%)	4	25
1	D	585/597 (98%)	515 (88%)	56 (10%)	14 (2%)	4	25
2	E	106/136 (78%)	87 (82%)	13 (12%)	6 (6%)	1	9
2	F	106/136 (78%)	86 (81%)	13 (12%)	7 (7%)	1	7
2	G	106/136 (78%)	85 (80%)	14 (13%)	7 (7%)	1	7
2	H	106/136 (78%)	86 (81%)	14 (13%)	6 (6%)	1	9
All	All	2764/2932 (94%)	2404 (87%)	279 (10%)	81 (3%)	3	22

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
2	E	499	VAL
2	E	521	HIS
2	E	571	VAL
2	E	578	ASN
1	B	146	PRO
2	F	499	VAL
2	F	521	HIS
2	F	571	VAL

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Mol	Chain	Res	Type
1	C	146	PRO
2	G	499	VAL
2	G	521	HIS
2	G	571	VAL
2	G	578	ASN
1	D	146	PRO
2	H	499	VAL
2	H	521	HIS
2	H	571	VAL
2	H	578	ASN
1	A	147	GLY
2	E	577	CYS
1	B	147	GLY
1	B	522	GLN
1	B	544	ILE
2	F	578	ASN
1	C	147	GLY
1	D	147	GLY
1	A	56	GLU
1	A	284	PRO
1	A	294	THR
1	A	522	GLN
1	A	544	ILE
1	B	56	GLU
1	B	284	PRO
1	B	294	THR
1	C	56	GLU
1	C	284	PRO
1	C	294	THR
1	C	522	GLN
1	D	56	GLU
1	D	284	PRO
1	D	294	THR
1	D	544	ILE
2	H	577	CYS
2	H	601	SER
1	A	254	SER
1	A	264	ALA
1	A	335	ASP
2	E	601	SER
1	B	335	ASP
1	B	505	HIS

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Mol	Chain	Res	Type
2	F	601	SER
1	C	335	ASP
1	C	505	HIS
2	G	601	SER
1	D	254	SER
1	D	335	ASP
1	D	522	GLN
1	D	608	THR
1	A	608	THR
1	B	291	ILE
1	B	504	PHE
2	F	577	CYS
1	C	277	ASN
1	C	291	ILE
1	C	504	PHE
2	G	577	CYS
1	D	264	ALA
1	A	291	ILE
1	B	254	SER
2	F	551	PRO
1	C	254	SER
1	C	544	ILE
1	D	291	ILE
1	D	352	GLY
1	A	107	VAL
1	B	352	GLY
2	G	551	PRO
1	A	352	GLY
1	D	107	VAL
1	C	185	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	523/527 (99%)	429 (82%)	94 (18%)	2 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	523/527 (99%)	435 (83%)	88 (17%)	2	11
1	C	523/527 (99%)	431 (82%)	92 (18%)	2	9
1	D	523/527 (99%)	431 (82%)	92 (18%)	2	9
2	E	98/121 (81%)	69 (70%)	29 (30%)	0	1
2	F	98/121 (81%)	70 (71%)	28 (29%)	0	1
2	G	98/121 (81%)	70 (71%)	28 (29%)	0	1
2	H	98/121 (81%)	70 (71%)	28 (29%)	0	1
All	All	2484/2592 (96%)	2005 (81%)	479 (19%)	1	7

All (479) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	21	ILE
1	A	29	LEU
1	A	31	LYS
1	A	39	LEU
1	A	43	SER
1	A	45	LEU
1	A	47	SER
1	A	51	ASN
1	A	52	THR
1	A	55	THR
1	A	56	GLU
1	A	57	GLU
1	A	62	MET
1	A	63	ASN
1	A	77	SER
1	A	78	THR
1	A	81	GLN
1	A	82	MET
1	A	87	GLU
1	A	89	GLN
1	A	91	LEU
1	A	93	VAL
1	A	95	LEU
1	A	97	LEU
1	A	100	LEU
1	A	120	LEU
1	A	131	LYS

