



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:39 AM UTC

PDB ID : 1H28 / pdb_00001h28
Title : CDK2/CyclinA in complex with an 11-residue recruitment peptide from p107
Authors : Tews, I.; Cheng, K.Y.; Lowe, E.D.; Noble, M.E.M.; Brown, N.R.; Gul, S.;
Gamblin, S.; Johnson, L.N.
Deposited on : 2002-07-31
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

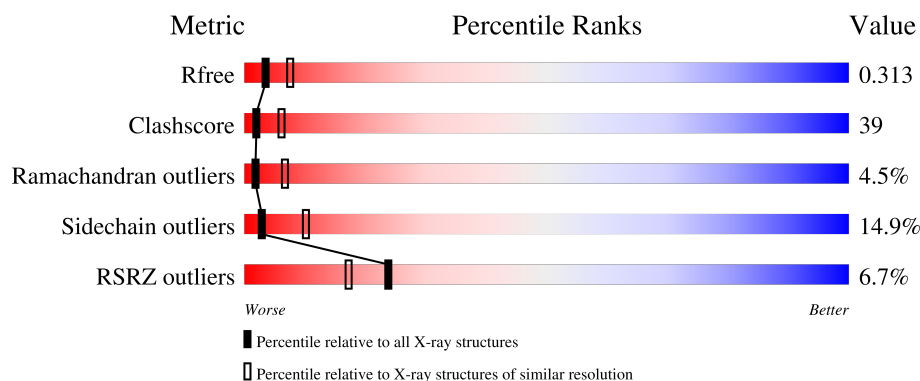
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	303	9% 36% 49% 13% .
1	C	303	8% 35% 48% 14% ..
2	B	259	3% 35% 50% 13% .
2	D	259	5% 32% 54% 11% .
3	E	11	18% 27% 36% 27% 9%

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Mol	Chain	Length	Quality of chain
3	F	11	

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
1	TPO	C	160	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9125 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called RETINOBLASTOMA-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			78	48	17	13			
3	F	8	Total	C	N	O	0	0	0
			68	43	15	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	11	Total	O	0	0
			11	11		
4	C	10	Total	O	0	0
			10	10		
4	D	3	Total	O	0	0
			3	3		

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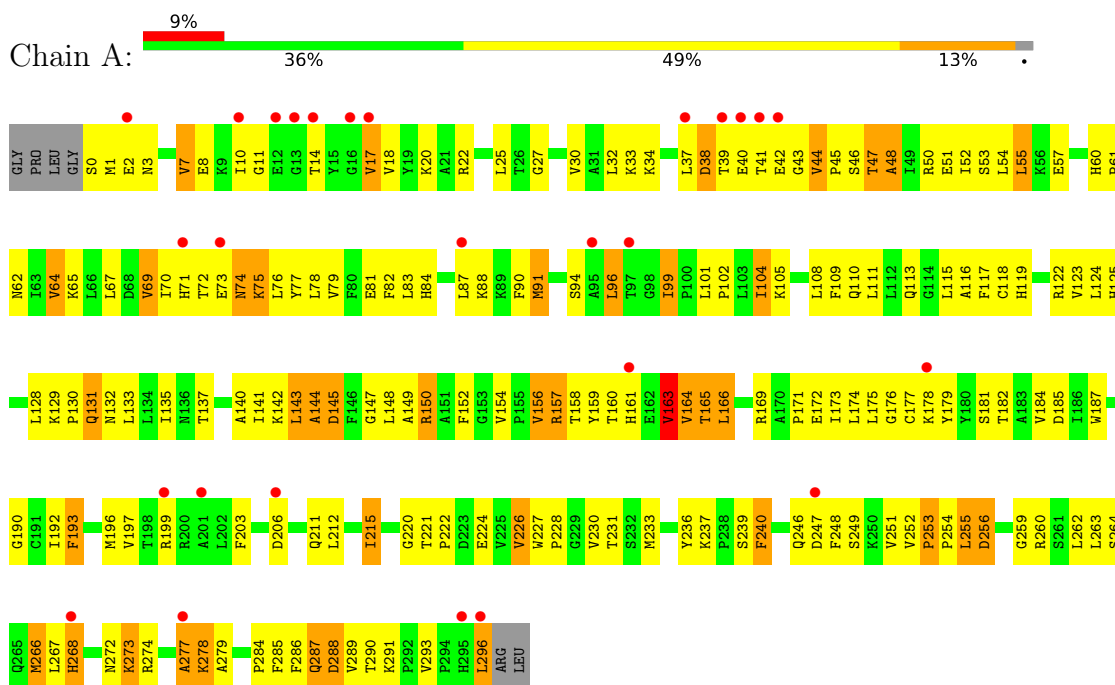
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	O	0	0
			1	1		

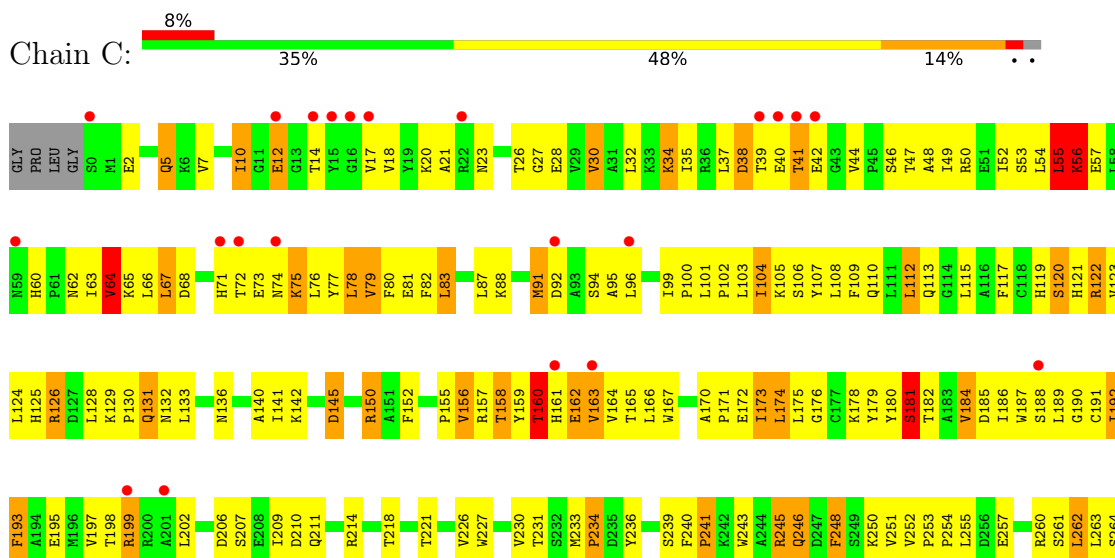
3 Residue-property plots

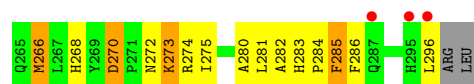
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CELL DIVISION PROTEIN KINASE 2

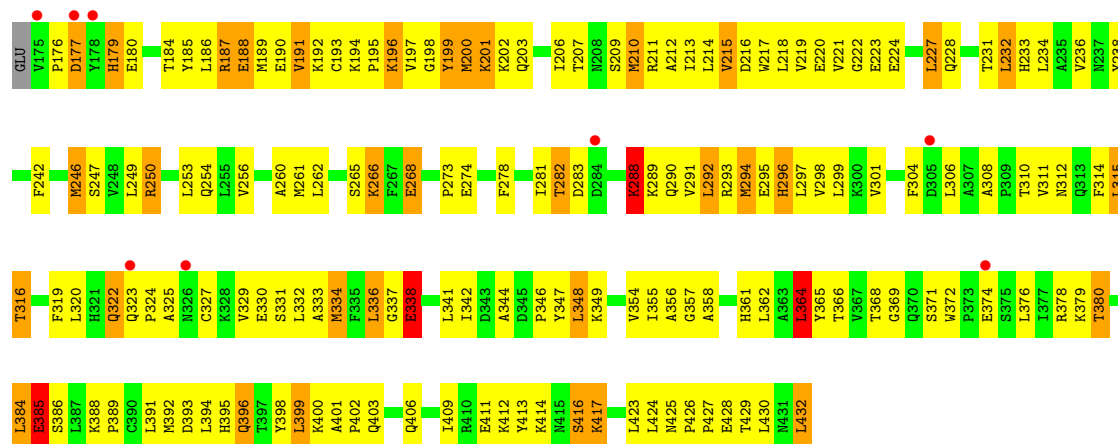


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

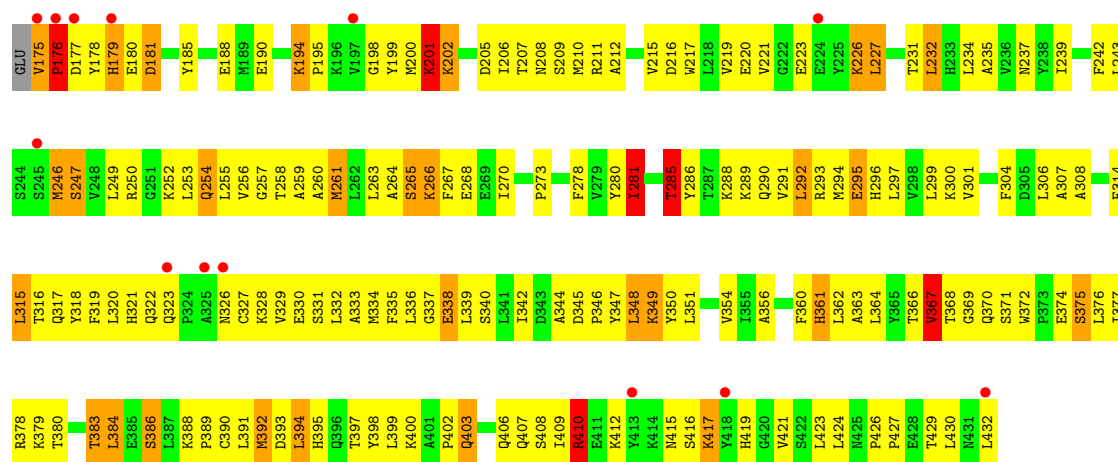




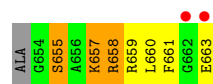
• Molecule 2: CYCLIN A2



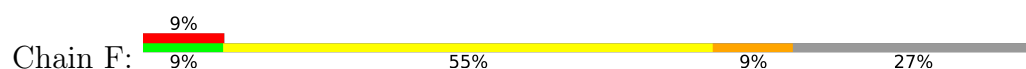
• Molecule 2: CYCLIN A2



• Molecule 3: RETINOBLASTOMA-LIKE PROTEIN 1



• Molecule 3: RETINOBLASTOMA-LIKE PROTEIN 1



ALA	GLY	SER	K656	K657	R658	R659	L660	F661	G662	E663
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.50Å 162.51Å 71.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.80 29.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.62-2.80) 95.0 (29.62-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.80Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.323 0.241 , 0.313	Depositor DCC
R_{free} test set	2095 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9125	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5558e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO

