



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:48 AM UTC

PDB ID : 1SJC / pdb_00001sjc
Title : x-ray structure of o-succinylbenzoate synthase complexed with N-succinyl methionine
Authors : Thoden, J.B.; Taylor-Ringia, E.A.; Garrett, J.B.; Gerlt, J.A.; Holden, H.M.; Rayment, I.
Deposited on : 2004-03-03
Resolution : 2.10 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

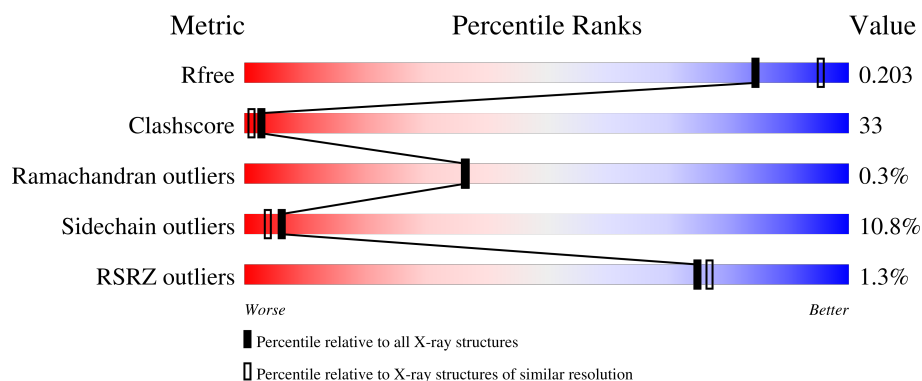
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	368	 51% 39% 8% 0.3%
1	B	368	 58% 35% 7% 0.3%
1	C	368	 57% 35% 8% 0.3%
1	D	368	 41% 46% 12% 3%

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	SMG	A	1000	-	-	X	-
3	SMG	B	1100	-	-	X	-
3	SMG	C	1200	-	-	X	-
3	SMG	D	1300	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12098 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.

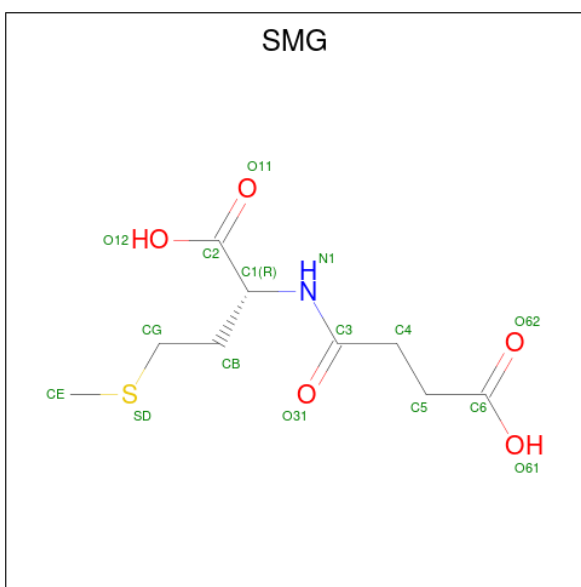
- Molecule 1 is a protein called N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	5	0
			2795	1776	490	517	12			
1	B	368	Total	C	N	O	S	0	3	0
			2786	1769	481	524	12			
1	C	367	Total	C	N	O	S	0	2	0
			2775	1764	480	519	12			
1	D	368	Total	C	N	O	S	0	1	0
			2779	1765	484	518	12			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is N-SUCCINYLMETHIONINE (CCD ID: SMG) (formula: C₉H₁₅NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			16	9	1	5	1		
3	B	1	Total	C	N	O	S	0	0
			16	9	1	5	1		
3	C	1	Total	C	N	O	S	0	0
			16	9	1	5	1		
3	D	1	Total	C	N	O	S	0	0
			16	9	1	5	1		

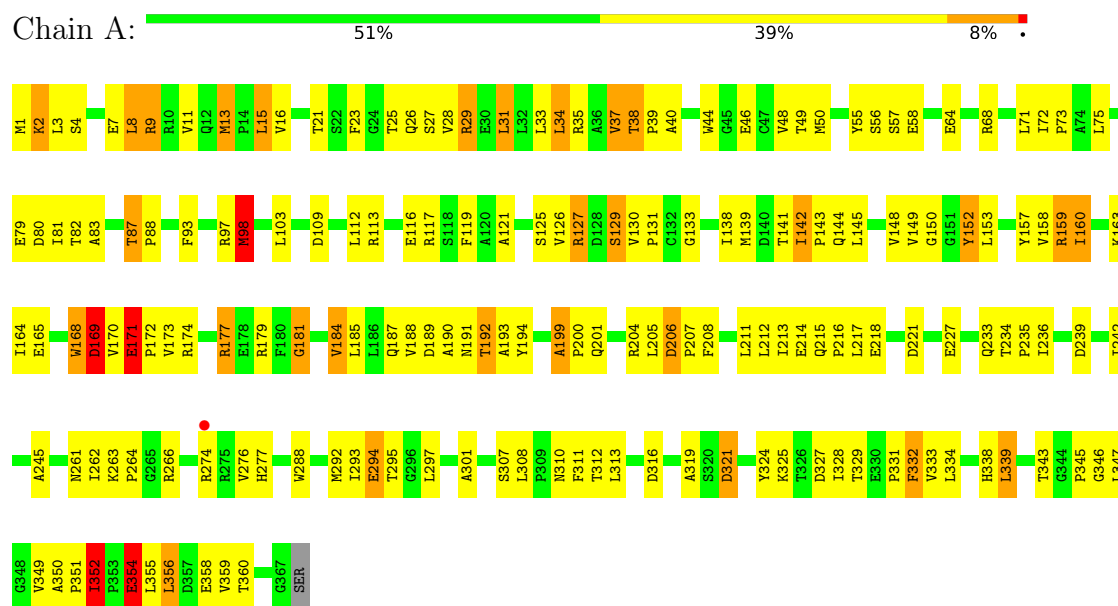
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total	O	0	0
			216	216		
4	B	295	Total	O	0	0
			295	295		
4	C	237	Total	O	0	0
			237	237		
4	D	147	Total	O	0	0
			147	147		

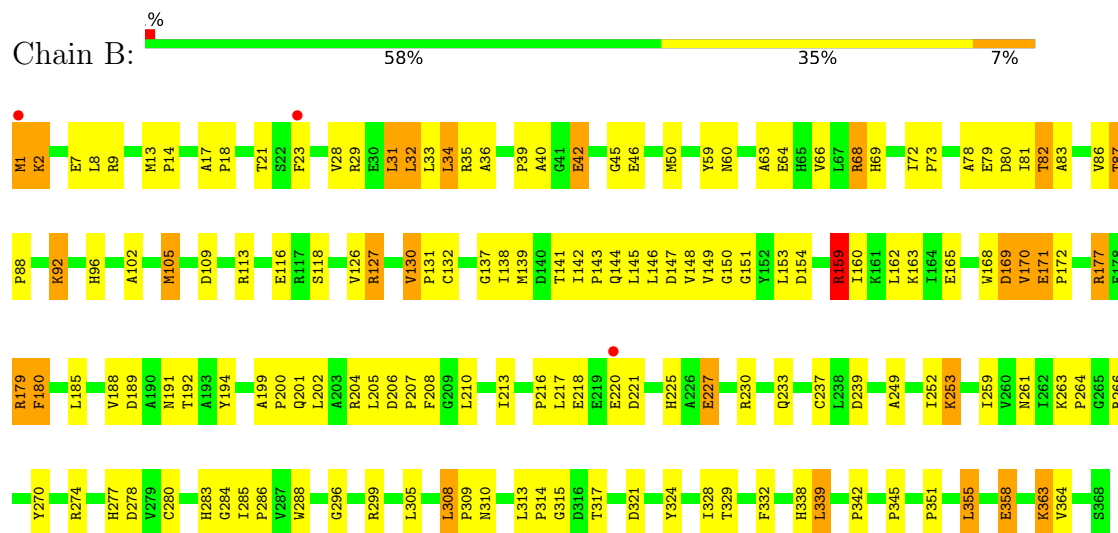
3 Residue-property plots

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.