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Mol	Chain	Res	Type
1	A	132	VAL
1	A	137	ASN
1	A	145	GLU
1	A	148	LEU
1	A	160	GLU
1	A	171	GLU
1	A	172	VAL
1	A	176	LEU
1	A	183	TYR
1	A	186	LEU
1	A	198	ASP
1	A	209	VAL
1	A	213	ASP
1	A	224	GLU
1	A	232	GLU
1	A	233	ILE
1	A	240	LEU
1	A	276	THR
1	A	287	GLN
1	A	291	ILE
1	A	294	THR
1	A	299	ASP
1	A	309	LYS
1	A	313	LYS
1	A	318	VAL
1	A	322	ASN
1	A	324	THR
1	A	330	ASN
1	A	333	LEU
1	A	341	LYS
1	A	351	LEU
1	A	364	VAL
1	A	365	THR
1	A	371	THR
1	A	380	GLN
1	A	401	HIS
1	A	407	ILE
1	A	418	LEU
1	A	421	ILE
1	A	423	LEU
1	A	427	ASP
1	A	429	GLN

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Mol	Chain	Res	Type
1	A	433	GLU
1	A	436	ILE
1	A	444	LEU
1	A	455	MET
1	A	481	LYS
1	A	485	VAL
1	A	488	VAL
1	A	503	LEU
1	A	513	ILE
1	A	519	THR
1	A	529	LEU
1	A	544	ILE
1	A	545	SER
1	A	546	ASN
1	A	557	MET
1	A	558	LEU
1	A	559	ARG
1	A	560	LEU
1	A	563	SER
1	A	573	VAL
1	A	577	LYS
1	A	582	ARG
1	A	604	VAL
1	A	608	THR
2	E	482	HIS
2	E	483	THR
2	E	486	ASN
2	E	488	THR
2	E	498	TYR
2	E	499	VAL
2	E	504	GLN
2	E	505	VAL
2	E	507	ILE
2	E	509	LEU
2	E	512	ASN
2	E	515	VAL
2	E	519	THR
2	E	520	SER
2	E	522	PHE
2	E	524	ILE
2	E	531	VAL
2	E	538	ASP

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Mol	Chain	Res	Type
2	E	545	LEU
2	E	549	THR
2	E	553	SER
2	E	569	SER
2	E	571	VAL
2	E	578	ASN
2	E	588	THR
2	E	591	THR
2	E	593	VAL
2	E	596	LEU
2	E	600	TRP
1	B	19	SER
1	B	21	ILE
1	B	27	THR
1	B	29	LEU
1	B	31	LYS
1	B	39	LEU
1	B	43	SER
1	B	45	LEU
1	B	52	THR
1	B	55	THR
1	B	56	GLU
1	B	57	GLU
1	B	62	MET
1	B	63	ASN
1	B	77	SER
1	B	78	THR
1	B	81	GLN
1	B	82	MET
1	B	87	GLU
1	B	89	GLN
1	B	91	LEU
1	B	93	VAL
1	B	95	LEU
1	B	97	LEU
1	B	100	LEU
1	B	120	LEU
1	B	131	LYS
1	B	145	GLU
1	B	160	GLU
1	B	171	GLU
1	B	176	LEU

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Mol	Chain	Res	Type
1	B	186	LEU
1	B	190	MET
1	B	198	ASP
1	B	209	VAL
1	B	213	ASP
1	B	224	GLU
1	B	232	GLU
1	B	233	ILE
1	B	240	LEU
1	B	287	GLN
1	B	291	ILE
1	B	294	THR
1	B	299	ASP
1	B	309	LYS
1	B	313	LYS
1	B	318	VAL
1	B	322	ASN
1	B	324	THR
1	B	330	ASN
1	B	333	LEU
1	B	341	LYS
1	B	351	LEU
1	B	364	VAL
1	B	365	THR
1	B	371	THR
1	B	380	GLN
1	B	401	HIS
1	B	407	ILE
1	B	421	ILE
1	B	423	LEU
1	B	427	ASP
1	B	429	GLN
1	B	433	GLU
1	B	436	ILE
1	B	444	LEU
1	B	455	MET
1	B	481	LYS
1	B	488	VAL
1	B	503	LEU
1	B	513	ILE
1	B	519	THR
1	B	529	LEU