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	1.23	5/2438 (0.2%)	1.25	13/3308 (0.4%)
1	C	1.26	5/2438 (0.2%)	1.28	13/3308 (0.4%)
2	B	1.33	6/2133 (0.3%)	1.28	8/2897 (0.3%)
2	D	1.32	7/2133 (0.3%)	1.29	9/2897 (0.3%)
3	E	1.24	0/78	1.34	1/100 (1.0%)
3	F	0.90	0/68	1.32	0/87
All	All	1.28	23/9288 (0.2%)	1.28	44/12597 (0.3%)

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	C	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	CA-CB	-10.76	1.43	1.54
2	B	210	MET	SD-CE	-8.60	1.58	1.79
2	B	200	MET	SD-CE	-7.92	1.59	1.79
1	C	266	MET	SD-CE	-7.89	1.59	1.79
2	D	281	ILE	CA-CB	-7.47	1.42	1.54
2	B	246	MET	SD-CE	6.94	1.96	1.79
2	B	338	GLU	C-O	-6.69	1.16	1.24
2	D	261	MET	CG-SD	6.53	1.97	1.80
1	A	144	ALA	CA-CB	-6.52	1.45	1.54
1	C	41	THR	CA-CB	6.39	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	MET	SD-CE	6.37	1.95	1.79
2	D	367	VAL	CA-CB	-6.12	1.48	1.54
2	B	294	MET	SD-CE	-6.08	1.64	1.79
1	A	99	ILE	CA-CB	5.80	1.59	1.54
2	D	337	GLY	CA-C	-5.57	1.45	1.52
2	D	259	ALA	CA-CB	-5.56	1.44	1.53
1	C	91	MET	SD-CE	-5.48	1.65	1.79
2	D	285	THR	C-O	-5.41	1.17	1.24
1	C	282	ALA	CA-CB	-5.28	1.46	1.53
1	C	158	THR	C-O	-5.24	1.17	1.23
1	A	48	ALA	C-O	-5.15	1.18	1.24
2	D	258	THR	C-O	-5.07	1.18	1.24
2	B	332	LEU	C-O	-5.04	1.18	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	GLU	N-CA-C	-8.41	103.61	114.04
1	A	253	PRO	N-CA-C	8.23	120.74	110.70
2	D	237	ASN	N-CA-C	8.02	121.03	111.33
1	A	163	VAL	N-CA-C	7.68	119.82	108.45
2	B	268	GLU	N-CA-C	7.60	122.85	112.90
1	A	44	VAL	N-CA-C	-7.21	102.43	108.63
2	D	410	ARG	N-CA-C	7.18	118.79	110.97
2	D	333	ALA	N-CA-C	6.86	118.76	111.28
1	C	55	LEU	N-CA-C	6.83	119.35	111.02
2	D	337	GLY	N-CA-C	-6.78	104.09	112.77
2	B	222	GLY	N-CA-C	6.59	122.03	113.27
1	A	47	THR	N-CA-C	-6.57	103.23	111.11
1	C	262	LEU	N-CA-C	-6.38	103.24	111.02
1	C	273	LYS	N-CA-C	-6.17	106.39	114.04
1	A	187	TRP	N-CA-C	-6.08	104.73	111.36
2	B	250	ARG	N-CA-C	5.88	118.19	111.02
1	C	184	VAL	N-CA-CB	5.75	116.89	110.62
1	A	197	VAL	N-CA-C	5.75	116.52	110.72
2	D	354	VAL	CB-CA-C	-5.70	104.36	112.22
1	C	202	LEU	N-CA-C	5.70	117.49	111.28
1	C	192	ILE	N-CA-C	-5.64	105.60	111.58
2	B	288	LYS	N-CA-C	-5.63	104.78	111.03
1	C	10	ILE	CB-CA-C	-5.56	106.16	111.06
1	A	289	VAL	N-CA-C	5.54	117.17	109.80
3	E	657	LYS	N-CA-C	-5.53	103.23	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	212	ALA	N-CA-C	5.47	117.67	111.11
1	C	167	TRP	N-CA-C	-5.43	105.78	112.90
2	D	261	MET	N-CA-C	-5.41	104.62	111.11
2	B	210	MET	N-CA-C	5.32	117.83	111.71
1	A	173	ILE	N-CA-C	-5.31	106.51	111.45
1	C	181	SER	N-CA-C	5.29	115.54	108.23
2	B	308	ALA	N-CA-C	5.28	117.95	110.24
1	A	296	LEU	CA-C-O	-5.27	111.84	120.80
2	B	253	LEU	N-CA-C	-5.26	105.44	111.07
1	C	12	GLU	N-CA-C	-5.24	101.34	109.14
2	D	273	PRO	CA-C-O	-5.23	115.49	121.56
1	C	270	ASP	CA-C-N	5.21	125.01	119.28
1	C	270	ASP	C-N-CA	5.21	125.01	119.28
1	C	241	PRO	N-CA-C	5.16	118.97	111.03
1	A	156	VAL	CB-CA-C	5.13	118.58	111.49
1	A	287	GLN	N-CA-CB	5.03	117.51	110.12
2	D	369	GLY	N-CA-C	-5.02	108.39	115.32
1	A	288	ASP	N-CA-C	5.01	118.43	112.72
1	A	215	ILE	N-CA-C	-5.01	105.61	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	TYR	Mainchain
1	C	160	TPO	Mainchain

5.2 Too-close contacts ⓘ

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	2388	0	2430	180	0
1	C	2388	0	2430	209	0
2	B	2083	0	2107	160	2
2	D	2083	0	2107	193	2
3	E	78	0	80	8	0
3	F	68	0	72	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	0	3	0
4	B	11	0	0	0	0
4	C	10	0	0	6	0
4	D	3	0	0	0	0
4	F	1	0	0	1	0
All	All	9125	0	9226	708	2

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 39.