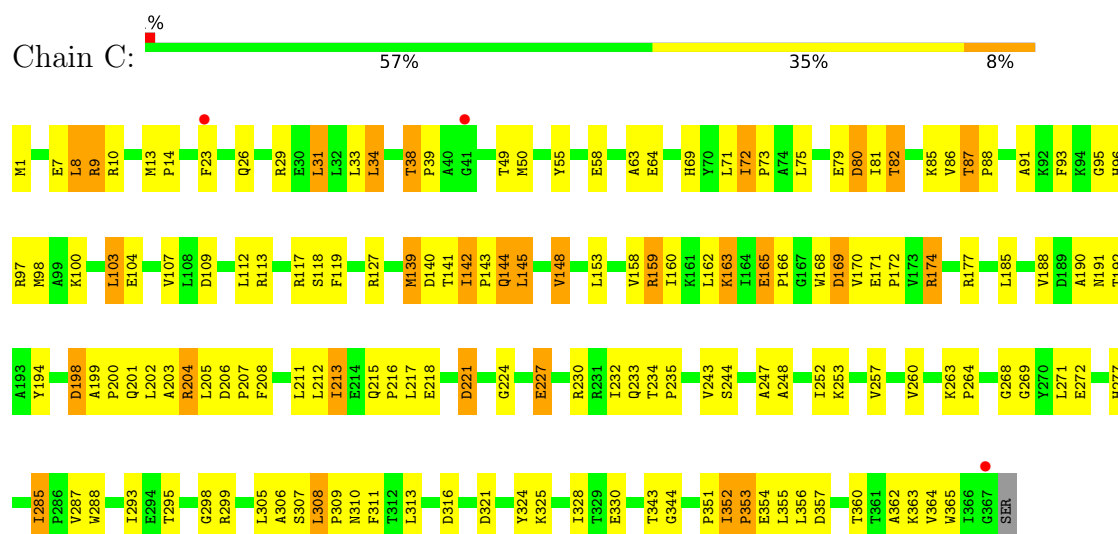
- Molecule 1: N-acylamino acid racemase



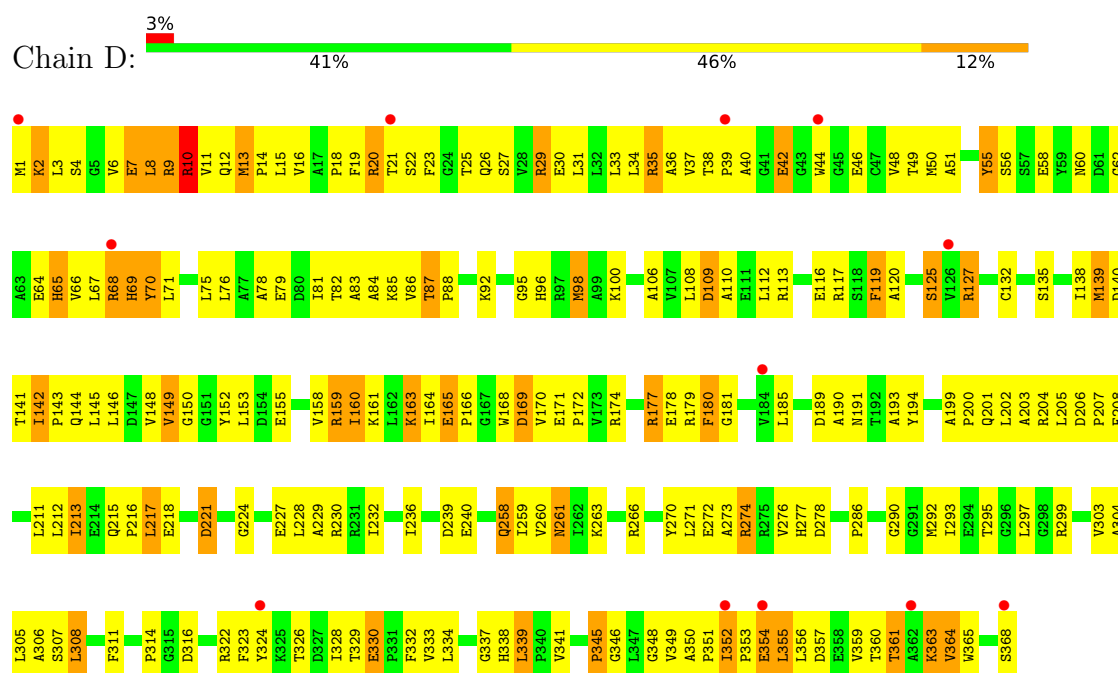
- Molecule 1: N-acylamino acid racemase



- Molecule 1: N-acylamino acid racemase



• Molecule 1: N-acylamino acid racemase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	215.70Å 215.70Å 259.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.10) 99.5 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.208 , 0.274 0.203 , 0.203	Depositor DCC
R_{free} test set	15319 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 147.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.010 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.004 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12098	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.18	3/2871 (0.1%)	1.64	37/3906 (0.9%)
1	B	1.21	1/2854 (0.0%)	1.66	30/3885 (0.8%)
1	C	1.21	3/2839 (0.1%)	1.64	28/3866 (0.7%)
1	D	1.18	2/2839 (0.1%)	1.69	39/3864 (1.0%)
All	All	1.19	9/11403 (0.1%)	1.66	134/15521 (0.9%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	GLY	CA-C	-7.06	1.44	1.52
1	D	10	ARG	NE-CZ	5.81	1.39	1.33
1	A	168	TRP	CA-CB	5.81	1.57	1.53
1	A	116	GLU	CD-OE2	5.69	1.36	1.25
1	C	72	ILE	CA-CB	-5.64	1.51	1.54
1	C	148	VAL	CA-CB	-5.56	1.47	1.54
1	D	70	TYR	CA-C	-5.49	1.47	1.52
1	A	87	THR	N-CA	-5.12	1.42	1.46
1	C	212	LEU	CA-C	-5.08	1.46	1.52

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	GLU	N-CA-CB	-10.46	101.44	111.27
1	C	80	ASP	CA-CB-CG	-9.40	103.20	112.60
1	B	208	PHE	CA-CB-CG	-8.40	105.40	113.80
1	B	126	VAL	CA-C-O	8.00	125.70	119.46
1	D	208	PHE	N-CA-C	7.99	122.12	112.38
1	D	180	PHE	CA-CB-CG	-7.97	105.83	113.80
1	A	171	GLU	O-C-N	7.82	126.56	120.38
1	C	72	ILE	CA-C-O	7.57	124.46	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	PRO	CA-C-N	-7.51	113.68	122.77
1	B	314	PRO	C-N-CA	-7.51	113.68	122.77
1	D	69	HIS	CA-CB-CG	-7.25	106.55	113.80
1	D	221	ASP	CA-CB-CG	-7.16	105.44	112.60
1	B	253	LYS	N-CA-CB	7.08	121.33	110.14
1	D	221	ASP	N-CA-C	7.08	120.52	110.68
1	A	71	LEU	N-CA-C	6.80	118.49	111.14
1	D	70	TYR	O-C-N	6.80	129.91	121.95
1	A	221	ASP	CA-CB-CG	-6.76	105.83	112.60
1	D	229	ALA	O-C-N	6.69	129.21	122.12
1	C	165	GLU	CB-CA-C	-6.60	99.19	109.55
1	A	98	MET	N-CA-CB	6.55	119.51	110.01
1	A	242	ILE	N-CA-C	6.54	113.21	106.21
1	A	116	GLU	CB-CA-C	6.46	121.06	111.89
1	D	6	VAL	CA-C-N	-6.45	114.19	122.77
1	D	6	VAL	C-N-CA	-6.45	114.19	122.77
1	C	352	ILE	CA-C-N	6.41	127.86	119.84
1	C	352	ILE	C-N-CA	6.41	127.86	119.84
1	A	169	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	221	ASP	N-CA-C	6.30	119.52	108.56
1	D	308	LEU	CA-C-N	6.29	127.70	119.84
1	D	308	LEU	C-N-CA	6.29	127.70	119.84
1	C	208	PHE	N-CA-C	6.27	120.77	113.18
1	D	333	VAL	N-CA-C	6.25	116.88	107.75
1	A	152	TYR	CA-CB-CG	-6.22	102.70	113.90
1	B	180	PHE	CA-C-N	-6.16	112.95	122.69
1	B	180	PHE	C-N-CA	-6.16	112.95	122.69
1	B	170	VAL	N-CA-C	6.16	116.83	110.36
1	D	259	ILE	CA-C-N	-6.12	115.21	123.10
1	D	259	ILE	C-N-CA	-6.12	115.21	123.10
1	A	294	GLU	N-CA-C	6.11	118.41	110.53
1	A	37	VAL	N-CA-C	6.04	116.31	107.37
1	C	325	LYS	N-CA-C	-6.00	104.31	111.69
1	D	109	ASP	CA-CB-CG	-5.98	106.62	112.60
1	D	290	GLY	CA-C-N	-5.95	117.98	122.33
1	D	290	GLY	C-N-CA	-5.95	117.98	122.33
1	D	193	ALA	N-CA-C	5.92	118.52	111.71
1	C	212	LEU	O-C-N	5.90	129.19	123.29
1	A	71	LEU	CA-C-N	-5.88	115.62	120.33
1	A	71	LEU	C-N-CA	-5.88	115.62	120.33
1	D	160	ILE	N-CA-C	5.85	116.42	107.77
1	D	208	PHE	CA-CB-CG	-5.85	107.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ARG	N-CA-C	-5.84	104.83	111.07
1	B	308	LEU	CA-C-O	5.83	127.06	120.70
1	B	358	GLU	N-CA-CB	5.83	119.20	110.22
1	C	260	VAL	N-CA-C	5.79	116.28	108.17
1	D	352	ILE	CA-C-N	5.78	127.07	119.84
1	D	352	ILE	C-N-CA	5.78	127.07	119.84
1	D	55	TYR	N-CA-C	-5.76	104.44	112.45
1	C	285	ILE	CA-C-O	5.76	123.63	119.25
1	A	87	THR	CA-C-O	5.75	124.54	119.08
1	D	314	PRO	N-CA-CB	5.74	108.44	103.27
1	B	299	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	A	93	PHE	CA-CB-CG	-5.72	108.08	113.80
1	B	69	HIS	CA-CB-CG	-5.71	108.09	113.80
1	C	221	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	332	PHE	CA-CB-CG	-5.71	108.09	113.80
1	D	258	GLN	CA-C-O	5.70	125.07	118.97
1	C	69	HIS	N-CA-C	5.69	120.36	112.90
1	D	87	THR	CA-C-O	5.68	124.47	119.08
1	B	96	HIS	CA-CB-CG	-5.67	108.13	113.80
1	A	206	ASP	CA-C-O	5.64	123.52	118.33
1	C	38	THR	O-C-N	5.60	125.92	121.55
1	A	359	VAL	N-CA-C	5.58	118.25	112.90
1	A	165	GLU	CB-CA-C	-5.56	102.75	110.37
1	C	308	LEU	CA-C-N	5.55	125.22	119.05
1	C	308	LEU	C-N-CA	5.55	125.22	119.05
1	A	133	GLY	N-CA-C	-5.52	103.03	112.64
1	D	96	HIS	CA-CB-CG	-5.51	108.28	113.80
1	B	270	TYR	CA-CB-CG	-5.50	104.00	113.90
1	C	69	HIS	CA-CB-CG	-5.48	108.32	113.80
1	A	325	LYS	N-CA-C	-5.48	105.23	111.14
1	A	333	VAL	N-CA-C	5.46	115.75	108.11
1	B	169	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	169	ASP	CA-C-N	5.42	127.59	120.60
1	A	169	ASP	C-N-CA	5.42	127.59	120.60
1	D	260	VAL	N-CA-C	5.42	116.39	108.53
1	D	65	HIS	CA-CB-CG	-5.42	108.38	113.80
1	B	102	ALA	CA-C-N	5.41	127.80	120.44
1	B	102	ALA	C-N-CA	5.41	127.80	120.44
1	A	264	PRO	CA-C-N	5.37	125.91	119.94
1	A	264	PRO	C-N-CA	5.37	125.91	119.94
1	C	87	THR	O-C-N	5.35	124.60	120.38
1	C	93	PHE	CA-CB-CG	-5.34	108.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ILE	N-CA-C	5.34	115.65	108.17
1	B	358	GLU	CA-CB-CG	-5.33	103.43	114.10
1	C	71	LEU	N-CA-C	5.32	116.77	110.97
1	C	55	TYR	N-CA-C	-5.32	105.93	112.90
1	D	341	VAL	CA-C-N	5.32	126.77	120.23
1	D	341	VAL	C-N-CA	5.32	126.77	120.23
1	C	170	VAL	N-CA-C	5.31	115.52	110.42
1	A	331	PRO	N-CA-CB	5.29	108.36	103.39
1	A	354	GLU	N-CA-C	-5.29	105.42	111.07
1	A	38	THR	O-C-N	5.28	125.95	121.20
1	C	203	ALA	CA-C-O	5.28	125.88	119.38
1	A	193	ALA	N-CA-C	5.26	119.33	113.01
1	C	23	PHE	CA-C-N	-5.25	115.00	121.83
1	C	23	PHE	C-N-CA	-5.25	115.00	121.83
1	A	181	GLY	N-CA-C	5.24	117.39	112.04
1	A	352	ILE	CA-C-N	5.24	126.38	119.84
1	A	352	ILE	C-N-CA	5.24	126.38	119.84
1	B	342	PRO	N-CA-CB	5.19	108.16	103.34
1	C	91	ALA	N-CA-C	5.19	117.67	111.71
1	D	330	GLU	N-CA-C	-5.15	103.23	109.57
1	B	82	THR	N-CA-C	-5.15	101.46	109.24
1	A	208	PHE	N-CA-C	5.15	119.43	113.20
1	B	13	MET	CA-C-O	5.14	124.94	119.69
1	B	159	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	A	158	VAL	N-CA-C	5.14	117.52	111.09
1	B	278	ASP	CA-CB-CG	-5.12	107.48	112.60
1	D	140	ASP	N-CA-C	-5.12	107.04	113.28
1	D	341	VAL	O-C-N	5.12	127.45	121.57
1	A	199	ALA	CA-C-O	5.11	123.25	118.44
1	D	349	VAL	N-CA-CB	5.10	121.32	111.62
1	B	171	GLU	O-C-N	5.09	124.40	120.38
1	D	354	GLU	O-C-N	5.09	127.52	122.08
1	C	198	ASP	CA-CB-CG	-5.08	107.52	112.60
1	B	314	PRO	N-CA-CB	5.08	107.83	103.31
1	A	152	TYR	CB-CA-C	-5.04	102.43	110.79
1	D	10	ARG	CD-NE-CZ	5.04	131.45	124.40
1	B	130	VAL	CA-C-N	5.03	125.18	119.90
1	B	130	VAL	C-N-CA	5.03	125.18	119.90
1	C	86	VAL	CA-C-O	5.02	126.17	120.95
1	D	354	GLU	N-CA-CB	5.01	117.44	109.82
1	D	345	PRO	N-CA-CB	5.00	108.50	103.25
1	B	87	THR	O-C-N	5.00	124.33	120.38

There are no chirality outliers.