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Mol	Chain	Res	Type
1	B	531	GLN
1	B	544	ILE
1	B	545	SER
1	B	546	ASN
1	B	552	GLN
1	B	557	MET
1	B	558	LEU
1	B	559	ARG
1	B	560	LEU
1	B	563	SER
1	B	573	VAL
1	B	577	LYS
1	B	582	ARG
1	B	604	VAL
1	B	608	THR
2	F	482	HIS
2	F	483	THR
2	F	486	ASN
2	F	497	CYS
2	F	498	TYR
2	F	499	VAL
2	F	504	GLN
2	F	505	VAL
2	F	509	LEU
2	F	512	ASN
2	F	515	VAL
2	F	519	THR
2	F	520	SER
2	F	522	PHE
2	F	524	ILE
2	F	525	ARG
2	F	531	VAL
2	F	538	ASP
2	F	545	LEU
2	F	549	THR
2	F	569	SER
2	F	571	VAL
2	F	578	ASN
2	F	588	THR
2	F	591	THR
2	F	593	VAL
2	F	596	LEU

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Mol	Chain	Res	Type
2	F	600	TRP
1	C	19	SER
1	C	21	ILE
1	C	27	THR
1	C	29	LEU
1	C	31	LYS
1	C	39	LEU
1	C	43	SER
1	C	45	LEU
1	C	52	THR
1	C	55	THR
1	C	56	GLU
1	C	57	GLU
1	C	62	MET
1	C	63	ASN
1	C	77	SER
1	C	78	THR
1	C	81	GLN
1	C	82	MET
1	C	87	GLU
1	C	89	GLN
1	C	91	LEU
1	C	93	VAL
1	C	95	LEU
1	C	97	LEU
1	C	100	LEU
1	C	117	ASN
1	C	120	LEU
1	C	131	LYS
1	C	145	GLU
1	C	148	LEU
1	C	160	GLU
1	C	171	GLU
1	C	172	VAL
1	C	176	LEU
1	C	186	LEU
1	C	190	MET
1	C	198	ASP
1	C	209	VAL
1	C	213	ASP
1	C	224	GLU
1	C	232	GLU

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Mol	Chain	Res	Type
1	C	233	ILE
1	C	240	LEU
1	C	287	GLN
1	C	291	ILE
1	C	294	THR
1	C	299	ASP
1	C	309	LYS
1	C	313	LYS
1	C	318	VAL
1	C	322	ASN
1	C	324	THR
1	C	330	ASN
1	C	333	LEU
1	C	341	LYS
1	C	351	LEU
1	C	364	VAL
1	C	365	THR
1	C	371	THR
1	C	380	GLN
1	C	401	HIS
1	C	407	ILE
1	C	421	ILE
1	C	423	LEU
1	C	427	ASP
1	C	429	GLN
1	C	433	GLU
1	C	436	ILE
1	C	444	LEU
1	C	455	MET
1	C	481	LYS
1	C	488	VAL
1	C	503	LEU
1	C	513	ILE
1	C	519	THR
1	C	529	LEU
1	C	531	GLN
1	C	544	ILE
1	C	545	SER
1	C	546	ASN
1	C	552	GLN
1	C	557	MET
1	C	558	LEU

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Mol	Chain	Res	Type
1	C	559	ARG
1	C	560	LEU
1	C	563	SER
1	C	573	VAL
1	C	577	LYS
1	C	582	ARG
1	C	597	ASP
1	C	604	VAL
1	C	608	THR
2	G	482	HIS
2	G	483	THR
2	G	486	ASN
2	G	497	CYS
2	G	498	TYR
2	G	499	VAL
2	G	504	GLN
2	G	505	VAL
2	G	509	LEU
2	G	512	ASN
2	G	515	VAL
2	G	519	THR
2	G	520	SER
2	G	522	PHE
2	G	524	ILE
2	G	531	VAL
2	G	533	SER
2	G	538	ASP
2	G	545	LEU
2	G	549	THR
2	G	553	SER
2	G	569	SER
2	G	571	VAL
2	G	578	ASN
2	G	588	THR
2	G	591	THR
2	G	596	LEU
2	G	600	TRP
1	D	19	SER
1	D	21	ILE
1	D	29	LEU
1	D	31	LYS
1	D	39	LEU