All (708) 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)
1:A:277:ALA:O	1:A:279:ALA:N	1.76	1.18
2:B:207:THR:OG1	2:B:210:MET:HG3	1.49	1.12
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.35	1.05
2:D:415:ASN:OD1	2:D:417:LYS:N	1.89	1.05
2:D:321:HIS:ND1	2:D:375:SER:OG	1.87	1.03
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.42	1.02
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.19	1.02
2:D:366:THR:HG23	2:D:427:PRO:HD3	1.44	0.99
1:A:190:GLY:HA2	1:A:266:MET:HE3	1.42	0.99
1:C:88:LYS:HE3	1:C:131:GLN:NE2	1.77	0.98
1:C:227:TRP:O	1:C:230:VAL:HG23	1.66	0.95
2:B:312:ASN:OD1	2:B:334:MET:HE1	1.68	0.94
2:D:175:VAL:O	2:D:177:ASP:N	2.00	0.93
1:A:0:SER:HA	4:A:2001:HOH:O	1.69	0.93
2:D:321:HIS:HD1	2:D:375:SER:HG	0.93	0.92
1:C:156:VAL:HG12	1:C:159:TYR:HE2	1.33	0.91
2:B:329:VAL:HG11	2:B:364:LEU:HD12	1.52	0.91
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.53	0.90
1:C:72:THR:HB	1:C:75:LYS:O	1.71	0.89
2:B:361:HIS:HD2	2:B:372:TRP:H	1.11	0.89
1:A:50:ARG:HH22	1:A:150:ARG:NH2	1.71	0.88
2:D:211:ARG:HG2	2:D:211:ARG:HH11	1.40	0.87
1:C:99:ILE:HG23	1:C:103:LEU:HD23	1.57	0.86
1:A:135:ILE:HG22	1:A:141:ILE:HG13	1.56	0.86
1:A:72:THR:O	1:A:74:ASN:N	2.07	0.86
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.56	0.85
1:A:116:ALA:HB2	1:A:277:ALA:HB1	1.59	0.85
1:A:7:VAL:HG11	1:A:20:LYS:HD3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:PHE:HB3	1:C:260:ARG:HD2	1.60	0.84
1:A:129:LYS:NZ	1:A:165:THR:OG1	2.11	0.83
1:A:81:GLU:OE1	1:A:142:LYS:NZ	2.10	0.82
1:A:39:THR:HG21	2:B:289:LYS:HG2	1.59	0.82
2:B:266:LYS:NZ	2:B:295:GLU:OE1	2.11	0.82
1:A:50:ARG:NH2	1:A:150:ARG:NH2	2.26	0.81
3:F:659:ARG:NH2	3:F:663:GLU:HA	1.94	0.81
1:A:255:LEU:HD23	1:A:260:ARG:N	1.96	0.80
1:C:60:HIS:CD2	1:C:62:ASN:H	1.99	0.80
2:B:391:LEU:HD23	2:B:432:LEU:HD11	1.65	0.79
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.62	0.79
1:C:71:HIS:HE1	2:D:304:PHE:HE2	1.29	0.79
1:A:266:MET:O	1:A:274:ARG:HD3	1.82	0.79
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.11	0.79
1:A:252:VAL:HG12	1:A:255:LEU:HB2	1.64	0.79
2:D:281:ILE:O	3:F:657:LYS:HA	1.83	0.79
1:C:268:HIS:NE2	1:C:273:LYS:HD2	1.99	0.78
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.65	0.78
2:D:329:VAL:HG22	2:D:367:VAL:HG21	1.64	0.78
1:C:245:ARG:HG3	1:C:245:ARG:NH1	1.98	0.78
1:C:117:PHE:O	1:C:120:SER:HB2	1.84	0.77
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.65	0.77
2:B:336:LEU:CD1	2:B:362:LEU:HD23	2.14	0.76
1:C:83:LEU:HD11	1:C:142:LYS:HD2	1.66	0.76
1:C:49:ILE:O	1:C:53:SER:OG	2.03	0.76
1:C:21:ALA:HB3	1:C:30:VAL:HG22	1.67	0.76
1:C:245:ARG:HH11	1:C:245:ARG:CG	1.96	0.76
2:D:175:VAL:C	2:D:177:ASP:H	1.93	0.75
2:B:319:PHE:O	2:B:322:GLN:HB2	1.85	0.75
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.16	0.75
1:A:64:VAL:HG23	1:A:143:LEU:O	1.86	0.75
1:A:154:VAL:O	2:B:316:THR:HG23	1.88	0.74
2:B:342:ILE:HD11	2:B:409:ILE:HD12	1.69	0.74
1:C:251:VAL:HG12	1:C:252:VAL:HG13	1.69	0.73
2:D:400:LYS:HA	2:D:403:GLN:HE21	1.51	0.73
1:A:96:LEU:HD12	1:A:96:LEU:H	1.54	0.73
1:C:60:HIS:HD2	1:C:62:ASN:H	1.36	0.73
2:D:285:THR:HG21	3:F:659:ARG:HG3	1.71	0.72
1:A:1:MET:O	4:A:2002:HOH:O	2.07	0.72
2:D:265:SER:O	2:D:267:PHE:N	2.22	0.72
1:C:296:LEU:O	4:C:2010:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:TYR:OH	2:D:394:LEU:HA	1.89	0.72
1:C:39:THR:HA	2:D:292:LEU:HD23	1.70	0.72
1:C:88:LYS:HE3	1:C:131:GLN:HE22	1.53	0.72
1:A:40:GLU:O	2:B:288:LYS:NZ	2.18	0.72
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.07	0.71
1:A:247:ASP:OD2	1:A:249:SER:OG	2.06	0.71
1:A:178:LYS:HE2	1:A:179:TYR:CE1	2.25	0.71
1:C:50:ARG:NH2	1:C:160:TPO:O2P	2.22	0.71
1:A:172:GLU:N	1:A:172:GLU:OE1	2.22	0.71
1:C:156:VAL:HG12	1:C:159:TYR:CE2	2.23	0.71
1:A:239:SER:O	1:A:240:PHE:C	2.31	0.70
2:D:400:LYS:HA	2:D:403:GLN:NE2	2.06	0.70
2:D:278:PHE:O	2:D:281:ILE:HG22	1.91	0.70
1:A:72:THR:O	1:A:72:THR:HG23	1.90	0.69
1:C:39:THR:O	2:D:292:LEU:CD2	2.40	0.69
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.27	0.69
1:C:157:ARG:NH1	2:D:268:GLU:OE2	2.22	0.69
2:D:392:MET:HE2	2:D:392:MET:HA	1.74	0.69
1:A:154:VAL:O	2:B:316:THR:CG2	2.41	0.69
2:B:412:LYS:HD3	2:B:413:TYR:CE1	2.27	0.69
2:B:223:GLU:OE2	2:B:412:LYS:HE3	1.92	0.69
2:B:361:HIS:O	2:B:362:LEU:C	2.35	0.69
1:A:2:GLU:OE1	1:C:73:GLU:HG2	1.91	0.69
2:B:411:GLU:O	2:B:414:LYS:HB2	1.93	0.69
2:D:306:LEU:O	2:D:308:ALA:N	2.19	0.69
1:A:108:LEU:HD23	1:A:286:PHE:HZ	1.56	0.68
2:B:196:LYS:O	2:B:199:TYR:HB3	1.92	0.68
3:F:661:PHE:O	3:F:663:GLU:N	2.21	0.68
1:A:33:LYS:NZ	1:A:51:GLU:OE2	2.26	0.68
2:B:223:GLU:CD	2:B:412:LYS:HE3	2.18	0.68
1:A:25:LEU:HD12	2:D:297:LEU:HD22	1.76	0.68
1:A:10:ILE:HG12	1:A:18:VAL:O	1.94	0.68
1:A:239:SER:O	1:A:240:PHE:O	2.12	0.68
3:F:662:GLY:O	3:F:663:GLU:HB2	1.94	0.67
1:C:37:LEU:O	1:C:38:ASP:CB	2.42	0.67
1:C:54:LEU:O	1:C:57:GLU:HB3	1.95	0.67
1:C:81:GLU:O	1:C:81:GLU:HG3	1.95	0.67
1:C:181:SER:OG	1:C:182:THR:N	2.27	0.67
2:D:221:VAL:HG13	2:D:281:ILE:CD1	2.25	0.67
1:C:37:LEU:O	1:C:38:ASP:HB2	1.94	0.67
1:C:160:TPO:O3P	1:C:160:TPO:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:SER:O	1:C:184:VAL:HG22	1.95	0.67
2:B:254:GLN:NE2	3:E:660:LEU:HG	2.09	0.66
2:B:361:HIS:CD2	2:B:372:TRP:H	2.03	0.66
3:F:658:ARG:HG2	3:F:660:LEU:HD23	1.77	0.66
1:A:157:ARG:NH2	2:B:268:GLU:OE1	2.24	0.66
2:D:363:ALA:O	2:D:367:VAL:HG22	1.96	0.66
1:C:115:LEU:HD11	1:C:119:HIS:CE1	2.30	0.66
2:D:383:THR:N	2:D:386:SER:OG	2.28	0.66
2:B:203:GLN:NE2	2:B:246:MET:O	2.28	0.66
2:D:384:LEU:HG	2:D:432:LEU:HD22	1.78	0.66
1:A:105:LYS:NZ	1:A:288:ASP:OD1	2.27	0.65
2:B:200:MET:SD	2:B:206:ILE:HG13	2.36	0.65
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.78	0.65
1:C:112:LEU:CD2	1:C:189:LEU:HD13	2.26	0.65
1:C:39:THR:CB	2:D:289:LYS:HD3	2.27	0.65
1:C:74:ASN:O	1:C:75:LYS:HB3	1.95	0.65
1:C:52:ILE:O	1:C:56:LYS:HG2	1.97	0.65
1:A:177:CYS:HB2	1:A:233:MET:HE1	1.79	0.65
1:A:277:ALA:O	1:A:278:LYS:C	2.37	0.65
2:B:344:ALA:O	2:B:348:LEU:HB2	1.96	0.65
1:C:245:ARG:NH1	1:C:245:ARG:CG	2.59	0.64
2:D:211:ARG:HG2	2:D:211:ARG:NH1	2.09	0.64
2:D:364:LEU:HG	2:D:370:GLN:HB2	1.79	0.64
1:C:68:ASP:O	1:C:79:VAL:HG23	1.98	0.64
2:B:388:LYS:HB3	2:B:389:PRO:CD	2.27	0.64
2:D:321:HIS:CE1	2:D:375:SER:HG	2.16	0.64
2:B:299:LEU:HD23	2:B:306:LEU:HD21	1.80	0.64
2:B:361:HIS:NE2	2:B:371:SER:OG	2.31	0.64
2:D:332:LEU:O	2:D:335:PHE:HB3	1.98	0.64
2:D:400:LYS:O	2:D:403:GLN:HG2	1.97	0.64
1:A:50:ARG:HH22	1:A:150:ARG:HH21	1.43	0.64
1:A:10:ILE:HD11	1:A:18:VAL:HG12	1.79	0.64
1:A:37:LEU:O	1:A:38:ASP:HB2	1.98	0.64
1:C:99:ILE:HG22	1:C:104:ILE:HG13	1.80	0.64
2:D:366:THR:CG2	2:D:427:PRO:HD3	2.23	0.64
1:C:10:ILE:HD13	1:C:82:PHE:HE1	1.63	0.63
1:C:112:LEU:HD23	1:C:189:LEU:HD13	1.80	0.63
2:B:342:ILE:CD1	2:B:409:ILE:HD12	2.28	0.63
2:D:299:LEU:HD22	2:D:304:PHE:CE1	2.34	0.63
1:A:2:GLU:O	1:A:2:GLU:HG2	1.98	0.63
1:A:65:LYS:HB3	1:A:81:GLU:OE2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:VAL:HG13	2:D:281:ILE:HD12	1.79	0.63
2:D:361:HIS:CD2	2:D:362:LEU:N	2.66	0.63
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.14	0.63
1:A:39:THR:CG2	2:B:289:LYS:HG2	2.29	0.63
2:D:416:SER:O	2:D:419:HIS:N	2.31	0.63
1:A:247:ASP:OD2	1:A:249:SER:N	2.32	0.62
2:B:412:LYS:HD3	2:B:413:TYR:HE1	1.62	0.62
1:C:210:ASP:O	1:C:214:ARG:HG3	1.99	0.62
1:C:42:GLU:O	2:D:266:LYS:NZ	2.24	0.62
1:A:239:SER:C	1:A:240:PHE:O	2.39	0.62
1:C:55:LEU:C	1:C:57:GLU:H	2.07	0.62
1:C:231:THR:HG22	1:C:236:TYR:CE2	2.35	0.62
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.80	0.62
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.81	0.62
1:C:248:PHE:CB	1:C:260:ARG:HD2	2.27	0.62
1:A:108:LEU:HD23	1:A:286:PHE:CZ	2.34	0.62
1:C:227:TRP:CH2	1:C:233:MET:HE1	2.35	0.62
2:D:384:LEU:HG	2:D:432:LEU:CD2	2.29	0.62
2:D:402:PRO:HA	2:D:407:GLN:HE22	1.64	0.62
3:F:659:ARG:HH21	3:F:663:GLU:HA	1.63	0.62
1:A:67:LEU:HD12	1:A:79:VAL:HG12	1.82	0.61