There are no planarity outliers.

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	2795	0	2841	186	1
1	B	2786	0	2814	137	0
1	C	2775	0	2809	169	0
1	D	2779	0	2819	249	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	13	9	0
3	B	16	0	13	9	0
3	C	16	0	13	13	0
3	D	16	0	13	11	0
4	A	216	0	0	11	0
4	B	295	0	0	4	0
4	C	237	0	0	11	0
4	D	147	0	0	15	0
All	All	12098	0	11335	741	1

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 33.

All (741) 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:B:46:GLU:H	1:B:105:MET:CE	1.52	1.21
1:A:144:GLN:O	1:A:148:VAL:HG23	1.47	1.12
1:B:46:GLU:N	1:B:105:MET:HE1	1.64	1.11
1:C:50:MET:HE1	3:C:1200:SMG:HE1	1.15	1.09
1:C:10:ARG:HD3	1:C:362:ALA:HB3	1.17	1.08
1:D:141:THR:HG22	1:D:143:PRO:HD2	1.30	1.06
1:D:38:THR:HB	1:D:39:PRO:HD2	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ALA:HB3	1:B:81:ILE:HD11	1.38	1.03
1:D:141:THR:CG2	1:D:143:PRO:HD2	1.88	1.03
1:C:38:THR:HB	1:C:39:PRO:HD2	1.39	1.01
1:C:269:GLY:C	4:C:1237:HOH:O	2.03	1.00
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.44	1.00
1:B:45:GLY:HA2	1:B:105:MET:HE3	1.42	0.99
1:D:9:ARG:HH12	1:D:363:LYS:HZ2	0.99	0.98
1:D:322:ARG:NH1	1:D:323:PHE:CE2	2.34	0.96
1:D:21:THR:HG21	1:D:23:PHE:CE2	2.01	0.95
1:C:58:GLU:HB2	1:C:98:MET:HE1	1.49	0.94
1:B:46:GLU:H	1:B:105:MET:HE1	0.79	0.94
1:C:141:THR:HG22	1:C:144:GLN:H	1.34	0.93
1:C:141:THR:HG23	1:C:143:PRO:HD2	1.49	0.93
1:C:58:GLU:HB2	1:C:98:MET:CE	2.00	0.91
1:C:87:THR:HB	1:C:88:PRO:HD3	1.52	0.89
1:D:110:ALA:HA	4:D:1395:HOH:O	1.73	0.88
1:B:142:ILE:N	1:B:143:PRO:HD2	1.89	0.88
1:B:45:GLY:CA	1:B:105:MET:HE3	2.03	0.87
1:D:159:ARG:HD2	4:D:1403:HOH:O	1.75	0.86
1:C:50:MET:CE	3:C:1200:SMG:HE1	2.05	0.85
1:C:139:MET:HB2	1:C:168:TRP:CH2	2.11	0.85
1:D:9:ARG:HH12	1:D:363:LYS:NZ	1.73	0.85
1:A:35:ARG:HD3	1:A:44:TRP:CZ2	2.11	0.84
1:D:58:GLU:OE1	1:D:98:MET:HG3	1.76	0.84
1:C:33:LEU:C	1:C:34:LEU:HD12	2.03	0.83
1:D:1:MET:SD	1:D:38:THR:HG21	2.17	0.83
1:D:353:PRO:HA	1:D:356:LEU:HB3	1.60	0.83
1:D:206:ASP:N	1:D:207:PRO:HD2	1.92	0.83
1:D:328:ILE:O	1:D:351:PRO:HA	1.78	0.82
1:A:7:GLU:OE2	1:A:9:ARG:NH1	2.13	0.82
1:D:9:ARG:NH1	1:D:363:LYS:HZ2	1.76	0.81
1:D:125:SER:HB2	1:D:307:SER:OG	1.79	0.81
1:D:352:ILE:O	1:D:355:LEU:HB2	1.79	0.81
1:A:263:LYS:HZ3	3:A:1000:SMG:C2	1.93	0.81
1:D:21:THR:HG22	1:D:22:SER:N	1.95	0.81
1:A:29:ARG:NE	1:A:31:LEU:HD23	1.94	0.81
1:D:20:ARG:HG2	1:D:138:ILE:HB	1.63	0.81
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.63	0.81
1:D:263:LYS:NZ	3:D:1300:SMG:O11	2.12	0.81
1:D:206:ASP:HB2	1:D:207:PRO:HD3	1.62	0.80
1:A:127:ARG:NH2	1:A:308:LEU:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ARG:HD2	1:B:31:LEU:HD21	1.64	0.80
1:D:38:THR:HB	1:D:39:PRO:CD	2.10	0.80
1:D:205:LEU:C	1:D:207:PRO:HD2	2.06	0.80
1:C:109:ASP:O	1:C:113:ARG:HG3	1.82	0.80
1:A:144:GLN:O	1:A:148:VAL:CG2	2.28	0.79
1:D:169:ASP:OD1	1:D:194:TYR:OH	1.99	0.79
1:A:169:ASP:O	1:A:173:VAL:HG23	1.83	0.79
1:C:159:ARG:NH2	1:C:316:ASP:OD1	2.14	0.79
1:C:75:LEU:CD1	1:C:103:LEU:HD13	2.12	0.79
1:D:139:MET:HE3	1:D:148:VAL:HG21	1.64	0.79
1:C:169:ASP:OD1	1:C:194:TYR:OH	2.01	0.79
1:D:221:ASP:OD2	1:D:224:GLY:HA3	1.82	0.78
1:D:141:THR:HG22	1:D:143:PRO:CD	2.13	0.78
1:D:263:LYS:HZ1	3:D:1300:SMG:C2	1.95	0.78
1:C:201:GLN:O	1:C:204:ARG:HB2	1.84	0.78
1:B:142:ILE:N	1:B:143:PRO:CD	2.47	0.78
1:A:329:THR:HB	1:A:349:VAL:HG13	1.65	0.78
1:C:34:LEU:HD12	1:C:34:LEU:N	1.98	0.78
1:B:1:MET:SD	1:B:39:PRO:HB2	2.24	0.78
1:B:78:ALA:HB3	1:B:81:ILE:CD1	2.13	0.77
1:A:40:ALA:HB3	4:A:1066:HOH:O	1.84	0.77
1:D:159:ARG:HG2	1:D:160:ILE:N	1.98	0.77
1:C:38:THR:CB	1:C:39:PRO:HD2	2.14	0.77
1:D:132:CYS:O	1:D:158:VAL:HG22	1.84	0.77
1:B:50:MET:SD	3:B:1100:SMG:CE	2.73	0.77
1:D:2:LYS:HD2	1:D:3:LEU:N	2.00	0.77
1:A:98:MET:CE	4:A:1065:HOH:O	2.33	0.76
1:B:163:LYS:NZ	1:B:189:ASP:OD2	2.18	0.76
1:C:10:ARG:CD	1:C:362:ALA:HB3	2.09	0.76
1:D:163:LYS:NZ	3:D:1300:SMG:H1	2.00	0.76
1:C:141:THR:CG2	1:C:143:PRO:HD2	2.15	0.76
1:D:169:ASP:HB2	1:D:170:VAL:HG23	1.67	0.76
1:B:46:GLU:N	1:B:105:MET:CE	2.34	0.75
1:C:87:THR:HB	1:C:88:PRO:CD	2.16	0.75
1:A:201:GLN:O	1:A:204[A]:ARG:HB2	1.86	0.75
1:A:149:VAL:HG13	1:A:160:ILE:HD13	1.68	0.75
1:D:62:GLY:O	4:D:1387:HOH:O	2.05	0.75
1:D:148:VAL:HG12	1:D:152:TYR:CE1	2.21	0.74
1:D:18:PRO:HA	1:D:26:GLN:O	1.86	0.74
1:B:29:ARG:HD2	1:B:31:LEU:CD2	2.18	0.74
1:C:58:GLU:CD	1:C:98:MET:HE2	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:HB2	1:A:207:PRO:HD3	1.67	0.74
1:D:206:ASP:N	1:D:207:PRO:CD	2.50	0.73
1:C:141:THR:HB	1:C:144:GLN:HB3	1.71	0.73
1:B:50:MET:SD	3:B:1100:SMG:HE3	2.29	0.73
1:D:19:PHE:HE2	3:D:1300:SMG:HE3	1.55	0.72
1:A:159:ARG:HG2	1:A:160:ILE:N	2.03	0.72
1:C:49:THR:HG22	1:C:98:MET:CE	2.20	0.72
1:B:8:LEU:CD2	1:B:34:LEU:HD22	2.19	0.72
1:C:127:ARG:HH11	1:C:307:SER:HA	1.52	0.72
1:C:49:THR:CG2	1:C:98:MET:HE3	2.20	0.72
1:A:201:GLN:O	1:A:204[B]:ARG:HB2	1.89	0.71
1:C:58:GLU:CB	1:C:98:MET:CE	2.67	0.71
1:C:205:LEU:C	1:C:207:PRO:HD2	2.15	0.71
1:A:117:ARG:HE	1:A:121:ALA:HB1	1.54	0.71
1:B:205:LEU:C	1:B:207:PRO:HD2	2.15	0.71
1:A:98:MET:HE1	4:A:1065:HOH:O	1.87	0.71
1:C:7:GLU:OE1	1:C:9:ARG:NH1	2.22	0.71
1:D:75:LEU:O	1:D:81:ILE:HD11	1.89	0.71
1:D:9:ARG:HG3	1:D:9:ARG:HH11	1.56	0.71
1:D:9:ARG:HH11	1:D:9:ARG:CG	2.04	0.70
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.72	0.70
1:A:33:LEU:C	1:A:34:LEU:HD23	2.16	0.70
1:C:248:ALA:O	1:C:252:ILE:HG13	1.91	0.70
1:A:329:THR:HG21	1:A:349:VAL:CG1	2.22	0.70
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.57	0.70
1:A:206:ASP:N	1:A:207:PRO:HD2	2.07	0.70
1:B:217:LEU:HB2	1:B:225:HIS:CE1	2.27	0.70
1:D:21:THR:HG22	1:D:22:SER:H	1.55	0.70
1:D:363:LYS:O	1:D:364:VAL:HG22	1.91	0.70
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.72	0.70
1:A:35:ARG:HD3	1:A:44:TRP:CH2	2.27	0.69
1:C:194:TYR:CE2	1:C:202:LEU:HD21	2.28	0.69
1:A:87:THR:HB	1:A:88:PRO:HD3	1.73	0.69
1:B:206:ASP:HB2	1:B:207:PRO:HD3	1.74	0.69
1:C:141:THR:CG2	1:C:144:GLN:H	2.04	0.69
1:C:75:LEU:HD11	1:C:103:LEU:HD13	1.72	0.69
1:D:216:PRO:C	1:D:217:LEU:HD23	2.18	0.69
1:A:112:LEU:HB3	1:A:117:ARG:O	1.92	0.69
1:D:363:LYS:HG2	1:D:364:VAL:N	2.08	0.68
1:A:356:LEU:HD22	1:A:360:THR:OG1	1.93	0.68
1:B:201:GLN:O	1:B:204:ARG:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:HB2	1:B:185:LEU:HB2	1.74	0.68
1:C:159:ARG:HD2	4:C:1296:HOH:O	1.92	0.68
1:A:293:ILE:HG22	1:A:293:ILE:O	1.91	0.68
3:C:1200:SMG:O62	4:C:1373:HOH:O	2.12	0.68
1:D:56:SER:OG	1:D:98:MET:HE2	1.94	0.68
1:A:21:THR:HG21	3:A:1000:SMG:HE2	1.76	0.68