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Mol	Chain	Res	Type
1	D	43	SER
1	D	45	LEU
1	D	51	ASN
1	D	52	THR
1	D	55	THR
1	D	56	GLU
1	D	57	GLU
1	D	62	MET
1	D	77	SER
1	D	78	THR
1	D	81	GLN
1	D	82	MET
1	D	87	GLU
1	D	89	GLN
1	D	91	LEU
1	D	93	VAL
1	D	95	LEU
1	D	97	LEU
1	D	100	LEU
1	D	120	LEU
1	D	131	LYS
1	D	132	VAL
1	D	137	ASN
1	D	145	GLU
1	D	148	LEU
1	D	160	GLU
1	D	171	GLU
1	D	176	LEU
1	D	186	LEU
1	D	198	ASP
1	D	209	VAL
1	D	213	ASP
1	D	224	GLU
1	D	232	GLU
1	D	233	ILE
1	D	240	LEU
1	D	287	GLN
1	D	291	ILE
1	D	294	THR
1	D	299	ASP
1	D	309	LYS
1	D	313	LYS

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Mol	Chain	Res	Type
1	D	318	VAL
1	D	322	ASN
1	D	324	THR
1	D	330	ASN
1	D	333	LEU
1	D	341	LYS
1	D	345	HIS
1	D	351	LEU
1	D	364	VAL
1	D	365	THR
1	D	371	THR
1	D	380	GLN
1	D	401	HIS
1	D	407	ILE
1	D	418	LEU
1	D	421	ILE
1	D	423	LEU
1	D	427	ASP
1	D	429	GLN
1	D	433	GLU
1	D	436	ILE
1	D	444	LEU
1	D	455	MET
1	D	481	LYS
1	D	485	VAL
1	D	488	VAL
1	D	503	LEU
1	D	513	ILE
1	D	519	THR
1	D	529	LEU
1	D	531	GLN
1	D	544	ILE
1	D	545	SER
1	D	546	ASN
1	D	557	MET
1	D	558	LEU
1	D	559	ARG
1	D	560	LEU
1	D	563	SER
1	D	573	VAL
1	D	577	LYS
1	D	582	ARG

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Mol	Chain	Res	Type
1	D	597	ASP
1	D	604	VAL
1	D	608	THR
2	H	482	HIS
2	H	483	THR
2	H	486	ASN
2	H	488	THR
2	H	498	TYR
2	H	499	VAL
2	H	504	GLN
2	H	505	VAL
2	H	507	ILE
2	H	509	LEU
2	H	512	ASN
2	H	515	VAL
2	H	519	THR
2	H	520	SER
2	H	522	PHE
2	H	524	ILE
2	H	531	VAL
2	H	533	SER
2	H	538	ASP
2	H	545	LEU
2	H	553	SER
2	H	569	SER
2	H	571	VAL
2	H	578	ASN
2	H	588	THR
2	H	591	THR
2	H	596	LEU
2	H	600	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	42	GLN
1	A	49	ASN
1	A	63	ASN
1	A	76	GLN
1	A	81	GLN
1	A	89	GLN

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	149	ASN
1	A	210	ASN
1	A	221	GLN
1	A	287	GLN
1	A	290	ASN
1	A	380	GLN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	526	GLN
1	A	531	GLN
1	A	535	HIS
1	A	556	ASN
1	A	580	ASN
1	A	586	ASN
2	E	482	HIS
2	E	504	GLN
2	E	578	ASN
1	B	34	HIS
1	B	42	GLN
1	B	49	ASN
1	B	63	ASN
1	B	76	GLN
1	B	81	GLN
1	B	96	GLN
1	B	137	ASN
1	B	139	GLN
1	B	210	ASN
1	B	287	GLN
1	B	290	ASN
1	B	380	GLN
1	B	493	HIS
1	B	505	HIS
1	B	524	GLN
1	B	526	GLN
1	B	531	GLN
1	B	535	HIS
1	B	556	ASN
1	B	580	ASN
1	B	586	ASN
2	F	482	HIS