1:C:35:ILE:HD12	1:C:78:LEU:HD21	1.80	0.61
1:A:1:MET:HE1	1:A:70:ILE:HD12	1.82	0.61
2:B:236:VAL:HG21	2:B:341:LEU:HD22	1.82	0.61
1:C:5:GLN:HE21	1:C:5:GLN:HA	1.65	0.61
1:C:39:THR:OG1	2:D:289:LYS:HD3	1.99	0.61
2:D:177:ASP:HB3	2:D:178:TYR:CD2	2.35	0.61
2:D:371:SER:O	2:D:372:TRP:C	2.44	0.61
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.83	0.61
2:B:234:LEU:HD23	2:B:310:THR:HG21	1.81	0.61
1:C:126:ARG:NH2	1:C:160:TPO:O1P	2.30	0.61
1:C:268:HIS:CE1	1:C:273:LYS:HD2	2.35	0.61
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.14	0.61
2:D:234:LEU:O	2:D:235:ALA:C	2.40	0.60
1:C:88:LYS:HA	1:C:91:MET:HE2	1.83	0.60
1:C:145:ASP:C	1:C:145:ASP:OD1	2.44	0.60
1:C:161:HIS:O	1:C:163:VAL:N	2.33	0.60
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.84	0.60
2:D:285:THR:HG22	3:F:659:ARG:HD2	1.83	0.60
2:D:216:ASP:HB2	2:D:406:GLN:HG2	1.83	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:GLN:O	2:D:254:GLN:HG3	2.01	0.60
2:D:265:SER:O	2:D:266:LYS:C	2.41	0.60
1:A:96:LEU:HD12	1:A:96:LEU:N	2.17	0.60
2:B:203:GLN:NE2	2:B:247:SER:HA	2.16	0.60
1:A:116:ALA:HB2	1:A:277:ALA:CB	2.31	0.60
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.84	0.60
2:D:289:LYS:HD2	2:D:293:ARG:HH21	1.67	0.60
2:D:368:THR:CB	2:D:370:GLN:HE21	2.14	0.60
2:D:416:SER:O	2:D:417:LYS:C	2.45	0.60
2:D:176:PRO:HA	2:D:179:HIS:CG	2.37	0.59
2:D:314:PHE:O	2:D:315:LEU:C	2.44	0.59
2:D:360:PHE:HD2	2:D:372:TRP:CZ3	2.20	0.59
2:B:232:LEU:HD23	2:B:261:MET:HE1	1.84	0.59
1:C:230:VAL:HG12	1:C:236:TYR:CD1	2.38	0.59
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.68	0.59
1:A:255:LEU:HD23	1:A:259:GLY:C	2.26	0.59
2:D:247:SER:O	2:D:247:SER:OG	2.16	0.58
2:B:392:MET:HE2	2:B:392:MET:HA	1.84	0.58
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.66	0.58
2:D:402:PRO:HB3	2:D:410:ARG:CZ	2.33	0.58
1:A:90:PHE:CE2	1:A:99:ILE:HD12	2.39	0.58
2:B:428:GLU:HG2	2:B:428:GLU:O	2.04	0.58
1:C:39:THR:CA	2:D:292:LEU:HD23	2.34	0.58
2:D:253:LEU:HD12	2:D:253:LEU:O	2.03	0.58
2:D:175:VAL:C	2:D:177:ASP:N	2.56	0.57
3:F:658:ARG:NE	4:F:2001:HOH:O	2.20	0.57
1:A:61:PRO:O	1:A:142:LYS:HD3	2.05	0.57
2:B:294:MET:O	2:B:295:GLU:C	2.47	0.57
2:D:178:TYR:O	2:D:180:GLU:N	2.38	0.57
1:A:54:LEU:HD13	1:A:123:VAL:HG13	1.86	0.57
2:B:203:GLN:HE22	2:B:247:SER:HA	1.67	0.57
1:C:110:GLN:HE22	1:C:140:ALA:HA	1.69	0.57
1:A:1:MET:CE	1:A:70:ILE:HD13	2.35	0.57
1:A:177:CYS:SG	1:A:178:LYS:N	2.77	0.57
1:C:128:LEU:HB2	4:C:2004:HOH:O	2.04	0.57
1:C:218:THR:HA	1:C:246:GLN:HG3	1.86	0.57
2:D:263:LEU:HD23	2:D:295:GLU:OE2	2.04	0.57
1:C:193:PHE:HD1	1:C:193:PHE:C	2.12	0.57
2:D:376:LEU:O	2:D:380:THR:OG1	2.16	0.57
2:D:388:LYS:N	2:D:389:PRO:CD	2.67	0.57
2:B:216:ASP:OD1	2:B:406:GLN:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:C	1:C:57:GLU:N	2.60	0.57
1:C:63:ILE:O	1:C:64:VAL:C	2.47	0.57
2:D:338:GLU:OE2	2:D:412:LYS:NZ	2.33	0.57
2:B:283:ASP:OD1	2:B:283:ASP:O	2.23	0.57
1:C:65:LYS:NZ	1:C:67:LEU:HD23	2.20	0.57
1:C:230:VAL:HG12	1:C:236:TYR:CE1	2.40	0.57
1:A:236:TYR:CD2	1:A:236:TYR:C	2.82	0.56
2:B:338:GLU:OE2	2:B:412:LYS:NZ	2.33	0.56
1:C:129:LYS:HE2	1:C:132:ASN:ND2	2.20	0.56
2:B:401:ALA:N	2:B:402:PRO:CD	2.69	0.56
1:C:109:PHE:CE2	1:C:113:GLN:NE2	2.73	0.56
1:A:84:HIS:CD2	1:A:296:LEU:HD13	2.41	0.56
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.41	0.56
2:D:256:VAL:HG22	2:D:294:MET:HE3	1.86	0.56
3:F:659:ARG:CZ	3:F:663:GLU:HA	2.34	0.56
1:C:21:ALA:HB3	1:C:30:VAL:CG2	2.34	0.56
1:C:227:TRP:CZ2	1:C:233:MET:HE1	2.40	0.56
2:B:391:LEU:HD23	2:B:432:LEU:CD1	2.32	0.56
2:B:365:TYR:O	2:B:369:GLY:HA2	2.04	0.56
1:C:108:LEU:CD2	1:C:193:PHE:CD2	2.88	0.56
1:A:256:ASP:O	1:A:260:ARG:HG3	2.05	0.56
2:B:189:MET:O	2:B:190:GLU:C	2.49	0.56
2:B:396:GLN:O	2:B:399:LEU:N	2.39	0.56
1:C:7:VAL:HB	1:C:20:LYS:HB3	1.88	0.56
2:B:215:VAL:HG22	2:B:236:VAL:HG22	1.88	0.56
1:C:113:GLN:HA	1:C:281:LEU:HD11	1.88	0.56
2:B:210:MET:HE1	2:B:250:ARG:HG2	1.88	0.55
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.71	0.55
1:A:52:ILE:O	1:A:53:SER:C	2.49	0.55
1:C:268:HIS:CE1	1:C:273:LYS:HB3	2.42	0.55
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.88	0.55
2:D:220:GLU:HG3	2:D:408:SER:HB3	1.87	0.55
1:C:193:PHE:C	1:C:193:PHE:CD1	2.82	0.55
2:D:265:SER:O	2:D:268:GLU:N	2.40	0.55
2:B:187:ARG:HG3	2:B:187:ARG:NH1	2.20	0.55
1:A:122:ARG:HA	1:A:152:PHE:CZ	2.41	0.55
1:A:124:LEU:HG	1:A:152:PHE:HD2	1.72	0.55
2:B:200:MET:SD	2:B:206:ILE:CD1	2.95	0.55
1:C:39:THR:O	2:D:292:LEU:HD23	2.06	0.55
2:D:306:LEU:C	2:D:308:ALA:H	2.12	0.55
1:A:1:MET:HE1	1:A:70:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:O	2:B:266:LYS:NZ	2.38	0.55
1:C:178:LYS:HG2	1:C:179:TYR:CE1	2.42	0.55
1:C:272:ASN:HB3	4:C:2009:HOH:O	2.07	0.55
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.42	0.55
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.88	0.55
2:D:227:LEU:N	2:D:227:LEU:HD23	2.22	0.55
2:B:322:GLN:CD	2:B:325:ALA:HA	2.33	0.54
1:C:35:ILE:HG22	1:C:35:ILE:O	2.06	0.54
2:D:383:THR:N	2:D:386:SER:HG	2.04	0.54
1:A:2:GLU:OE1	1:C:73:GLU:CG	2.55	0.54
1:C:101:LEU:HB3	1:C:102:PRO:CD	2.37	0.54
1:A:1:MET:CE	1:A:70:ILE:CD1	2.86	0.54
2:D:317:GLN:NE2	2:D:379:LYS:NZ	2.56	0.54
1:C:34:LYS:HB2	1:C:77:TYR:CE1	2.42	0.54
1:C:233:MET:O	1:C:234:PRO:C	2.50	0.54
2:D:175:VAL:N	2:D:176:PRO:CD	2.70	0.54
2:D:329:VAL:HG22	2:D:367:VAL:CG2	2.37	0.54
2:B:221:VAL:HG11	2:B:281:ILE:HD13	1.90	0.54
1:C:109:PHE:O	1:C:113:GLN:HB2	2.07	0.54
1:A:104:ILE:HG23	1:A:196:MET:HE3	1.90	0.54
1:A:110:GLN:HE22	1:A:140:ALA:HA	1.72	0.54
1:A:226:VAL:HG22	1:A:226:VAL:O	2.07	0.54
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.39	0.54
2:B:361:HIS:CD2	2:B:371:SER:OG	2.61	0.54
2:D:200:MET:HE3	2:D:207:THR:C	2.32	0.54
2:B:314:PHE:O	2:B:315:LEU:C	2.49	0.53
1:A:1:MET:C	1:A:3:ASN:H	2.16	0.53
1:A:172:GLU:O	1:A:177:CYS:HB2	2.08	0.53
1:C:50:ARG:O	1:C:54:LEU:HD12	2.08	0.53
1:A:171:PRO:HD2	1:A:172:GLU:OE1	2.07	0.53
2:D:392:MET:O	2:D:395:HIS:HB3	2.08	0.53
1:A:27:GLY:HA3	2:D:249:LEU:HD12	1.90	0.53
1:C:180:TYR:C	1:C:180:TYR:CD1	2.86	0.53
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.90	0.53
1:A:122:ARG:HD2	1:A:122:ARG:O	2.08	0.53
2:B:185:TYR:O	2:B:188:GLU:HB3	2.09	0.53
2:B:221:VAL:CG1	2:B:281:ILE:HD13	2.39	0.53
2:B:336:LEU:O	2:B:337:GLY:C	2.51	0.53
2:D:368:THR:HB	2:D:370:GLN:HE21	1.73	0.53
2:D:326:ASN:HB3	2:D:329:VAL:HG23	1.91	0.53
2:D:415:ASN:OD1	2:D:416:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:MET:CE	2:D:250:ARG:HB2	2.39	0.53
2:B:211:ARG:O	2:B:214:LEU:HB3	2.08	0.52
2:B:234:LEU:HD23	2:B:310:THR:CG2	2.40	0.52
2:D:260:ALA:O	2:D:261:MET:C	2.52	0.52
1:A:211:GLN:O	1:A:215:ILE:HG13	2.09	0.52
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.91	0.52
1:A:181:SER:O	1:A:184:VAL:HG22	2.10	0.52
2:B:384:LEU:O	2:B:385:GLU:C	2.53	0.52
1:C:170:ALA:HB1	1:C:171:PRO:CD	2.39	0.52
3:E:659:ARG:HE	3:E:663:GLU:HA	1.73	0.52
1:C:39:THR:HB	2:D:289:LYS:HD3	1.91	0.52
1:C:156:VAL:CG1	1:C:159:TYR:HE2	2.14	0.52
2:D:221:VAL:HG22	2:D:281:ILE:CD1	2.39	0.52
2:D:317:GLN:NE2	2:D:379:LYS:HZ1	2.07	0.52
2:D:392:MET:HE3	2:D:430:LEU:HD12	1.91	0.52
1:A:42:GLU:HA	1:A:42:GLU:OE1	2.09	0.52
1:C:37:LEU:HD22	1:C:44:VAL:HA	1.91	0.52
1:C:160:TPO:HG23	1:C:161:HIS:N	2.25	0.52
1:A:17:VAL:C	1:A:18:VAL:HG23	2.35	0.52
2:B:330:GLU:O	2:B:333:ALA:HB3	2.10	0.52
1:C:103:LEU:O	1:C:104:ILE:C	2.53	0.52
2:D:216:ASP:CB	2:D:406:GLN:HG2	2.40	0.52
1:C:40:GLU:O	2:D:288:LYS:NZ	2.43	0.52
1:C:155:PRO:CD	2:D:316:THR:HG22	2.39	0.52
1:C:284:PRO:C	1:C:286:PHE:N	2.62	0.52
1:A:60:HIS:HD2	1:A:62:ASN:H	1.55	0.51
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.92	0.51
2:D:210:MET:HE1	2:D:250:ARG:CB	2.40	0.51
2:D:285:THR:CG2	3:F:659:ARG:HD2	2.40	0.51
2:B:196:LYS:HB2	2:B:196:LYS:NZ	2.25	0.51
1:C:178:LYS:HG2	1:C:179:TYR:CD1	2.45	0.51
1:C:266:MET:O	1:C:274:ARG:HD3	2.10	0.51
1:A:33:LYS:NZ	1:A:51:GLU:CD	2.68	0.51
2:B:262:LEU:O	2:B:265:SER:HB2	2.11	0.51