1:B:199:ALA:HB3	1:B:200:PRO:HD3	1.77	0.67
1:C:206:ASP:N	1:C:207:PRO:CD	2.57	0.67
1:C:353:PRO:HA	4:C:1285:HOH:O	1.94	0.67
1:D:297:LEU:HD23	1:D:329:THR:HG21	1.76	0.67
1:D:334:LEU:HD12	1:D:339:LEU:HD13	1.75	0.67
1:D:227:GLU:O	1:D:230:ARG:HB2	1.95	0.67
1:A:329:THR:HB	1:A:349:VAL:CG1	2.24	0.67
1:D:33:LEU:O	1:D:34:LEU:HD23	1.94	0.67
1:D:81:ILE:HD12	4:D:1361:HOH:O	1.95	0.67
1:C:29:ARG:CZ	1:C:50:MET:HE2	2.25	0.66
1:C:50:MET:HE1	3:C:1200:SMG:CE	2.09	0.66
1:D:8:LEU:CD1	1:D:34:LEU:HD22	2.25	0.66
1:A:206:ASP:N	1:A:207:PRO:CD	2.58	0.66
1:C:271:LEU:N	4:C:1237:HOH:O	2.29	0.66
1:C:293:ILE:CD1	3:C:1200:SMG:CE	2.73	0.66
1:D:44:TRP:O	1:D:106:ALA:HA	1.95	0.66
1:A:75:LEU:O	1:A:81:ILE:HD11	1.95	0.66
1:A:163:LYS:NZ	3:A:1000:SMG:H1	2.11	0.66
1:D:199:ALA:N	1:D:200:PRO:HD2	2.11	0.66
1:D:355:LEU:O	1:D:359:VAL:HG22	1.95	0.66
1:B:33:LEU:CD2	1:B:46:GLU:HG3	2.26	0.65
1:C:8:LEU:CD2	1:C:64:GLU:HG3	2.26	0.65
1:A:73:PRO:O	4:A:1175:HOH:O	2.13	0.65
1:D:35:ARG:HG3	1:D:44:TRP:CH2	2.31	0.65
1:D:201:GLN:O	1:D:204:ARG:HB2	1.97	0.65
1:B:92:LYS:HE3	4:B:1146:HOH:O	1.95	0.65
1:B:163:LYS:HE3	1:B:191:ASN:OD1	1.96	0.65
1:C:141:THR:HG23	1:C:143:PRO:CD	2.24	0.65
1:C:141:THR:CG2	1:C:143:PRO:CD	2.74	0.65
1:C:58:GLU:CB	1:C:98:MET:HE1	2.26	0.64
1:D:58:GLU:HB2	1:D:98:MET:HE3	1.78	0.64
1:D:213:ILE:HG12	1:D:216:PRO:HG3	1.78	0.64
1:C:49:THR:HG22	1:C:98:MET:HE3	1.77	0.64
1:D:29:ARG:NH1	1:D:49:THR:O	2.30	0.64
1:D:30:GLU:O	1:D:60:ASN:ND2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:TYR:CE2	1:D:202:LEU:HD21	2.32	0.64
1:B:72:ILE:HB	1:B:73:PRO:HD3	1.80	0.64
1:C:75:LEU:HD12	1:C:103:LEU:HD13	1.79	0.63
1:A:4:SER:HB2	1:A:37:VAL:HG12	1.80	0.63
1:B:87:THR:HB	1:B:88:PRO:HD3	1.79	0.63
1:C:352:ILE:HB	1:C:355:LEU:HD12	1.81	0.63
1:C:288:TRP:HB3	1:C:313:LEU:HB2	1.79	0.63
1:D:95:GLY:O	1:D:100:LYS:HE3	1.97	0.63
1:D:163:LYS:HZ1	3:D:1300:SMG:H1	1.61	0.63
1:A:329:THR:CG2	1:A:349:VAL:CG1	2.77	0.63
1:A:319:ALA:HB1	1:A:332:PHE:O	1.99	0.63
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.63	0.63
1:A:199:ALA:HB3	1:A:200:PRO:CD	2.26	0.63
1:A:171:GLU:N	1:A:172:PRO:HD2	2.14	0.63
1:A:139:MET:HG3	1:A:145:LEU:HA	1.80	0.62
1:C:29:ARG:NH2	1:C:50:MET:HE2	2.14	0.62
1:A:8:LEU:HD11	1:A:34:LEU:HD22	1.82	0.62
1:C:293:ILE:CD1	3:C:1200:SMG:HE2	2.30	0.62
1:D:21:THR:CG2	1:D:22:SER:N	2.61	0.62
1:C:38:THR:HB	1:C:39:PRO:CD	2.23	0.62
1:C:127:ARG:NH1	1:C:307:SER:HA	2.13	0.62
1:D:19:PHE:CE2	3:D:1300:SMG:HE3	2.34	0.62
1:C:204:ARG:HG2	1:C:204:ARG:NH1	2.13	0.62
1:D:21:THR:CG2	1:D:22:SER:H	2.12	0.62
1:D:15:LEU:HD23	1:D:324:TYR:HE1	1.64	0.62
1:D:109:ASP:OD1	1:D:346:GLY:HA3	2.00	0.62
1:D:352:ILE:CG2	1:D:355:LEU:HD22	2.29	0.62
1:B:358:GLU:O	1:B:358:GLU:HG2	1.99	0.62
1:A:75:LEU:HD12	1:A:103:LEU:HD21	1.82	0.62
1:B:159:ARG:HG2	1:B:160:ILE:N	2.14	0.61
1:D:274:ARG:O	1:D:277:HIS:HB3	1.99	0.61
1:A:263:LYS:NZ	3:A:1000:SMG:O11	2.33	0.61
1:D:112:LEU:HD12	1:D:119:PHE:CD1	2.35	0.61
1:A:15:LEU:HB2	1:A:27:SER:O	2.00	0.61
1:A:185:LEU:HD22	1:A:211:LEU:HD11	1.83	0.61
1:C:227:GLU:O	1:C:230:ARG:HB2	2.00	0.61
1:A:87:THR:N	1:A:88:PRO:HD2	2.14	0.61
1:B:288:TRP:HB3	1:B:313:LEU:HB2	1.83	0.60
1:C:243:VAL:O	1:C:244:SER:HB3	2.01	0.60
1:A:33:LEU:HD21	1:A:46:GLU:HG3	1.83	0.60
1:D:8:LEU:HD12	1:D:34:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ILE:HG21	1:D:355:LEU:HD22	1.83	0.60
1:B:201:GLN:OE1	1:B:201:GLN:HA	2.01	0.60
1:B:252:ILE:HG12	1:B:285:ILE:HG13	1.82	0.60
1:A:8:LEU:CD1	1:A:34:LEU:HD22	2.31	0.60
1:A:49:THR:HG22	1:A:98:MET:HE3	1.84	0.60
1:C:142:ILE:N	1:C:143:PRO:HD2	2.17	0.60
1:A:205:LEU:C	1:A:207:PRO:HD2	2.26	0.60
1:B:280:CYS:HB3	1:B:285:ILE:O	2.01	0.60
1:C:34:LEU:N	1:C:34:LEU:CD1	2.65	0.60
1:C:58:GLU:OE1	1:C:98:MET:HE2	2.01	0.60
1:A:263:LYS:NZ	3:A:1000:SMG:C2	2.63	0.60
1:B:227:GLU:OE1	1:B:230:ARG:NH1	2.35	0.59
1:C:139:MET:CG	1:C:145:LEU:HB2	2.31	0.59
1:D:338:HIS:O	1:D:339:LEU:HD12	2.03	0.59
1:B:29:ARG:CD	1:B:31:LEU:HD21	2.31	0.59
1:C:293:ILE:HG13	3:C:1200:SMG:HE3	1.84	0.59
1:A:28:VAL:HG12	1:A:29:ARG:N	2.15	0.59
1:B:171:GLU:HB2	1:B:172:PRO:HD3	1.84	0.59
1:D:29:ARG:CZ	1:D:31:LEU:HD23	2.33	0.59
1:D:270:TYR:O	1:D:273:ALA:HB3	2.02	0.59
1:A:8:LEU:CD2	1:A:64:GLU:HG3	2.33	0.59
1:A:21:THR:HG22	1:A:163:LYS:HE3	1.85	0.59
3:D:1300:SMG:O11	4:D:1421:HOH:O	2.16	0.59
1:C:252:ILE:HD13	1:C:285:ILE:HG13	1.84	0.58
1:D:159:ARG:NH2	1:D:316:ASP:OD1	2.26	0.58
1:D:363:LYS:C	1:D:364:VAL:HG22	2.27	0.58
1:A:113:ARG:HA	1:A:345:PRO:HB2	1.84	0.58
1:D:164:ILE:HB	1:D:168:TRP:O	2.03	0.58
1:A:191:ASN:C	1:A:192:THR:HG23	2.28	0.58
1:C:82:THR:CG2	1:C:85:LYS:HD2	2.33	0.58
1:A:199:ALA:N	1:A:200:PRO:HD2	2.18	0.58
1:A:332:PHE:HB3	1:A:339:LEU:HD21	1.86	0.58
1:A:349:VAL:CG1	1:A:350:ALA:N	2.65	0.58
1:C:190:ALA:HB3	1:C:216:PRO:HA	1.84	0.58
1:C:82:THR:HG23	1:C:85:LYS:HD2	1.85	0.58
1:C:364:VAL:HG23	4:C:1383:HOH:O	2.03	0.58
1:D:87:THR:HB	1:D:88:PRO:HD3	1.86	0.58
1:B:7:GLU:OE2	1:B:363:LYS:HD2	2.04	0.58
1:D:23:PHE:HZ	3:D:1300:SMG:HG1	1.68	0.58
1:D:199:ALA:HB3	1:D:200:PRO:CD	2.33	0.58
1:D:50:MET:HE1	1:D:293:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:NZ	3:D:1300:SMG:O31	2.37	0.57
1:A:125:SER:HB2	1:A:307:SER:OG	2.04	0.57
1:B:50:MET:HE1	3:B:1100:SMG:CE	2.34	0.57
1:D:119:PHE:HB2	4:D:1341:HOH:O	2.03	0.57
1:D:217:LEU:HD21	1:D:228:LEU:HD22	1.86	0.57
1:A:129:SER:OG	1:A:338:HIS:ND1	2.32	0.57
1:C:127:ARG:HB2	1:C:307:SER:HB2	1.85	0.57
1:D:21:THR:HG21	1:D:23:PHE:CD2	2.39	0.57
1:B:141:THR:CB	1:B:143:PRO:HD2	2.33	0.57
1:B:237:CYS:HA	1:B:259:ILE:O	2.04	0.57
1:D:68[B]:ARG:NH2	1:D:364:VAL:HG21	2.19	0.57
1:B:263:LYS:HB2	1:B:266:ARG:NH1	2.20	0.57
1:C:38:THR:CB	1:C:39:PRO:CD	2.82	0.57
1:C:139:MET:HB2	1:C:168:TRP:HH2	1.69	0.57
1:D:297:LEU:CD2	1:D:329:THR:HG21	2.33	0.57
1:A:57:SER:HB3	4:A:1090:HOH:O	2.05	0.57
1:D:141:THR:HG22	1:D:142:ILE:N	2.18	0.57
1:B:33:LEU:HD21	1:B:46:GLU:HG3	1.86	0.57
1:C:293:ILE:HD12	3:C:1200:SMG:CE	2.35	0.57
1:D:62:GLY:CA	4:D:1387:HOH:O	2.52	0.57
1:D:148:VAL:O	1:D:149:VAL:C	2.46	0.57
1:C:58:GLU:HB2	1:C:98:MET:HE2	1.84	0.56
1:B:45:GLY:HA2	1:B:105:MET:CE	2.26	0.56
1:C:87:THR:CB	1:C:88:PRO:HD3	2.30	0.56
1:D:363:LYS:C	1:D:364:VAL:CG2	2.79	0.56
1:A:329:THR:CB	1:A:349:VAL:CG1	2.82	0.56
1:C:141:THR:HG22	1:C:144:GLN:N	2.14	0.56
1:A:149:VAL:HG13	1:A:160:ILE:CD1	2.35	0.56
1:D:353:PRO:O	1:D:357:ASP:OD2	2.24	0.56
1:A:38:THR:HB	1:A:39:PRO:HD2	1.86	0.56
1:C:139:MET:HG2	1:C:145:LEU:HB2	1.86	0.56
1:D:261:ASN:C	1:D:261:ASN:OD1	2.49	0.56