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Mol	Chain	Res	Type
2	F	504	GLN
2	F	578	ASN
2	F	586	HIS
1	C	34	HIS
1	C	49	ASN
1	C	63	ASN
1	C	76	GLN
1	C	81	GLN
1	C	96	GLN
1	C	137	ASN
1	C	139	GLN
1	C	210	ASN
1	C	287	GLN
1	C	290	ASN
1	C	322	ASN
1	C	380	GLN
1	C	493	HIS
1	C	505	HIS
1	C	526	GLN
1	C	531	GLN
1	C	535	HIS
1	C	556	ASN
1	C	580	ASN
1	C	586	ASN
2	G	482	HIS
2	G	504	GLN
2	G	578	ASN
2	G	586	HIS
1	D	34	HIS
1	D	42	GLN
1	D	49	ASN
1	D	63	ASN
1	D	76	GLN
1	D	81	GLN
1	D	89	GLN
1	D	96	GLN
1	D	149	ASN
1	D	210	ASN
1	D	287	GLN
1	D	290	ASN
1	D	380	GLN
1	D	493	HIS

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Mol	Chain	Res	Type
1	D	505	HIS
1	D	524	GLN
1	D	526	GLN
1	D	531	GLN
1	D	535	HIS
1	D	556	ASN
1	D	580	ASN
1	D	586	ASN
2	H	482	HIS
2	H	504	GLN
2	H	578	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	800	1	14,14,15	0.47	0	17,19,21	1.93	5 (29%)
3	NAG	A	800	1	14,14,15	0.40	0	17,19,21	1.80	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	801	1	14,14,15	1.10	1 (7%)	17,19,21	2.52	7 (41%)
3	NAG	B	801	1	14,14,15	1.20	1 (7%)	17,19,21	2.53	8 (47%)
3	NAG	D	800	1	14,14,15	0.43	0	17,19,21	1.82	2 (11%)
3	NAG	H	1512	2	14,14,15	0.70	0	17,19,21	2.36	7 (41%)
3	NAG	G	1512	2	14,14,15	0.71	0	17,19,21	2.44	6 (35%)
3	NAG	C	801	1	14,14,15	1.14	1 (7%)	17,19,21	2.47	7 (41%)
3	NAG	D	801	1	14,14,15	1.06	1 (7%)	17,19,21	2.48	7 (41%)
3	NAG	E	1486	2	14,14,15	0.67	0	17,19,21	0.95	1 (5%)
3	NAG	F	1512	2	14,14,15	0.71	1 (7%)	17,19,21	2.42	5 (29%)
3	NAG	H	1486	2	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
3	NAG	F	1486	2	14,14,15	0.66	0	17,19,21	0.81	0
3	NAG	E	1512	2	14,14,15	0.58	0	17,19,21	2.35	6 (35%)
3	NAG	B	800	1	14,14,15	0.55	0	17,19,21	2.00	5 (29%)
3	NAG	G	1486	2	14,14,15	0.66	0	17,19,21	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	800	1	-	1/6/23/26	0/1/1/1
3	NAG	A	800	1	-	1/6/23/26	0/1/1/1
3	NAG	A	801	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	B	801	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	H	1512	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	D	800	1	-	1/6/23/26	0/1/1/1
3	NAG	G	1512	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	801	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	D	801	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	E	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1512	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	H	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	1512	2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	B	800	1	-	1/6/23/26	0/1/1/1
3	NAG	G	1486	2	1/1/5/7	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	NAG	C1-C2	3.62	1.57	1.52
3	C	801	NAG	C1-C2	3.52	1.57	1.52
3	A	801	NAG	C1-C2	3.36	1.56	1.52
3	D	801	NAG	C1-C2	3.31	1.56	1.52
3	F	1512	NAG	C1-C2	2.06	1.55	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1512	NAG	C1-O5-C5	7.37	122.06	112.19