1:C:57:GLU:HG3	2:D:185:TYR:OH	2.11	0.51
1:A:259:GLY:O	1:A:260:ARG:C	2.52	0.51
2:B:211:ARG:HD3	2:B:344:ALA:HB2	1.91	0.51
1:A:38:ASP:HB3	4:A:2004:HOH:O	2.10	0.51
2:B:190:GLU:O	2:B:191:VAL:C	2.53	0.51
1:A:17:VAL:HG12	1:A:18:VAL:H	1.75	0.51
1:C:106:SER:O	1:C:107:TYR:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:O	2:D:252:LYS:HG3	2.10	0.51
2:B:217:TRP:CE3	3:E:660:LEU:HD11	2.46	0.51
2:B:388:LYS:N	2:B:389:PRO:HD2	2.26	0.51
1:C:160:TPO:HA	2:D:270:ILE:HG23	1.92	0.51
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.93	0.51
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.46	0.51
2:D:199:TYR:CD1	2:D:199:TYR:C	2.88	0.51
2:B:249:LEU:HD12	1:C:27:GLY:HA3	1.92	0.50
1:A:132:ASN:OD1	1:A:145:ASP:HB3	2.12	0.50
1:C:101:LEU:N	1:C:102:PRO:HD2	2.26	0.50
1:C:123:VAL:HG12	1:C:124:LEU:N	2.25	0.50
1:C:128:LEU:CB	4:C:2004:HOH:O	2.59	0.50
2:D:221:VAL:HG22	2:D:281:ILE:HD11	1.93	0.50
2:D:350:TYR:CE1	2:D:390:CYS:HB2	2.47	0.50
2:D:397:THR:O	2:D:398:TYR:C	2.55	0.50
1:A:266:MET:O	1:A:274:ARG:CD	2.58	0.50
2:D:205:ASP:O	2:D:206:ILE:CG2	2.59	0.50
2:D:231:THR:HG23	2:D:264:ALA:C	2.36	0.50
2:B:187:ARG:CG	2:B:187:ARG:HH11	2.24	0.50
2:B:342:ILE:HD11	2:B:409:ILE:CD1	2.39	0.50
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.46	0.50
3:E:657:LYS:O	3:E:658:ARG:HB2	2.12	0.50
1:A:165:THR:O	1:A:166:LEU:C	2.54	0.50
2:B:278:PHE:O	2:B:282:THR:HG23	2.12	0.50
1:C:101:LEU:O	1:C:104:ILE:HB	2.12	0.50
1:C:284:PRO:O	1:C:285:PHE:C	2.55	0.50
1:A:268:HIS:HB2	1:A:274:ARG:HA	1.92	0.50
1:C:253:PRO:CB	1:C:254:PRO:CD	2.83	0.50
2:D:175:VAL:N	2:D:176:PRO:HD2	2.26	0.50
2:D:339:LEU:HD23	2:D:409:ILE:HG21	1.92	0.50
2:B:296:HIS:O	2:B:297:LEU:C	2.55	0.50
1:C:108:LEU:HD11	1:C:112:LEU:HD21	1.93	0.50
1:A:40:GLU:H	2:B:292:LEU:HD23	1.75	0.50
1:A:115:LEU:HD21	1:A:185:ASP:HB3	1.93	0.50
1:C:39:THR:C	2:D:292:LEU:HD23	2.37	0.50
1:C:261:SER:O	1:C:262:LEU:C	2.54	0.50
2:D:256:VAL:CG2	2:D:294:MET:HE3	2.42	0.50
1:C:197:VAL:HG21	1:C:255:LEU:HD13	1.94	0.49
2:D:395:HIS:O	2:D:398:TYR:HB3	2.12	0.49
1:A:124:LEU:HG	1:A:152:PHE:CD2	2.46	0.49
1:A:174:LEU:HD13	1:A:212:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:HIS:HD2	2:D:391:LEU:HD11	1.76	0.49
2:D:200:MET:SD	2:D:206:ILE:HG13	2.52	0.49
2:D:252:LYS:O	2:D:253:LEU:C	2.54	0.49
2:D:327:CYS:SG	2:D:328:LYS:N	2.86	0.49
2:D:423:LEU:O	2:D:424:LEU:C	2.49	0.49
2:B:423:LEU:O	2:B:424:LEU:C	2.54	0.49
1:A:37:LEU:O	1:A:38:ASP:CB	2.61	0.49
2:B:409:ILE:O	2:B:412:LYS:HB3	2.13	0.49
1:C:60:HIS:HD2	1:C:62:ASN:N	2.08	0.49
2:D:253:LEU:HD12	2:D:253:LEU:C	2.35	0.49
3:F:659:ARG:HH21	3:F:663:GLU:CA	2.25	0.49
1:A:142:LYS:O	1:A:143:LEU:C	2.55	0.49
2:B:203:GLN:OE1	2:B:247:SER:HA	2.13	0.49
1:C:65:LYS:HZ3	1:C:67:LEU:HD23	1.76	0.49
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.49
2:B:212:ALA:O	2:B:213:ILE:C	2.54	0.49
2:B:385:GLU:O	2:B:386:SER:C	2.56	0.49
2:B:227:LEU:HD21	2:B:273:PRO:CG	2.43	0.49
1:C:241:PRO:HB2	1:C:243:TRP:CZ3	2.48	0.49
1:C:39:THR:O	2:D:292:LEU:HD22	2.11	0.48
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.48	0.48
2:D:326:ASN:OD1	2:D:329:VAL:HG23	2.12	0.48
1:A:1:MET:C	1:A:3:ASN:N	2.71	0.48
1:A:7:VAL:HG12	1:A:8:GLU:N	2.28	0.48
1:C:48:ALA:O	1:C:49:ILE:C	2.53	0.48
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.95	0.48
1:A:124:LEU:O	1:A:149:ALA:HA	2.13	0.48
1:A:47:THR:O	1:A:51:GLU:N	2.40	0.48
2:B:278:PHE:HD1	2:B:281:ILE:HD11	1.78	0.48
1:C:239:SER:O	1:C:240:PHE:C	2.57	0.48
1:C:260:ARG:O	1:C:264:SER:HB3	2.13	0.48
1:C:284:PRO:C	1:C:286:PHE:H	2.20	0.48
1:C:57:GLU:CG	2:D:185:TYR:OH	2.61	0.48
2:D:255:LEU:HB2	2:D:286:TYR:CZ	2.47	0.48
1:A:284:PRO:O	1:A:287:GLN:HG2	2.14	0.48
2:B:203:GLN:CD	2:B:247:SER:HA	2.38	0.48
2:B:288:LYS:O	2:B:289:LYS:C	2.56	0.48
1:C:95:ALA:O	1:C:199:ARG:NH1	2.44	0.48
2:D:246:MET:HG2	2:D:301:VAL:HG11	1.96	0.48
2:D:392:MET:CE	2:D:430:LEU:HD12	2.44	0.48
2:B:203:GLN:HE22	2:B:246:MET:C	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:PRO:O	2:B:348:LEU:N	2.47	0.48
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.49	0.48
1:C:123:VAL:CG1	1:C:124:LEU:N	2.76	0.48
1:C:209:ILE:CG2	1:C:210:ASP:N	2.76	0.48
1:C:284:PRO:O	1:C:286:PHE:N	2.47	0.48
2:D:378:ARG:CB	2:D:378:ARG:HH11	2.27	0.48
1:A:131:GLN:OE1	1:A:131:GLN:N	2.47	0.47
2:B:400:LYS:HG2	2:B:403:GLN:HE21	1.79	0.47
1:C:99:ILE:CG2	1:C:104:ILE:HG13	2.43	0.47
1:A:190:GLY:O	1:A:193:PHE:HB3	2.13	0.47
2:B:198:GLY:O	2:B:201:LYS:HG3	2.14	0.47
1:C:10:ILE:HD11	1:C:20:LYS:HA	1.96	0.47
1:A:17:VAL:C	1:A:18:VAL:CG2	2.87	0.47
1:A:237:LYS:HG2	1:A:240:PHE:CZ	2.49	0.47
1:A:266:MET:O	1:A:274:ARG:HG3	2.14	0.47
2:B:299:LEU:HD21	2:B:306:LEU:HD11	1.96	0.47
2:B:395:HIS:O	2:B:396:GLN:C	2.58	0.47
1:A:2:GLU:O	1:A:2:GLU:CG	2.63	0.47
1:C:221:THR:OG1	1:C:241:PRO:O	2.24	0.47
1:A:171:PRO:HA	1:A:174:LEU:HB2	1.97	0.47
1:A:220:GLY:O	1:A:221:THR:C	2.55	0.47
2:B:329:VAL:HG11	2:B:364:LEU:CD1	2.35	0.47
2:B:398:TYR:CZ	2:B:426:PRO:HB3	2.49	0.47
1:C:87:LEU:O	1:C:91:MET:HE2	2.15	0.47
2:B:293:ARG:CG	1:C:2:GLU:OE2	2.63	0.47
2:B:428:GLU:O	2:B:429:THR:HG23	2.15	0.47
1:C:88:LYS:HB2	1:C:130:PRO:CB	2.36	0.47
2:D:205:ASP:O	2:D:206:ILE:HG23	2.14	0.47
2:D:366:THR:HG23	2:D:427:PRO:CD	2.31	0.47
3:F:661:PHE:C	3:F:663:GLU:H	2.16	0.47
1:A:11:GLY:O	1:A:18:VAL:HB	2.14	0.47
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.71	0.47
2:B:201:LYS:HE2	2:B:201:LYS:HB2	1.64	0.47
2:D:254:GLN:HG2	2:D:286:TYR:CE2	2.49	0.47
2:D:226:LYS:HB3	2:D:226:LYS:HE3	1.52	0.47
2:D:252:LYS:O	2:D:255:LEU:N	2.47	0.47
1:C:46:SER:O	1:C:50:ARG:HG3	2.14	0.47
1:C:156:VAL:HG22	4:C:2006:HOH:O	2.15	0.47
1:A:33:LYS:HZ3	1:A:51:GLU:CD	2.21	0.46
1:A:174:LEU:C	1:A:176:GLY:H	2.23	0.46
2:B:398:TYR:O	2:B:398:TYR:CD1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ASN:O	1:C:75:LYS:CB	2.63	0.46
2:D:178:TYR:O	2:D:181:ASP:N	2.46	0.46
1:C:131:GLN:CD	1:C:131:GLN:H	2.22	0.46
2:D:360:PHE:CD2	2:D:372:TRP:CZ3	3.03	0.46
1:A:64:VAL:HG12	1:A:65:LYS:N	2.29	0.46
1:A:226:VAL:O	1:A:226:VAL:CG2	2.63	0.46
1:C:241:PRO:HB2	1:C:243:TRP:CE3	2.50	0.46
2:D:223:GLU:CD	2:D:412:LYS:HD2	2.40	0.46
1:A:10:ILE:HG13	1:A:11:GLY:N	2.30	0.46
2:B:214:LEU:HD12	2:B:214:LEU:C	2.40	0.46
1:C:17:VAL:HG12	1:C:18:VAL:N	2.30	0.46
2:B:398:TYR:O	2:B:398:TYR:HD1	1.99	0.46
1:C:23:ASN:CG	1:C:26:THR:OG1	2.58	0.46
1:C:186:ILE:O	1:C:187:TRP:C	2.57	0.46
1:C:270:ASP:C	1:C:270:ASP:OD1	2.59	0.46
2:B:256:VAL:HG22	2:B:294:MET:CE	2.46	0.46
1:C:157:ARG:O	1:C:158:THR:C	2.59	0.46
1:A:268:HIS:CD2	1:A:273:LYS:HB3	2.50	0.46
1:C:129:LYS:HE3	1:C:131:GLN:HG2	1.98	0.46
2:D:360:PHE:HD2	2:D:372:TRP:CE3	2.32	0.46
2:B:423:LEU:C	2:B:424:LEU:O	2.57	0.45
2:D:190:GLU:HG3	2:D:351:LEU:HD22	1.97	0.45
1:C:108:LEU:CD1	1:C:112:LEU:HD21	2.46	0.45
1:C:125:HIS:O	1:C:126:ARG:HB2	2.16	0.45
1:C:170:ALA:HB1	1:C:171:PRO:HD2	1.97	0.45
1:A:125:HIS:NE2	1:A:144:ALA:O	2.35	0.45
1:A:166:LEU:HD13	1:A:169:ARG:NH1	2.31	0.45
2:B:260:ALA:O	2:B:261:MET:C	2.55	0.45
1:C:30:VAL:HB	1:C:80:PHE:O	2.17	0.45
2:D:239:ILE:HD11	2:D:257:GLY:HA2	1.99	0.45
1:A:75:LYS:NZ	1:A:77:TYR:OH	2.48	0.45
1:A:203:PHE:O	1:A:211:GLN:NE2	2.46	0.45
2:D:288:LYS:HB3	2:D:288:LYS:HE2	1.56	0.45
2:D:265:SER:C	2:D:267:PHE:N	2.74	0.45
2:D:338:GLU:C	2:D:340:SER:N	2.72	0.45
2:D:360:PHE:CD2	2:D:372:TRP:HZ3	2.35	0.45
1:A:41:THR:C	1:A:43:GLY:H	2.25	0.45
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.98	0.45
1:A:87:LEU:O	1:A:87:LEU:HG	2.17	0.45
1:A:90:PHE:HE2	1:A:99:ILE:HD12	1.79	0.45
1:C:173:ILE:O	1:C:174:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:VAL:HG21	2:B:409:ILE:CG1	2.47	0.45
2:B:394:LEU:HA	2:B:394:LEU:HD12	1.59	0.45
2:B:398:TYR:CD1	2:B:398:TYR:C	2.92	0.45
2:D:278:PHE:C	2:D:281:ILE:HG22	2.42	0.45
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.99	0.45
1:C:188:SER:O	1:C:189:LEU:C	2.60	0.45
1:A:45:PRO:O	1:A:48:ALA:HB3	2.16	0.44
1:A:82:PHE:C	1:A:83:LEU:HG	2.43	0.44