1:A:199:ALA:N	1:A:200:PRO:CD	2.68	0.56
1:B:141:THR:C	1:B:143:PRO:HD2	2.31	0.56
1:D:135:SER:HB2	1:D:161:LYS:HD3	1.88	0.56
1:D:148:VAL:CG1	1:D:152:TYR:CE1	2.88	0.56
1:D:363:LYS:HG2	1:D:364:VAL:H	1.70	0.56
1:B:283:HIS:CE1	1:C:253:LYS:HE2	2.40	0.56
1:D:82:THR:HG22	1:D:84:ALA:H	1.69	0.56
1:A:21:THR:HG21	3:A:1000:SMG:CE	2.36	0.55
1:A:72:ILE:N	1:A:73:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:O	1:D:145:LEU:N	2.39	0.55
1:A:321:ASP:HA	1:A:324:TYR:O	2.05	0.55
1:B:169:ASP:OD2	1:B:194:TYR:OH	2.21	0.55
1:A:138:ILE:HG23	1:A:168:TRP:CD1	2.40	0.55
1:C:95:GLY:O	1:C:100:LYS:HE3	2.07	0.55
1:D:217:LEU:HD21	1:D:228:LEU:CD2	2.37	0.55
1:D:85:LYS:C	1:D:88:PRO:HD2	2.31	0.55
1:A:187:GLN:HB2	1:A:212:LEU:CD1	2.36	0.55
1:C:87:THR:CB	1:C:88:PRO:CD	2.83	0.55
1:C:206:ASP:N	1:C:207:PRO:HD2	2.22	0.55
1:C:269:GLY:O	4:C:1237:HOH:O	2.17	0.55
1:D:143:PRO:O	1:D:144:GLN:C	2.49	0.55
1:C:49:THR:HG22	1:C:98:MET:HE1	1.87	0.55
1:D:334:LEU:HD12	1:D:339:LEU:CD1	2.36	0.55
1:A:8:LEU:HD23	1:A:64:GLU:HG3	1.86	0.55
1:C:127:ARG:NH1	1:C:306:ALA:O	2.40	0.55
1:C:328:ILE:O	1:C:351:PRO:HA	2.07	0.55
1:D:3:LEU:HD23	1:D:76:LEU:HD23	1.89	0.55
1:A:11:VAL:HB	1:A:31:LEU:HD12	1.90	0.54
1:A:163:LYS:HZ3	3:A:1000:SMG:H1	1.70	0.54
1:D:2:LYS:O	1:D:39:PRO:HD3	2.07	0.54
1:D:141:THR:CG2	1:D:142:ILE:N	2.69	0.54
1:D:353:PRO:O	1:D:354:GLU:C	2.50	0.54
1:C:139:MET:HE3	1:C:148:VAL:HG21	1.89	0.54
1:D:87:THR:N	1:D:88:PRO:HD2	2.21	0.54
1:A:352:ILE:HG22	1:A:355:LEU:HG	1.90	0.54
1:C:293:ILE:HD11	3:C:1200:SMG:HE2	1.88	0.54
1:C:194:TYR:CD2	1:C:202:LEU:HD21	2.42	0.54
1:C:352:ILE:O	1:C:355:LEU:HB2	2.06	0.54
1:A:192:THR:HB	1:A:218:GLU:HA	1.90	0.54
1:B:227:GLU:CD	1:B:230:ARG:HH11	2.15	0.53
1:C:139:MET:HB2	1:C:168:TRP:CZ2	2.43	0.53
1:C:362:ALA:O	1:C:363:LYS:HB2	2.07	0.53
1:B:139:MET:HG3	1:B:145:LEU:HA	1.90	0.53
1:D:194:TYR:CD2	1:D:202:LEU:HD21	2.43	0.53
1:D:218:GLU:HG2	4:D:1357:HOH:O	2.09	0.53
1:B:249:ALA:O	1:B:253:LYS:HG3	2.08	0.53
1:C:118:SER:HB3	1:C:344:GLY:O	2.08	0.53
1:B:216:PRO:C	1:B:217:LEU:HD23	2.33	0.53
1:C:162:LEU:O	1:C:188:VAL:HA	2.08	0.53
1:B:206:ASP:N	1:B:207:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:CD2	1:A:311:PHE:CE1	2.96	0.53
1:D:4:SER:HB2	1:D:37:VAL:O	2.09	0.53
1:A:72:ILE:N	1:A:73:PRO:CD	2.72	0.53
1:A:356:LEU:CD2	1:A:360:THR:OG1	2.57	0.53
1:C:169:ASP:OD2	1:C:201:GLN:NE2	2.38	0.53
1:D:62:GLY:HA2	4:D:1387:HOH:O	2.06	0.53
1:B:35:ARG:HD2	1:B:42:GLU:OE2	2.09	0.53
1:C:142:ILE:N	1:C:143:PRO:CD	2.72	0.53
1:D:159:ARG:HH21	1:D:161:LYS:HB3	1.74	0.53
1:D:215:GLN:HG3	1:D:240:GLU:OE1	2.08	0.53
1:A:329:THR:HG21	1:A:349:VAL:HG11	1.90	0.52
1:B:179:ARG:O	1:B:179:ARG:HG3	1.99	0.52
1:C:264:PRO:HG3	1:C:305:LEU:HD22	1.90	0.52
1:D:58:GLU:HB2	1:D:98:MET:CE	2.39	0.52
1:D:142:ILE:HB	1:D:143:PRO:CD	2.37	0.52
1:A:87:THR:CB	1:A:88:PRO:HD3	2.37	0.52
1:C:287:VAL:O	1:C:311:PHE:HA	2.09	0.52
1:A:33:LEU:CD2	1:A:46:GLU:HG3	2.39	0.52
1:B:283:HIS:ND1	1:C:253:LYS:HE2	2.24	0.52
1:B:179:ARG:HG2	1:B:180:PHE:CE1	2.45	0.52
1:D:60:ASN:HB2	4:D:1352:HOH:O	2.09	0.52
1:B:332:PHE:HB3	1:B:339:LEU:HD21	1.92	0.52
1:C:49:THR:HG23	1:C:98:MET:HE3	1.92	0.52
1:C:293:ILE:O	1:C:293:ILE:HG22	2.10	0.52
1:D:120:ALA:HB1	1:D:125:SER:HB3	1.92	0.52
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.75	0.52
1:D:199:ALA:N	1:D:200:PRO:CD	2.73	0.51
1:A:87:THR:N	1:A:88:PRO:CD	2.73	0.51
1:A:352:ILE:CG2	1:A:355:LEU:HG	2.40	0.51
1:A:87:THR:CB	1:A:88:PRO:CD	2.88	0.51
1:B:8:LEU:HD23	1:B:34:LEU:HD22	1.92	0.51
1:D:22:SER:OG	1:D:191:ASN:HB2	2.11	0.51
1:A:192:THR:HG22	1:A:215:GLN:HG2	1.91	0.51
1:B:162:LEU:O	1:B:188:VAL:HA	2.11	0.51
1:A:297:LEU:HD23	1:A:329:THR:HG21	1.93	0.51
1:A:354:GLU:O	1:A:358:GLU:HG3	2.11	0.51
1:C:8:LEU:HD22	1:C:64:GLU:HG3	1.92	0.51
1:D:46:GLU:OE2	1:D:295:THR:HG23	2.11	0.51
1:A:329:THR:HG21	1:A:349:VAL:HG12	1.92	0.51
1:A:352:ILE:O	1:A:355:LEU:N	2.43	0.51
1:B:139:MET:HG3	1:B:145:LEU:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HB	1:B:143:PRO:HD3	1.93	0.51
1:D:62:GLY:C	4:D:1387:HOH:O	2.52	0.51
1:A:46:GLU:OE2	1:A:294:GLU:HB3	2.11	0.51
1:A:170:VAL:HG21	1:A:204[B]:ARG:HB3	1.93	0.51
1:B:8:LEU:O	1:B:363:LYS:HA	2.10	0.51
1:B:227:GLU:CD	1:B:230:ARG:NH1	2.69	0.51
1:D:203:ALA:HA	1:D:232:ILE:HG22	1.92	0.51
1:A:213:ILE:HG22	1:A:234:THR:HG22	1.92	0.51
1:A:328:ILE:O	1:A:351:PRO:HA	2.10	0.51
1:D:2:LYS:HD2	1:D:2:LYS:C	2.34	0.51
1:D:58:GLU:CD	1:D:98:MET:HG3	2.36	0.51
1:D:142:ILE:HG22	1:D:146:LEU:HD12	1.93	0.51
1:D:206:ASP:CB	1:D:207:PRO:HD3	2.36	0.51
1:A:58:GLU:HB2	1:A:98:MET:HE2	1.93	0.51
1:B:264:PRO:HG3	1:B:305:LEU:HD22	1.93	0.50
1:D:171:GLU:HB2	1:D:172:PRO:CD	2.39	0.50
1:D:272:GLU:O	1:D:276:VAL:HG23	2.11	0.50
1:B:145:LEU:O	1:B:149:VAL:HG23	2.11	0.50
1:A:139:MET:HG3	1:A:145:LEU:CA	2.41	0.50
1:B:50:MET:HE1	3:B:1100:SMG:HE2	1.94	0.50
1:A:82:THR:O	1:A:83:ALA:C	2.53	0.50
1:A:310:ASN:O	1:A:312:THR:N	2.44	0.50
1:B:29:ARG:CD	1:B:31:LEU:CD2	2.88	0.50
1:D:56:SER:OG	1:D:98:MET:CE	2.58	0.50
1:C:257:VAL:HG13	1:C:257:VAL:O	2.10	0.50
1:D:348:GLY:HA2	4:D:1374:HOH:O	2.12	0.50
1:A:159:ARG:NH2	1:A:316:ASP:OD1	2.26	0.50
1:B:146:LEU:O	1:B:180:PHE:HZ	1.94	0.50
1:B:200:PRO:HA	4:B:1331:HOH:O	2.12	0.50
1:D:148:VAL:HG12	1:D:152:TYR:HE1	1.74	0.50
1:A:169:ASP:OD1	1:A:194:TYR:OH	2.22	0.49
1:C:272:GLU:N	4:C:1237:HOH:O	2.13	0.49
1:D:25:THR:HG22	1:D:26:GLN:N	2.26	0.49
1:D:194:TYR:N	1:D:194:TYR:CD1	2.79	0.49
1:D:215:GLN:HG2	1:D:239:ASP:H	1.77	0.49
1:B:206:ASP:N	1:B:207:PRO:HD2	2.27	0.49
1:C:356:LEU:HD12	1:C:356:LEU:O	2.11	0.49
1:A:349:VAL:HG12	1:A:350:ALA:N	2.28	0.49
1:D:15:LEU:CD2	1:D:324:TYR:HE1	2.25	0.49
1:A:2:LYS:O	1:A:38:THR:HG22	2.12	0.49
1:B:148:VAL:O	1:B:149:VAL:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:TYR:OH	1:D:266:ARG:HD3	2.12	0.49
1:D:78:ALA:HB3	1:D:81:ILE:HD11	1.93	0.49
1:A:277:HIS:NE2	1:A:310:ASN:HB3	2.28	0.49
1:D:329:THR:O	1:D:330:GLU:C	2.56	0.49
1:A:212:LEU:C	1:A:212:LEU:HD12	2.37	0.49
1:A:301:ALA:HB2	1:A:347:LEU:CD2	2.42	0.49
1:B:64:GLU:O	1:B:68:ARG:HB2	2.13	0.49
1:B:109:ASP:OD2	1:B:113:ARG:NH1	2.45	0.49
1:D:293:ILE:HD11	3:D:1300:SMG:CE	2.43	0.49
1:A:212:LEU:HD12	1:A:212:LEU:O	2.13	0.49
1:C:58:GLU:CB	1:C:98:MET:HE2	2.42	0.49
1:C:204:ARG:HH11	1:C:204:ARG:CG	2.25	0.49
1:C:198:ASP:C	1:C:200:PRO:HD2	2.38	0.49
1:B:23:PHE:HE2	1:B:191:ASN:CG	2.21	0.49
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.95	0.49
1:B:83:ALA:O	1:B:86:VAL:HB	2.13	0.48
1:C:141:THR:HG22	1:C:143:PRO:N	2.29	0.48
1:D:212:LEU:C	1:D:212:LEU:HD12	2.37	0.48