3	G	1512	NAG	C1-O5-C5	7.32	122.00	112.19
3	E	1512	NAG	C1-O5-C5	7.09	121.68	112.19
3	H	1512	NAG	C1-O5-C5	6.62	121.05	112.19
3	D	800	NAG	C1-O5-C5	5.93	120.14	112.19
3	A	800	NAG	C1-O5-C5	5.80	119.95	112.19
3	B	800	NAG	C1-O5-C5	5.62	119.72	112.19
3	C	800	NAG	C1-O5-C5	5.41	119.44	112.19
3	D	801	NAG	C1-O5-C5	5.23	119.19	112.19
3	A	801	NAG	C2-N2-C7	5.00	129.60	122.90
3	A	801	NAG	C1-O5-C5	4.90	118.75	112.19
3	B	801	NAG	C2-N2-C7	4.83	129.37	122.90
3	B	801	NAG	C1-O5-C5	4.76	118.56	112.19
3	C	801	NAG	C1-O5-C5	4.71	118.49	112.19
3	C	801	NAG	C1-C2-N2	4.68	117.80	110.43
3	B	801	NAG	C1-C2-N2	4.64	117.74	110.43
3	D	801	NAG	C2-N2-C7	4.55	129.00	122.90
3	D	801	NAG	C1-C2-N2	4.51	117.54	110.43
3	C	801	NAG	C2-N2-C7	4.37	128.76	122.90
3	A	801	NAG	C1-C2-N2	4.34	117.27	110.43
3	G	1512	NAG	C2-N2-C7	3.68	127.83	122.90
3	H	1512	NAG	C2-N2-C7	3.56	127.67	122.90
3	C	801	NAG	O5-C1-C2	-3.35	106.11	111.29
3	F	1512	NAG	O5-C5-C4	3.33	118.92	110.83
3	G	1512	NAG	O5-C5-C4	3.30	118.86	110.83
3	F	1512	NAG	C2-N2-C7	3.27	127.28	122.90
3	E	1512	NAG	C2-N2-C7	3.26	127.27	122.90
3	E	1512	NAG	O5-C5-C4	3.18	118.56	110.83
3	H	1512	NAG	O5-C5-C4	3.15	118.48	110.83
3	B	801	NAG	O5-C1-C2	-3.03	106.60	111.29
3	D	801	NAG	O5-C1-C2	-2.91	106.79	111.29
3	A	801	NAG	O5-C1-C2	-2.85	106.88	111.29
3	A	801	NAG	C3-C4-C5	-2.84	105.09	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	NAG	C2-N2-C7	2.77	126.61	122.90
3	A	801	NAG	O7-C7-C8	-2.76	117.15	122.05
3	D	801	NAG	C3-C4-C5	-2.73	105.29	110.23
3	C	801	NAG	C3-C4-C5	-2.67	105.38	110.23
3	B	801	NAG	O7-C7-N2	2.67	126.70	121.98
3	C	800	NAG	C2-N2-C7	2.65	126.45	122.90
3	B	801	NAG	O7-C7-C8	-2.61	117.40	122.05
3	H	1512	NAG	C6-C5-C4	-2.60	106.64	113.02
3	E	1512	NAG	C6-C5-C4	-2.60	106.65	113.02
3	H	1512	NAG	C3-C4-C5	2.57	114.90	110.23
3	E	1486	NAG	C1-O5-C5	2.50	115.54	112.19
3	C	801	NAG	O7-C7-N2	2.48	126.36	121.98
3	D	800	NAG	C1-C2-N2	2.46	114.30	110.43
3	A	800	NAG	C1-C2-N2	2.43	114.26	110.43
3	B	801	NAG	C3-C4-C5	-2.40	105.89	110.23
3	F	1512	NAG	C6-C5-C4	-2.39	107.14	113.02
3	A	801	NAG	O7-C7-N2	2.34	126.12	121.98
3	H	1486	NAG	C1-O5-C5	2.33	115.31	112.19
3	G	1512	NAG	C6-C5-C4	-2.30	107.38	113.02
3	E	1512	NAG	C3-C4-C5	2.29	114.39	110.23
3	B	800	NAG	C1-C2-N2	2.28	114.03	110.43
3	C	801	NAG	O7-C7-C8	-2.28	117.99	122.05
3	B	800	NAG	C6-C5-C4	-2.27	107.45	113.02
3	E	1512	NAG	O5-C1-C2	-2.27	107.78	111.29
3	C	800	NAG	C1-C2-N2	2.26	113.99	110.43
3	F	1512	NAG	C3-C4-C5	2.25	114.32	110.23
3	G	1512	NAG	C3-C4-C5	2.21	114.25	110.23
3	D	801	NAG	O7-C7-C8	-2.16	118.20	122.05
3	C	800	NAG	C6-C5-C4	-2.13	107.79	113.02
3	B	800	NAG	O5-C5-C6	2.13	111.81	107.66
3	B	801	NAG	O3-C3-C2	2.13	113.82	109.40
3	H	1512	NAG	O5-C1-C2	-2.13	108.00	111.29
3	D	801	NAG	O7-C7-N2	2.09	125.67	121.98
3	H	1512	NAG	C1-C2-N2	2.05	113.67	110.43
3	G	1512	NAG	O5-C1-C2	-2.04	108.13	111.29
3	C	800	NAG	O5-C5-C6	2.02	111.59	107.66