1:A:104:ILE:O	1:A:105:LYS:C	2.59	0.44
1:A:248:PHE:CE2	1:A:264:SER:HB3	2.52	0.44
1:A:252:VAL:CG1	1:A:255:LEU:HB2	2.42	0.44
2:B:200:MET:SD	2:B:206:ILE:CG1	3.05	0.44
1:A:172:GLU:O	1:A:177:CYS:CB	2.65	0.44
2:B:364:LEU:O	2:B:365:TYR:C	2.59	0.44
1:C:55:LEU:O	1:C:57:GLU:N	2.50	0.44
2:B:283:ASP:OD1	2:B:283:ASP:C	2.59	0.44
2:B:358:ALA:HA	2:B:391:LEU:HD13	1.99	0.44
1:C:10:ILE:HD11	1:C:20:LYS:CA	2.47	0.44
2:D:217:TRP:O	2:D:221:VAL:HG23	2.18	0.44
2:D:281:ILE:O	2:D:281:ILE:HG12	2.17	0.44
2:D:318:TYR:HA	2:D:376:LEU:HD21	1.99	0.44
1:A:111:LEU:HD21	1:A:133:LEU:HD22	2.00	0.44
2:B:354:VAL:O	2:B:355:ILE:C	2.60	0.44
2:D:201:LYS:HE3	2:D:202:LYS:NZ	2.32	0.44
2:D:211:ARG:HH12	2:D:215:VAL:HG21	1.82	0.44
2:D:361:HIS:CD2	2:D:391:LEU:HD11	2.51	0.44
1:A:50:ARG:NH2	1:A:150:ARG:CZ	2.80	0.44
1:A:109:PHE:O	1:A:113:GLN:HG3	2.18	0.44
2:B:293:ARG:HG2	1:C:2:GLU:OE2	2.18	0.44
1:C:37:LEU:O	1:C:38:ASP:CG	2.61	0.44
1:C:119:HIS:CE1	1:C:185:ASP:OD2	2.57	0.44
1:C:209:ILE:HG23	1:C:210:ASP:N	2.33	0.44
2:D:292:LEU:HD12	2:D:292:LEU:HA	1.75	0.44
2:D:342:ILE:HD11	2:D:409:ILE:HD12	2.00	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.74	0.44
1:A:71:HIS:CE1	2:B:304:PHE:CE1	3.05	0.44
1:A:110:GLN:O	1:A:111:LEU:C	2.58	0.44
2:B:218:LEU:O	2:B:219:VAL:C	2.59	0.44
2:D:398:TYR:O	2:D:399:LEU:C	2.60	0.44
2:D:415:ASN:CG	2:D:416:SER:N	2.75	0.44
1:A:268:HIS:CB	1:A:274:ARG:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:ARG:HG3	2:B:187:ARG:HH11	1.82	0.44
2:B:207:THR:HG1	2:B:210:MET:HG3	1.73	0.44
1:A:71:HIS:HE1	2:B:304:PHE:CD1	2.36	0.44
2:B:214:LEU:HD12	2:B:214:LEU:O	2.17	0.44
1:C:12:GLU:HA	1:C:17:VAL:HA	2.00	0.44
1:C:17:VAL:HG12	1:C:18:VAL:H	1.81	0.44
1:C:115:LEU:CD1	1:C:119:HIS:CE1	3.00	0.44
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.48	0.44
1:C:262:LEU:O	1:C:263:LEU:C	2.60	0.44
2:D:278:PHE:O	2:D:281:ILE:CG2	2.62	0.43
2:D:350:TYR:CD1	2:D:390:CYS:HB2	2.53	0.43
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.82	0.43
2:B:190:GLU:O	2:B:192:LYS:N	2.51	0.43
1:C:18:VAL:HA	1:C:32:LEU:O	2.18	0.43
1:C:71:HIS:CE1	2:D:304:PHE:HE2	2.21	0.43
1:C:112:LEU:HD13	1:C:280:ALA:HB3	2.00	0.43
2:D:242:PHE:O	2:D:246:MET:HB2	2.18	0.43
2:B:354:VAL:O	2:B:357:GLY:N	2.52	0.43
1:C:261:SER:HB3	1:C:283:HIS:CE1	2.53	0.43
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.87	0.43
2:D:315:LEU:HD13	2:D:356:ALA:HB1	2.00	0.43
1:A:115:LEU:HD11	1:A:185:ASP:HB3	2.00	0.43
1:A:262:LEU:O	1:A:263:LEU:C	2.61	0.43
2:B:315:LEU:HD13	2:B:356:ALA:HB1	2.01	0.43
1:A:72:THR:O	1:A:72:THR:CG2	2.60	0.43
1:A:203:PHE:HB2	1:A:211:GLN:HE22	1.84	0.43
2:B:247:SER:OG	1:C:28:GLU:OE2	2.37	0.43
2:B:281:ILE:O	3:E:657:LYS:HA	2.18	0.43
1:C:230:VAL:HA	1:C:233:MET:HE2	2.00	0.43
3:E:661:PHE:O	3:E:663:GLU:N	2.52	0.43
2:B:374:GLU:O	2:B:374:GLU:HG3	2.19	0.43
2:B:401:ALA:N	2:B:402:PRO:HD3	2.33	0.43
2:D:242:PHE:CD1	2:D:242:PHE:C	2.97	0.43
1:A:46:SER:HB3	2:B:266:LYS:HG2	2.01	0.43
2:B:249:LEU:HD12	1:C:27:GLY:CA	2.48	0.43
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.54	0.43
1:C:160:TPO:HA	2:D:270:ILE:CG2	2.49	0.43
1:A:33:LYS:NZ	1:A:51:GLU:OE1	2.52	0.43
1:A:277:ALA:O	1:A:279:ALA:CA	2.60	0.43
1:C:63:ILE:O	1:C:64:VAL:O	2.37	0.43
1:C:73:GLU:CD	1:C:73:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:THR:C	2:D:209:SER:N	2.73	0.43
2:D:384:LEU:HD12	2:D:384:LEU:HA	1.69	0.43
1:A:255:LEU:CD2	1:A:259:GLY:C	2.91	0.42
2:D:345:ASP:C	2:D:345:ASP:OD1	2.60	0.42
2:B:366:THR:OG1	2:B:427:PRO:HD3	2.19	0.42
2:D:232:LEU:O	2:D:232:LEU:HD22	2.19	0.42
1:A:40:GLU:H	2:B:292:LEU:CD2	2.32	0.42
1:A:142:LYS:C	1:A:143:LEU:O	2.63	0.42
1:A:105:LYS:O	1:A:286:PHE:HE1	2.01	0.42
1:C:40:GLU:C	2:D:288:LYS:HZ1	2.28	0.42
1:A:57:GLU:OE2	2:B:189:MET:CE	2.67	0.42
2:B:416:SER:O	2:B:417:LYS:C	2.62	0.42
1:C:121:HIS:O	1:C:122:ARG:HD2	2.18	0.42
2:D:198:GLY:C	2:D:200:MET:N	2.74	0.42
2:D:415:ASN:OD1	2:D:417:LYS:CB	2.67	0.42
1:C:176:GLY:O	1:C:234:PRO:HG2	2.19	0.42
1:C:227:TRP:CD2	1:C:230:VAL:HG22	2.55	0.42
2:D:350:TYR:CZ	2:D:390:CYS:HA	2.55	0.42
1:C:64:VAL:CG1	1:C:65:LYS:N	2.78	0.42
2:D:198:GLY:C	2:D:200:MET:H	2.26	0.42
2:D:200:MET:C	2:D:202:LYS:H	2.28	0.42
2:D:372:TRP:CH2	2:D:376:LEU:HD13	2.54	0.42
1:A:221:THR:HA	1:A:222:PRO:HD3	1.95	0.42
1:A:247:ASP:OD2	1:A:249:SER:CB	2.67	0.42
2:B:186:LEU:C	2:B:188:GLU:H	2.28	0.42
2:B:247:SER:OG	1:C:28:GLU:CD	2.62	0.42
2:B:294:MET:O	2:B:298:VAL:HG23	2.20	0.42
1:C:190:GLY:N	1:C:266:MET:HE2	2.34	0.42
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.55	0.42
3:F:661:PHE:C	3:F:663:GLU:N	2.76	0.42
1:A:158:THR:HG23	1:A:178:LYS:O	2.20	0.42
1:A:278:LYS:HE2	2:B:177:ASP:O	2.20	0.42
2:B:233:HIS:CD2	2:B:311:VAL:HB	2.55	0.42
2:B:323:GLN:HA	2:B:324:PRO:HA	1.80	0.42
1:C:71:HIS:HE1	2:D:304:PHE:CE2	2.21	0.42
1:A:227:TRP:O	1:A:228:PRO:C	2.62	0.42
1:A:252:VAL:HG21	1:A:263:LEU:CD2	2.50	0.42
2:B:322:GLN:O	2:B:324:PRO:HA	2.20	0.42
2:D:178:TYR:O	2:D:179:HIS:C	2.62	0.42
2:D:362:LEU:HD12	2:D:362:LEU:HA	1.81	0.42
2:B:216:ASP:CG	2:B:406:GLN:HB3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:H	1:C:162:GLU:CD	2.26	0.41
1:A:192:ILE:O	1:A:193:PHE:C	2.62	0.41
2:B:346:PRO:HG3	2:B:393:ASP:OD2	2.20	0.41
1:C:173:ILE:O	1:C:175:LEU:N	2.53	0.41
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.55	0.41
2:D:344:ALA:O	2:D:348:LEU:HB2	2.20	0.41
1:A:42:GLU:OE2	2:B:274:GLU:HG2	2.20	0.41
1:A:110:GLN:O	1:A:113:GLN:HB2	2.20	0.41
1:A:174:LEU:CD1	1:A:212:LEU:HD23	2.49	0.41
2:B:242:PHE:CD2	2:B:242:PHE:C	2.97	0.41
2:D:323:GLN:OE1	2:D:323:GLN:HA	2.20	0.41
2:B:290:GLN:O	2:B:291:VAL:C	2.63	0.41
1:C:110:GLN:HB2	1:C:141:ILE:CG2	2.50	0.41
1:C:166:LEU:O	1:C:211:GLN:CD	2.63	0.41
2:D:317:GLN:O	2:D:320:LEU:HB2	2.20	0.41
2:D:331:SER:HB2	2:D:421:VAL:HG11	2.01	0.41
2:B:376:LEU:O	2:B:380:THR:HG23	2.21	0.41
2:B:184:THR:O	2:B:185:TYR:C	2.61	0.41
2:D:190:GLU:O	2:D:194:LYS:HB3	2.21	0.41
2:D:280:TYR:CE1	3:F:657:LYS:HD3	2.55	0.41
2:D:392:MET:O	2:D:393:ASP:C	2.64	0.41
1:A:99:ILE:HG22	1:A:104:ILE:HG13	2.02	0.41
1:C:88:LYS:HD3	1:C:92:ASP:OD2	2.20	0.41
1:C:136:ASN:OD1	1:C:140:ALA:N	2.41	0.41
1:C:173:ILE:HG22	1:C:174:LEU:N	2.35	0.41
2:D:346:PRO:O	2:D:349:LYS:HG2	2.21	0.41
2:D:348:LEU:HD12	2:D:348:LEU:HA	1.78	0.41
1:A:141:ILE:C	1:A:142:LYS:HG2	2.45	0.41
2:B:388:LYS:O	2:B:392:MET:N	2.45	0.41
1:C:99:ILE:O	1:C:100:PRO:C	2.62	0.41
3:E:659:ARG:HH21	3:E:663:GLU:N	2.19	0.41
1:A:69:VAL:HG22	1:A:71:HIS:CE1	2.56	0.41
1:A:130:PRO:C	1:A:132:ASN:H	2.27	0.41
1:A:284:PRO:O	1:A:285:PHE:C	2.63	0.41
1:C:262:LEU:HD23	1:C:285:PHE:CD2	2.56	0.41
2:D:290:GLN:O	2:D:291:VAL:C	2.63	0.41
3:E:655:SER:O	3:E:655:SER:OG	2.31	0.41
2:B:189:MET:HE3	2:B:193:CYS:SG	2.61	0.41
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.81	0.41
1:C:189:LEU:O	1:C:193:PHE:N	2.40	0.41
2:D:326:ASN:HB3	2:D:329:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.56	0.41
1:A:115:LEU:HD13	1:A:128:LEU:HD11	2.03	0.40
1:A:157:ARG:HD3	2:B:228:GLN:OE1	2.21	0.40
1:A:177:CYS:CB	1:A:233:MET:HE1	2.49	0.40
1:C:173:ILE:HD11	1:C:184:VAL:HG11	2.04	0.40
1:C:188:SER:O	1:C:192:ILE:HG13	2.22	0.40
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.76	0.40
4:C:2006:HOH:O	2:D:175:VAL:HG21	2.22	0.40
1:A:117:PHE:O	1:A:118:CYS:C	2.64	0.40
1:A:71:HIS:CE1	2:B:304:PHE:HE1	2.39	0.40
1:A:174:LEU:HB3	1:A:212:LEU:HD21	2.02	0.40
2:B:238:TYR:OH	2:B:306:LEU:HB3	2.21	0.40
1:C:125:HIS:ND1	1:C:125:HIS:C	2.79	0.40
1:C:150:ARG:HH21	1:C:160:TPO:P	2.44	0.40
1:C:171:PRO:O	1:C:172:GLU:C	2.60	0.40
2:D:342:ILE:HD13	2:D:342:ILE:HG21	1.91	0.40
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.36	0.40
1:C:191:CYS:O	1:C:195:GLU:HB2	2.22	0.40
3:F:662:GLY:O	3:F:663:GLU:CB	2.66	0.40
2:B:180:GLU:HA	2:B:180:GLU:OE1	2.21	0.40
2:B:216:ASP:CB	2:B:406:GLN:HG2	2.51	0.40
2:B:315:LEU:HD12	2:B:315:LEU:HA	1.94	0.40
1:C:209:ILE:O	1:C:210:ASP:C	2.65	0.40
2:D:207:THR:O	2:D:208:ASN:C	2.65	0.40