1:B:29:ARG:CZ	1:B:31:LEU:HD23	2.43	0.48
1:B:21:THR:HG22	1:B:163:LYS:HG2	1.96	0.48
1:D:149:VAL:O	1:D:150:GLY:C	2.57	0.48
1:D:55:TYR:OH	1:D:239:ASP:OD1	2.27	0.48
1:A:171:GLU:N	1:A:172:PRO:CD	2.76	0.48
1:C:96:HIS:O	1:C:100:LYS:HG3	2.14	0.48
1:A:206:ASP:OD1	4:A:1155:HOH:O	2.20	0.48
1:C:127:ARG:NH2	1:C:308:LEU:O	2.47	0.48
1:C:142:ILE:O	1:C:145:LEU:HB3	2.13	0.48
1:D:68[A]:ARG:HB3	1:D:69:HIS:CD2	2.49	0.48
1:A:190:ALA:O	1:A:191:ASN:C	2.57	0.47
1:C:298:GLY:O	1:C:299:ARG:C	2.57	0.47
1:D:16:VAL:HG23	1:D:323:PHE:O	2.14	0.47
1:A:9:ARG:HG3	1:A:9:ARG:HH11	1.79	0.47
1:A:56:SER:OG	1:A:98:MET:HE2	2.14	0.47
1:A:113:ARG:HG2	1:A:113:ARG:NH1	2.26	0.47
1:C:213:ILE:HG22	1:C:234:THR:HG22	1.95	0.47
1:D:148:VAL:CG1	1:D:152:TYR:HE1	2.27	0.47
1:C:171:GLU:N	1:C:172:PRO:HD2	2.30	0.47
1:B:50:MET:CE	3:B:1100:SMG:HE3	2.43	0.47
1:B:194:TYR:CD2	1:B:202:LEU:HD21	2.50	0.47
1:D:142:ILE:O	1:D:143:PRO:C	2.56	0.47
1:D:206:ASP:CB	1:D:207:PRO:CD	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HD3	1:A:31:LEU:CD2	2.44	0.47
1:D:9:ARG:NH1	1:D:9:ARG:CG	2.70	0.47
1:D:356:LEU:O	1:D:359:VAL:HG23	2.14	0.47
1:B:105:MET:HE3	1:B:105:MET:HB3	1.61	0.47
1:B:118:SER:HB2	4:B:1159:HOH:O	2.14	0.47
1:C:198:ASP:O	1:C:201:GLN:HB3	2.14	0.47
1:D:36:ALA:O	1:D:42:GLU:HB3	2.15	0.47
1:D:169:ASP:O	1:D:172:PRO:HD2	2.14	0.47
1:A:171:GLU:HA	1:A:171:GLU:OE2	2.13	0.47
1:B:130:VAL:O	1:B:338:HIS:HA	2.15	0.47
1:C:263:LYS:HZ1	3:C:1200:SMG:C2	2.28	0.47
1:D:46:GLU:OE1	1:D:297:LEU:HB2	2.15	0.47
1:D:113:ARG:HG2	1:D:345:PRO:HB2	1.96	0.47
1:C:174:ARG:HG2	4:C:1368:HOH:O	2.15	0.47
1:D:206:ASP:HB2	1:D:207:PRO:CD	2.39	0.47
1:A:142:ILE:O	1:A:143:PRO:C	2.56	0.47
1:C:75:LEU:HD12	1:C:103:LEU:CD1	2.44	0.47
1:C:199:ALA:N	1:C:200:PRO:CD	2.78	0.47
1:D:179:ARG:HG2	1:D:180:PHE:CE1	2.50	0.47
1:B:127:ARG:NH2	1:B:308:LEU:O	2.47	0.47
1:B:50:MET:HE1	3:B:1100:SMG:HE3	1.97	0.46
1:C:63:ALA:O	1:C:64:GLU:C	2.57	0.46
1:C:141:THR:HG22	1:C:143:PRO:CD	2.45	0.46
1:D:48:VAL:HB	1:D:292:MET:HG3	1.98	0.46
1:D:145:LEU:O	1:D:146:LEU:C	2.59	0.46
1:B:87:THR:HB	1:B:88:PRO:CD	2.45	0.46
1:D:326:THR:HG22	1:D:326:THR:O	2.14	0.46
1:A:321:ASP:OD1	1:A:321:ASP:C	2.58	0.46
1:C:192:THR:HG22	1:C:215:GLN:HG2	1.96	0.46
1:D:51:ALA:HB3	4:D:1351:HOH:O	2.15	0.46
1:A:190:ALA:HB3	1:A:216:PRO:HA	1.97	0.46
1:B:308:LEU:CB	1:B:309:PRO:HD2	2.45	0.46
1:D:360:THR:HG22	1:D:361:THR:N	2.29	0.46
1:A:159:ARG:CD	4:A:1077:HOH:O	2.62	0.46
1:B:82:THR:O	1:B:86:VAL:HG23	2.16	0.46
1:D:67:LEU:HD23	1:D:71:LEU:HB2	1.97	0.46
1:A:97:ARG:HD2	4:A:1027:HOH:O	2.14	0.46
1:A:329:THR:CB	1:A:349:VAL:HG11	2.46	0.46
1:C:233:GLN:O	1:C:235:PRO:HD3	2.15	0.46
1:D:8:LEU:CD1	1:D:34:LEU:CD2	2.94	0.46
1:D:205:LEU:C	1:D:207:PRO:CD	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:NZ	3:C:1200:SMG:H1	2.31	0.46
1:D:356:LEU:C	1:D:356:LEU:HD12	2.39	0.46
1:C:353:PRO:O	1:C:354:GLU:C	2.58	0.46
1:C:353:PRO:O	1:C:357:ASP:OD2	2.34	0.46
1:D:85:LYS:O	1:D:86:VAL:C	2.57	0.46
1:D:127:ARG:NH2	1:D:308:LEU:O	2.49	0.46
1:D:127:ARG:HH22	1:D:311:PHE:HB2	1.80	0.46
1:D:171:GLU:N	1:D:172:PRO:HD2	2.31	0.46
1:D:328:ILE:HG13	1:D:329:THR:HG23	1.98	0.46
1:A:29:ARG:HE	1:A:31:LEU:HD23	1.78	0.46
1:B:138:ILE:HG23	1:B:168:TRP:CD1	2.51	0.45
1:D:199:ALA:O	1:D:203:ALA:N	2.48	0.45
1:A:164:ILE:HG12	1:A:188:VAL:HB	1.98	0.45
1:C:31:LEU:HD22	1:C:295:THR:HG23	1.98	0.45
1:C:142:ILE:HD13	1:C:168:TRP:CZ3	2.52	0.45
1:D:263:LYS:HB2	1:D:266:ARG:NH1	2.31	0.45
1:A:29:ARG:HD3	1:A:31:LEU:HD21	1.98	0.45
1:A:29:ARG:NH1	1:A:50:MET:CE	2.79	0.45
1:B:227:GLU:HA	1:B:230:ARG:NH1	2.32	0.45
1:C:159:ARG:HG2	1:C:160:ILE:N	2.32	0.45
1:C:171:GLU:O	1:C:172:PRO:C	2.57	0.45
1:D:58:GLU:CB	1:D:98:MET:HE3	2.46	0.45
1:D:239:ASP:OD1	1:D:266:ARG:NH1	2.49	0.45
1:B:50:MET:CE	3:B:1100:SMG:CE	2.94	0.45
1:A:117:ARG:HE	1:A:121:ALA:CB	2.25	0.45
1:B:17:ALA:HA	1:B:18:PRO:HD3	1.83	0.45
1:C:72:ILE:HB	1:C:73:PRO:CD	2.47	0.45
1:D:356:LEU:O	1:D:356:LEU:HD12	2.16	0.45
1:A:28:VAL:HG12	1:A:29:ARG:H	1.81	0.45
1:D:3:LEU:HB3	4:D:1361:HOH:O	2.16	0.45
1:D:216:PRO:HB2	1:D:217:LEU:HD23	1.98	0.45
1:A:9:ARG:HH11	1:A:9:ARG:CG	2.30	0.45
1:A:239:ASP:OD1	1:A:266:ARG:NH1	2.46	0.45
1:B:202:LEU:C	1:B:204:ARG:N	2.72	0.45
1:C:364:VAL:HG12	1:C:365:TRP:N	2.31	0.45
1:B:113:ARG:HG2	1:B:345:PRO:HB2	1.97	0.45
1:D:334:LEU:CD2	1:D:337:GLY:HA2	2.47	0.45
1:A:350:ALA:HB1	1:A:351:PRO:HD2	1.98	0.45
1:B:46:GLU:N	1:B:105:MET:HE3	2.29	0.45
1:C:97:ARG:O	1:C:268:GLY:HA2	2.15	0.45
1:D:299:ARG:O	1:D:303:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB3	1:B:1:MET:HE2	1.61	0.45
1:B:32:LEU:HA	1:B:32:LEU:HD23	1.70	0.45
1:D:37:VAL:HG21	1:D:365:TRP:CH2	2.52	0.45
1:D:170:VAL:HG23	1:D:170:VAL:H	1.44	0.45
1:B:23:PHE:CE2	1:B:191:ASN:HB3	2.52	0.44
1:D:334:LEU:HD21	1:D:337:GLY:HA2	1.99	0.44
1:A:28:VAL:CG1	1:A:29:ARG:N	2.79	0.44
1:B:284:GLY:O	1:B:286:PRO:HD3	2.17	0.44
1:C:1:MET:HE1	1:C:107:VAL:O	2.16	0.44
1:D:2:LYS:CD	1:D:3:LEU:N	2.77	0.44
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.99	0.44
1:C:81:ILE:C	1:C:82:THR:CG2	2.91	0.44
1:C:352:ILE:HA	1:C:353:PRO:HD3	1.64	0.44
1:D:169:ASP:C	1:D:172:PRO:HD2	2.42	0.44
1:D:201:GLN:OE1	1:D:201:GLN:HA	2.17	0.44
1:D:258:GLN:O	1:D:286:PRO:HD2	2.18	0.44
1:D:299:ARG:HG2	1:D:332:PHE:CD1	2.53	0.44
1:A:170:VAL:CG2	1:A:204[B]:ARG:HB3	2.47	0.44
1:A:187:GLN:HB2	1:A:212:LEU:HD12	2.00	0.44
1:D:13:MET:HA	1:D:14:PRO:HD3	1.50	0.44
1:D:82:THR:O	1:D:83:ALA:C	2.60	0.44
1:D:274:ARG:HH11	1:D:274:ARG:HD2	1.66	0.44
1:A:33:LEU:O	1:A:34:LEU:HD23	2.16	0.44
1:C:351:PRO:CB	1:C:356:LEU:HD22	2.48	0.44
1:D:142:ILE:N	4:D:1381:HOH:O	2.38	0.44
1:D:211:LEU:O	1:D:212:LEU:HB3	2.18	0.44
1:B:137:GLY:HA2	1:B:163:LYS:HB2	2.00	0.44
1:B:141:THR:HB	1:B:143:PRO:HD2	1.99	0.44
1:B:261:ASN:C	1:B:261:ASN:OD1	2.61	0.44
1:A:159:ARG:HD3	4:A:1077:HOH:O	2.18	0.44
1:A:49:THR:HG22	1:A:58:GLU:HB3	2.00	0.43
1:A:152:TYR:CD2	1:A:157:TYR:CD1	3.06	0.43
1:A:293:ILE:N	3:A:1000:SMG:O62	2.44	0.43
1:C:277:HIS:CD2	1:C:310:ASN:HB3	2.53	0.43
1:D:216:PRO:HB2	1:D:217:LEU:CD2	2.48	0.43
1:D:351:PRO:O	1:D:353:PRO:HD3	2.18	0.43
1:A:1:MET:HE3	1:A:38:THR:HG21	2.00	0.43
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.79	0.43
1:A:245:ALA:HA	1:A:276:VAL:HG22	2.00	0.43
1:B:151:GLY:O	1:B:154:ASP:HB2	2.19	0.43
1:C:13:MET:HE2	1:C:324:TYR:CG	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:SER:HB2	4:C:1203:HOH:O	2.17	0.43
1:C:205:LEU:C	1:C:207:PRO:CD	2.87	0.43
1:D:363:LYS:NZ	1:D:363:LYS:CB	2.81	0.43
1:A:125:SER:OG	1:A:126:VAL:N	2.51	0.43