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	801	NAG	C1
3	E	1486	NAG	C1

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Mol	Chain	Res	Type	Atom
3	E	1512	NAG	C1
3	B	801	NAG	C1
3	F	1486	NAG	C1
3	F	1512	NAG	C1
3	C	801	NAG	C1
3	G	1486	NAG	C1
3	G	1512	NAG	C1
3	D	801	NAG	C1
3	H	1486	NAG	C1
3	H	1512	NAG	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1512	NAG	O5-C5-C6-O6
3	F	1512	NAG	O5-C5-C6-O6
3	G	1512	NAG	O5-C5-C6-O6
3	H	1512	NAG	O5-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6
3	D	801	NAG	O5-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
3	G	1512	NAG	C4-C5-C6-O6
3	F	1512	NAG	C4-C5-C6-O6
3	E	1512	NAG	C4-C5-C6-O6
3	H	1512	NAG	C4-C5-C6-O6
3	C	801	NAG	C4-C5-C6-O6
3	B	801	NAG	C4-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6
3	D	801	NAG	C4-C5-C6-O6
3	B	800	NAG	O5-C5-C6-O6
3	C	800	NAG	O5-C5-C6-O6
3	A	800	NAG	O5-C5-C6-O6
3	D	800	NAG	O5-C5-C6-O6
3	A	801	NAG	C1-C2-N2-C7
3	B	801	NAG	C1-C2-N2-C7
3	C	801	NAG	C1-C2-N2-C7
3	G	1486	NAG	C1-C2-N2-C7
3	D	801	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1512	NAG	1	0
3	F	1512	NAG	1	0
3	E	1512	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	593/597 (99%)	-0.93	0 100 100	43, 46, 48, 52	0
1	B	593/597 (99%)	-0.73	0 100 100	43, 46, 48, 51	0
1	C	593/597 (99%)	-0.75	1 (0%) 91 86	43, 46, 48, 52	0
1	D	593/597 (99%)	-0.89	2 (0%) 90 82	43, 46, 48, 52	0
2	E	110/136 (80%)	-1.10	0 100 100	27, 46, 48, 54	0
2	F	110/136 (80%)	-0.67	1 (0%) 81 66	27, 46, 48, 54	0
2	G	110/136 (80%)	-0.83	0 100 100	27, 46, 48, 54	0
2	H	110/136 (80%)	-1.11	0 100 100	27, 46, 48, 54	0
All	All	2812/2932 (95%)	-0.84	4 (0%) 92 91	27, 46, 48, 54	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	496	SER	3.2
1	C	42	GLN	3.1
1	D	70	SER	2.2
1	D	136	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	801	14/15	0.93	0.12	65,70,74,75	0
3	NAG	F	1512	14/15	0.93	0.10	94,105,108,109	0
3	NAG	A	800	14/15	0.94	0.09	76,81,85,85	0
3	NAG	D	800	14/15	0.94	0.07	76,81,85,85	0
3	NAG	H	1512	14/15	0.94	0.10	94,105,108,109	0
3	NAG	G	1512	14/15	0.95	0.07	94,105,108,109	0
3	NAG	B	800	14/15	0.95	0.08	76,81,85,85	0
3	NAG	C	801	14/15	0.95	0.09	65,70,74,75	0
3	NAG	F	1486	14/15	0.96	0.07	86,104,108,109	0
3	NAG	C	800	14/15	0.96	0.08	76,81,84,85	0
3	NAG	E	1486	14/15	0.97	0.08	86,104,108,109	0
3	NAG	E	1512	14/15	0.97	0.07	94,105,108,109	0
3	NAG	D	801	14/15	0.97	0.08	65,70,74,75	0
3	NAG	G	1486	14/15	0.97	0.06	86,104,108,109	0
3	NAG	H	1486	14/15	0.98	0.05	86,104,108,109	0
3	NAG	A	801	14/15	0.98	0.06	65,70,74,75	0

6.5 Other polymers

There are no such residues in this entry.