All (2) 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)
2:B:379:LYS:O	2:D:378:ARG:NH2[2_665]	1.84	0.36
2:B:378:ARG:NH1	2:D:320:LEU:O[2_665]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	294/303 (97%)	232 (79%)	47 (16%)	15 (5%)	1	5
1	C	294/303 (97%)	242 (82%)	37 (13%)	15 (5%)	1	5
2	B	256/259 (99%)	204 (80%)	42 (16%)	10 (4%)	2	8
2	D	256/259 (99%)	201 (78%)	48 (19%)	7 (3%)	4	15
3	E	8/11 (73%)	4 (50%)	2 (25%)	2 (25%)	0	0
3	F	6/11 (54%)	4 (67%)	1 (17%)	1 (17%)	0	0
All	All	1114/1146 (97%)	887 (80%)	177 (16%)	50 (4%)	2	7

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	73	GLU
1	A	137	THR
1	A	277	ALA
1	A	278	LYS
2	B	197	VAL
1	C	14	THR
1	C	145	ASP
1	C	174	LEU
2	D	176	PRO
2	D	266	LYS
1	A	145	ASP
1	A	164	VAL
1	A	175	LEU
2	B	320	LEU
2	B	347	TYR
1	C	38	ASP
1	C	75	LYS
1	C	164	VAL
1	C	173	ILE
2	D	179	HIS
2	D	307	ALA
2	D	417	LYS
3	E	658	ARG
3	F	662	GLY
1	A	38	ASP
1	A	143	LEU