1:B:1:MET:SD	1:B:40:ALA:HB2	2.58	0.43
1:B:163:LYS:HZ1	3:B:1100:SMG:C2	2.32	0.43
1:C:264:PRO:HG3	1:C:305:LEU:CD2	2.48	0.43
1:A:35:ARG:CD	1:A:44:TRP:CZ2	2.93	0.43
1:B:277:HIS:CD2	1:B:310:ASN:HB3	2.54	0.43
1:C:29:ARG:NH2	1:C:50:MET:CE	2.82	0.43
1:D:8:LEU:HD11	1:D:34:LEU:HD22	1.98	0.43
1:D:112:LEU:HB3	1:D:117:ARG:O	2.19	0.43
1:D:356:LEU:O	1:D:359:VAL:CG2	2.66	0.43
1:A:38:THR:CB	1:A:39:PRO:HD2	2.48	0.43
1:A:189:ASP:HA	1:A:214:GLU:HB3	2.01	0.43
1:A:233:GLN:O	1:A:235:PRO:HD3	2.18	0.43
1:B:2:LYS:HE3	1:B:2:LYS:O	2.19	0.43
1:D:141:THR:CG2	1:D:143:PRO:CD	2.79	0.43
1:D:166:PRO:HD3	1:D:194:TYR:CZ	2.53	0.43
1:B:2:LYS:HE3	1:B:2:LYS:C	2.43	0.43
1:B:29:ARG:NE	1:B:31:LEU:HD21	2.34	0.43
1:B:153:LEU:HD23	1:B:153:LEU:HA	1.85	0.43
1:B:239:ASP:OD1	1:B:266:ARG:NH1	2.49	0.43
1:C:87:THR:N	1:C:88:PRO:HD2	2.34	0.43
1:D:139:MET:HG2	1:D:145:LEU:HB2	2.00	0.43
1:D:153:LEU:HA	1:D:153:LEU:HD23	1.73	0.43
1:D:227:GLU:HA	1:D:230:ARG:NH1	2.34	0.43
1:A:13:MET:HB3	1:A:324:TYR:CE2	2.54	0.43
1:A:29:ARG:NH1	1:A:292:MET:O	2.52	0.43
1:A:143:PRO:O	1:A:144:GLN:C	2.62	0.43
1:B:23:PHE:HE2	1:B:191:ASN:HB3	1.84	0.43
1:B:217:LEU:HD23	1:B:217:LEU:N	2.34	0.43
1:B:328:ILE:O	1:B:351:PRO:HA	2.18	0.43
1:C:9:ARG:HG2	1:C:360:THR:HG23	2.01	0.43
1:C:165:GLU:O	1:C:166:PRO:C	2.61	0.43
1:C:192:THR:HB	1:C:218:GLU:HA	1.99	0.43
1:D:11:VAL:HG13	1:D:359:VAL:HB	2.00	0.43
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.90	0.43
1:B:59:TYR:O	1:B:60:ASN:C	2.61	0.43
1:B:63:ALA:O	1:B:66:VAL:HG12	2.19	0.43
1:C:112:LEU:HB3	1:C:117:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:SER:N	1:D:37:VAL:O	2.49	0.43
1:A:4:SER:HB2	1:A:37:VAL:O	2.19	0.42
1:B:130:VAL:HA	1:B:131:PRO:HD3	1.91	0.42
1:B:194:TYR:CE2	1:B:202:LEU:HD21	2.54	0.42
1:C:29:ARG:NE	1:C:50:MET:HE2	2.33	0.42
1:A:288:TRP:HB3	1:A:313:LEU:HB2	2.00	0.42
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.76	0.42
1:B:355:LEU:HA	1:B:355:LEU:HD12	1.67	0.42
1:D:159:ARG:HA	1:D:185:LEU:HB2	2.01	0.42
1:A:159:ARG:HD2	1:A:187:GLN:OE1	2.19	0.42
1:C:271:LEU:HD23	1:C:271:LEU:HA	1.81	0.42
1:D:58:GLU:OE1	1:D:98:MET:CG	2.60	0.42
1:D:148:VAL:HG12	1:D:152:TYR:CD1	2.54	0.42
1:A:129:SER:HA	1:A:339:LEU:O	2.19	0.42
1:A:277:HIS:CD2	1:A:310:ASN:HB3	2.54	0.42
1:B:142:ILE:HD12	1:B:172:PRO:HA	2.01	0.42
1:B:192:THR:HB	1:B:218:GLU:HA	2.00	0.42
1:C:191:ASN:C	1:C:192:THR:HG23	2.44	0.42
1:C:321:ASP:HA	1:C:324:TYR:O	2.19	0.42
1:B:14:PRO:HA	1:B:28:VAL:HG22	2.00	0.42
1:B:141:THR:O	1:B:144:GLN:HB3	2.20	0.42
1:D:35:ARG:HG3	1:D:44:TRP:CZ2	2.53	0.42
1:D:85:LYS:O	1:D:88:PRO:HD2	2.19	0.42
1:C:316:ASP:HB3	3:C:1200:SMG:H42	2.01	0.42
1:D:38:THR:CB	1:D:39:PRO:HD2	2.19	0.42
1:D:66:VAL:O	1:D:70:TYR:N	2.48	0.42
1:D:142:ILE:N	1:D:143:PRO:HD2	2.35	0.42
1:A:58:GLU:HB2	1:A:98:MET:CE	2.49	0.42
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.67	0.42
1:A:171:GLU:O	1:A:174:ARG:HB3	2.20	0.42
1:B:358:GLU:O	1:B:358:GLU:CG	2.66	0.42
1:D:305:LEU:O	1:D:307:SER:N	2.52	0.42
1:B:132:CYS:SG	1:B:317:THR:O	2.78	0.42
1:C:293:ILE:HG13	3:C:1200:SMG:CE	2.50	0.42
1:A:25:THR:HG22	1:A:26:GLN:N	2.34	0.42
1:A:334:LEU:HD12	1:A:338:HIS:O	2.20	0.42
1:D:7:GLU:HB2	1:D:365:TRP:HE3	1.84	0.42
1:D:38:THR:CB	1:D:39:PRO:CD	2.82	0.42
1:D:163:LYS:HE3	1:D:189:ASP:HB3	2.02	0.42
1:D:217:LEU:HD23	1:D:217:LEU:N	2.35	0.42
1:A:277:HIS:NE2	1:A:310:ASN:N	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:C	1:A:297:LEU:N	2.77	0.41
1:A:352:ILE:HG22	1:A:355:LEU:H	1.84	0.41
1:C:75:LEU:CD1	1:C:103:LEU:CD1	2.93	0.41
1:D:23:PHE:CZ	3:D:1300:SMG:HG1	2.53	0.41
1:A:352:ILE:HG22	1:A:352:ILE:O	2.20	0.41
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.93	0.41
1:D:65:HIS:O	1:D:69:HIS:HD2	2.02	0.41
1:D:190:ALA:O	1:D:191:ASN:C	2.60	0.41
1:A:141:THR:OG1	1:A:144:GLN:CB	2.68	0.41
1:A:152:TYR:HD2	1:A:157:TYR:CD1	2.38	0.41
1:C:127:ARG:NH2	1:C:311:PHE:O	2.53	0.41
1:A:29:ARG:NH1	1:A:50:MET:HE3	2.35	0.41
1:B:205:LEU:C	1:B:207:PRO:CD	2.90	0.41
1:C:221:ASP:OD2	1:C:224:GLY:HA3	2.20	0.41
1:D:8:LEU:O	1:D:363:LYS:HA	2.20	0.41
1:A:113:ARG:HG3	1:A:346:GLY:HA3	2.01	0.41
1:A:239:ASP:CG	1:A:263:LYS:HE3	2.45	0.41
1:A:327:ASP:OD1	1:A:328:ILE:N	2.54	0.41
1:D:49:THR:HG22	1:D:98:MET:HE3	2.02	0.41
1:A:181:GLY:O	1:A:184:VAL:HG23	2.21	0.41
1:B:177:ARG:HA	1:B:177:ARG:HD3	1.69	0.41
1:B:296:GLY:HA3	1:B:329:THR:OG1	2.21	0.41
1:C:158:VAL:O	1:C:185:LEU:HD12	2.20	0.41
1:C:308:LEU:CB	1:C:309:PRO:CD	2.98	0.41
1:D:165:GLU:HG2	1:D:166:PRO:N	2.34	0.41
1:A:109:ASP:OD1	1:A:346:GLY:HA3	2.21	0.41
1:A:234:THR:HA	1:A:235:PRO:HD2	1.92	0.41
1:B:50:MET:SD	3:B:1100:SMG:HE1	2.58	0.41
1:B:127:ARG:HG3	4:B:1387:HOH:O	2.20	0.41
1:B:147:ASP:O	1:B:150:GLY:N	2.54	0.41
1:C:244:SER:O	1:C:247:ALA:HB3	2.20	0.41
1:D:82:THR:HG22	1:D:84:ALA:N	2.35	0.41
1:A:130:VAL:HA	1:A:131:PRO:HD3	1.92	0.41
1:C:72:ILE:N	1:C:73:PRO:HD2	2.36	0.41
1:D:3:LEU:CD2	1:D:76:LEU:HD23	2.50	0.41
1:B:308:LEU:HA	1:B:309:PRO:HD3	1.96	0.41
1:C:13:MET:HA	1:C:14:PRO:HD3	1.91	0.41
1:C:72:ILE:CB	1:C:73:PRO:CD	2.99	0.41
1:C:103:LEU:O	1:C:104:GLU:C	2.62	0.41
1:C:355:LEU:HA	1:C:355:LEU:HD23	1.81	0.41
1:D:21:THR:CG2	1:D:23:PHE:CD2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:VAL:HG21	1:D:365:TRP:CZ3	2.56	0.41
1:D:68[B]:ARG:NH2	1:D:364:VAL:HG11	2.36	0.41
1:D:177:ARG:HD3	1:D:177:ARG:HA	1.51	0.41
1:D:354:GLU:HG3	1:D:355:LEU:HD13	2.03	0.41
1:A:192:THR:HG22	1:A:215:GLN:CG	2.51	0.41
1:D:200:PRO:O	1:D:203:ALA:HB3	2.21	0.41
1:D:304:ALA:O	1:D:305:LEU:C	2.64	0.41
1:A:177:ARG:HD3	1:A:177:ARG:HA	1.87	0.40
1:C:163:LYS:HA	1:C:163:LYS:HD2	1.50	0.40
1:D:83:ALA:CB	1:D:108:LEU:HD13	2.50	0.40
1:D:174:ARG:O	1:D:178:GLU:HB2	2.21	0.40
1:D:177:ARG:HD2	1:D:181:GLY:O	2.20	0.40
1:A:149:VAL:O	1:A:150:GLY:C	2.64	0.40
1:A:277:HIS:NE2	1:A:310:ASN:CB	2.84	0.40
1:B:210:LEU:HA	1:B:210:LEU:HD23	1.73	0.40
1:D:7:GLU:HA	1:D:364:VAL:O	2.22	0.40
1:D:271:LEU:O	1:D:272:GLU:C	2.62	0.40
1:A:48:VAL:HG22	4:A:1057:HOH:O	2.21	0.40
1:A:55:TYR:OH	1:A:266:ARG:HD3	2.21	0.40
1:A:159:ARG:HD2	4:A:1077:HOH:O	2.20	0.40
1:B:36:ALA:O	1:B:42:GLU:HA	2.21	0.40
1:B:321:ASP:HA	1:B:324:TYR:O	2.22	0.40
1:D:350:ALA:HB1	1:D:351:PRO:CD	2.51	0.40
1:A:201:GLN:OE1	1:A:204[A]:ARG:HD2	2.22	0.40
1:A:352:ILE:O	1:A:355:LEU:HB2	2.21	0.40
1:C:159:ARG:CD	4:C:1296:HOH:O	2.62	0.40
1:C:185:LEU:HB3	1:C:211:LEU:HD11	2.02	0.40
1:D:293:ILE:O	1:D:293:ILE:HG22	2.20	0.40
1:A:23:PHE:CZ	3:A:1000:SMG:HE2	2.57	0.40
1:B:142:ILE:HG22	1:B:143:PRO:N	2.37	0.40
1:D:171:GLU:OE1	1:D:171:GLU:HA	2.21	0.40