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Mol	Chain	Res	Type
2	B	191	VAL
2	B	364	LEU
1	C	41	THR
1	C	56	LYS
1	C	285	PHE
3	E	655	SER
1	A	193	PHE
1	A	256	ASP
2	B	385	GLU
2	B	396	GLN
1	C	64	VAL
1	C	120	SER
2	B	179	HIS
2	B	336	LEU
1	C	104	ILE
1	C	234	PRO
2	D	265	SER
2	B	327	CYS
2	D	201	LYS
1	A	104	ILE
1	A	147	GLY
1	A	240	PHE
1	C	275	ILE

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	261/265 (98%)	223 (85%)	38 (15%)	3	11
1	C	261/265 (98%)	223 (85%)	38 (15%)	3	11
2	B	232/233 (100%)	194 (84%)	38 (16%)	2	8
2	D	232/233 (100%)	197 (85%)	35 (15%)	3	10
3	E	7/7 (100%)	7 (100%)	0	100	100
3	F	6/7 (86%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	999/1010 (99%)	850 (85%)	149 (15%)	3 10

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	17	VAL
1	A	22	ARG
1	A	30	VAL
1	A	34	LYS
1	A	44	VAL
1	A	55	LEU
1	A	69	VAL
1	A	74	ASN
1	A	75	LYS
1	A	76	LEU
1	A	78	LEU
1	A	91	MET
1	A	94	SER
1	A	96	LEU
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	156	VAL
1	A	157	ARG
1	A	161	HIS
1	A	163	VAL
1	A	165	THR
1	A	166	LEU
1	A	182	THR
1	A	199	ARG
1	A	206	ASP
1	A	226	VAL
1	A	230	VAL
1	A	246	GLN
1	A	255	LEU
1	A	266	MET
1	A	268	HIS
1	A	272	ASN
1	A	273	LYS
1	A	290	THR
1	A	291	LYS

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Mol	Chain	Res	Type
1	A	293	VAL
2	B	177	ASP
2	B	187	ARG
2	B	196	LYS
2	B	199	TYR
2	B	201	LYS
2	B	202	LYS
2	B	209	SER
2	B	215	VAL
2	B	220	GLU
2	B	224	GLU
2	B	227	LEU
2	B	231	THR
2	B	232	LEU
2	B	266	LYS
2	B	282	THR
2	B	288	LYS
2	B	292	LEU
2	B	296	HIS
2	B	301	VAL
2	B	315	LEU
2	B	316	THR
2	B	322	GLN
2	B	331	SER
2	B	334	MET
2	B	338	GLU
2	B	348	LEU
2	B	349	LYS
2	B	364	LEU
2	B	368	THR
2	B	380	THR
2	B	384	LEU
2	B	385	GLU
2	B	399	LEU
2	B	416	SER
2	B	417	LYS
2	B	425	ASN
2	B	430	LEU
2	B	432	LEU
1	C	5	GLN
1	C	30	VAL
1	C	34	LYS

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Mol	Chain	Res	Type
1	C	47	THR
1	C	55	LEU
1	C	56	LYS
1	C	64	VAL
1	C	66	LEU
1	C	67	LEU
1	C	76	LEU
1	C	78	LEU
1	C	79	VAL
1	C	83	LEU
1	C	94	SER
1	C	96	LEU
1	C	105	LYS
1	C	112	LEU
1	C	122	ARG
1	C	126	ARG
1	C	131	GLN
1	C	133	LEU
1	C	150	ARG
1	C	156	VAL
1	C	162	GLU
1	C	163	VAL
1	C	165	THR
1	C	181	SER
1	C	193	PHE
1	C	198	THR
1	C	199	ARG
1	C	206	ASP
1	C	207	SER
1	C	226	VAL
1	C	245	ARG
1	C	246	GLN
1	C	248	PHE
1	C	250	LYS
1	C	257	GLU
2	D	175	VAL
2	D	176	PRO
2	D	181	ASP
2	D	188	GLU
2	D	194	LYS
2	D	201	LYS
2	D	202	LYS

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Mol	Chain	Res	Type
2	D	226	LYS
2	D	227	LEU
2	D	232	LEU
2	D	243	LEU
2	D	246	MET
2	D	247	SER
2	D	254	GLN
2	D	281	ILE
2	D	285	THR
2	D	292	LEU
2	D	295	GLU
2	D	315	LEU
2	D	322	GLN
2	D	334	MET
2	D	338	GLU
2	D	348	LEU
2	D	349	LYS
2	D	361	HIS
2	D	367	VAL
2	D	375	SER
2	D	383	THR
2	D	384	LEU
2	D	386	SER
2	D	392	MET
2	D	394	LEU
2	D	403	GLN
2	D	410	ARG
2	D	429	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	74	ASN
1	A	85	GLN
1	A	119	HIS
1	A	268	HIS
2	B	233	HIS
2	B	370	GLN
2	B	395	HIS
2	B	403	GLN
2	B	419	HIS

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Mol	Chain	Res	Type
1	C	3	ASN
1	C	5	GLN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	85	GLN
1	C	110	GLN
1	C	119	HIS
1	C	131	GLN
2	D	179	HIS
2	D	296	HIS
2	D	317	GLN
2	D	361	HIS
2	D	370	GLN
2	D	396	GLN
2	D	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	C	160	1	8,10,11	1.45	1 (12%)	10,14,16	1.88	3 (30%)
1	TPO	A	160	1	8,10,11	1.83	2 (25%)	10,14,16	2.07	3 (30%)

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
1	TPO	C	160	1	-	2/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	3.78	1.62	1.50
1	A	160	TPO	P-O3P	2.56	1.64	1.54
1	C	160	TPO	P-O1P	2.41	1.58	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	P-OG1-CB	-4.55	110.96	123.33
1	C	160	TPO	OG1-P-O1P	3.30	121.11	109.33
1	A	160	TPO	O2P-P-OG1	3.26	118.53	105.85
1	C	160	TPO	O-C-CA	-2.65	117.94	124.77
1	C	160	TPO	O3P-P-O2P	2.47	117.05	107.80
1	A	160	TPO	CG2-CB-CA	2.11	117.38	113.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	C-CA-CB-CG2
1	C	160	TPO	C-CA-CB-CG2
1	C	160	TPO	N-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	7	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	159:TYR	C	160:TPO	N	1.66

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	296/303 (97%)	0.69	27 (9%)	15 11	13, 32, 60, 75	0
1	C	296/303 (97%)	0.60	25 (8%)	17 12	12, 32, 58, 71	0
2	B	258/259 (99%)	0.26	8 (3%)	51 41	9, 25, 48, 59	0
2	D	258/259 (99%)	0.36	13 (5%)	34 26	11, 28, 47, 64	0
3	E	10/11 (90%)	1.05	2 (20%)	3 2	33, 41, 46, 46	0
3	F	8/11 (72%)	1.06	1 (12%)	8 6	42, 45, 54, 57	0
All	All	1126/1146 (98%)	0.50	76 (6%)	24 17	9, 29, 54, 75	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	ASN	5.5
2	B	177	ASP	5.2
2	B	323	GLN	4.6
1	C	199	ARG	4.5
1	C	42	GLU	4.3
2	D	245	SER	4.2
2	D	175	VAL	4.0
1	C	16	GLY	3.9
2	D	176	PRO	3.6
2	B	374	GLU	3.6
1	A	41	THR	3.6
1	A	206	ASP	3.5
1	C	39	THR	3.4
1	A	40	GLU	3.3
1	A	42	GLU	3.3
1	C	92	ASP	3.2
1	A	199	ARG	3.2
1	A	14	THR	3.1
1	A	13	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	15	TYR	3.0
1	C	14	THR	2.9
1	C	296	LEU	2.9
1	A	39	THR	2.9
1	A	247	ASP	2.8
1	A	161	HIS	2.8
2	D	418	TYR	2.8
2	B	305	ASP	2.8
2	D	197	VAL	2.8
1	C	287	GLN	2.7
1	C	17	VAL	2.7
2	D	325	ALA	2.6
2	D	323	GLN	2.5
1	A	95	ALA	2.5
1	A	268	HIS	2.5
1	A	2	GLU	2.5
1	C	12	GLU	2.5
1	A	277	ALA	2.5
1	A	296	LEU	2.5
2	D	432	LEU	2.4
1	A	12	GLU	2.4
1	A	71	HIS	2.4
1	C	188	SER	2.4
1	C	201	ALA	2.4
1	A	97	THR	2.4
1	C	41	THR	2.4
1	C	163	VAL	2.3
2	B	326	ASN	2.3
3	F	662	GLY	2.3
1	C	40	GLU	2.3
2	D	179	HIS	2.3
2	B	175	VAL	2.3
1	C	161	HIS	2.3
1	C	22	ARG	2.3
2	B	284	ASP	2.3
1	C	72	THR	2.3
1	A	295	HIS	2.2
1	C	71	HIS	2.2
2	B	178	TYR	2.2
2	D	413	TYR	2.2
3	E	662	GLY	2.2
1	A	178	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLU	2.2
1	A	87	LEU	2.2
1	C	295	HIS	2.1
1	A	17	VAL	2.1
2	D	177	ASP	2.1
1	C	96	LEU	2.1
3	E	663	GLU	2.1
1	C	59	ASN	2.1
2	D	326	ASN	2.1
1	A	16	GLY	2.1
1	A	10	ILE	2.1
2	D	224	GLU	2.1
1	C	0	SER	2.0
1	A	201	ALA	2.0
1	A	37	LEU	2.0

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

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
1	TPO	C	160	11/12	0.96	0.08	14,19,24,25	0
1	TPO	A	160	11/12	0.98	0.08	4,14,21,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.