All (1) 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:274[A]:ARG:NH2	1:D:278:ASP:OD2[17_555]	1.80	0.40

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	370/368 (100%)	348 (94%)	22 (6%)	0	100	100
1	B	369/368 (100%)	353 (96%)	16 (4%)	0	100	100
1	C	367/368 (100%)	345 (94%)	21 (6%)	1 (0%)	36	36
1	D	367/368 (100%)	326 (89%)	37 (10%)	4 (1%)	11	8
All	All	1473/1472 (100%)	1372 (93%)	96 (6%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	ALA
1	D	306	ALA
1	D	149	VAL
1	D	142	ILE
1	C	353	PRO

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	295/291 (101%)	259 (88%)	36 (12%)	5	2
1	B	294/291 (101%)	267 (91%)	27 (9%)	8	6
1	C	292/291 (100%)	267 (91%)	25 (9%)	10	7
1	D	292/291 (100%)	252 (86%)	40 (14%)	3	2
All	All	1173/1164 (101%)	1045 (89%)	128 (11%)	6	4

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	8	LEU
1	A	9	ARG
1	A	13	MET
1	A	15	LEU
1	A	16	VAL
1	A	29	ARG
1	A	31	LEU
1	A	34	LEU
1	A	68[A]	ARG
1	A	68[B]	ARG
1	A	79	GLU
1	A	80	ASP
1	A	98	MET
1	A	119	PHE
1	A	127	ARG
1	A	129	SER
1	A	142	ILE
1	A	159	ARG
1	A	169	ASP
1	A	171	GLU
1	A	177	ARG
1	A	179	ARG
1	A	184	VAL
1	A	192	THR
1	A	217	LEU
1	A	227	GLU
1	A	236	ILE
1	A	261	ASN
1	A	262	ILE
1	A	321	ASP
1	A	339	LEU
1	A	343	THR
1	A	352	ILE
1	A	354	GLU
1	A	356	LEU
1	B	1	MET
1	B	2	LYS
1	B	9	ARG
1	B	31	LEU
1	B	32	LEU
1	B	34	LEU

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Mol	Chain	Res	Type
1	B	42	GLU
1	B	68	ARG
1	B	79[A]	GLU
1	B	79[B]	GLU
1	B	80	ASP
1	B	92	LYS
1	B	105	MET
1	B	116	GLU
1	B	127	ARG
1	B	159	ARG
1	B	170	VAL
1	B	177	ARG
1	B	179	ARG
1	B	213	ILE
1	B	227	GLU
1	B	233	GLN
1	B	274	ARG
1	B	339	LEU
1	B	355	LEU
1	B	363	LYS
1	B	364	VAL
1	C	8	LEU
1	C	9	ARG
1	C	26	GLN
1	C	31	LEU
1	C	34	LEU
1	C	80	ASP
1	C	82	THR
1	C	103	LEU
1	C	119	PHE
1	C	139	MET
1	C	140	ASP
1	C	142	ILE
1	C	144	GLN
1	C	145	LEU
1	C	159	ARG
1	C	163	LYS
1	C	169	ASP
1	C	177	ARG
1	C	204	ARG
1	C	213	ILE
1	C	217	LEU

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Mol	Chain	Res	Type
1	C	227	GLU
1	C	232	ILE
1	C	330	GLU
1	C	343	THR
1	D	2	LYS
1	D	7	GLU
1	D	8	LEU
1	D	9	ARG
1	D	10	ARG
1	D	12	GLN
1	D	13	MET
1	D	20	ARG
1	D	27	SER
1	D	29	ARG
1	D	35	ARG
1	D	42	GLU
1	D	64	GLU
1	D	68[A]	ARG
1	D	68[B]	ARG
1	D	79	GLU
1	D	92	LYS
1	D	98	MET
1	D	116	GLU
1	D	119	PHE
1	D	125	SER
1	D	127	ARG
1	D	139	MET
1	D	155	GLU
1	D	159	ARG
1	D	163	LYS
1	D	165	GLU
1	D	169	ASP
1	D	177	ARG
1	D	213	ILE
1	D	217	LEU
1	D	236	ILE
1	D	261	ASN
1	D	274	ARG
1	D	339	LEU
1	D	355	LEU
1	D	361	THR
1	D	363	LYS

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Mol	Chain	Res	Type
1	D	364	VAL
1	D	368	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	258	GLN
1	B	12	GLN
1	B	69	HIS
1	B	233	GLN
1	B	258	GLN
1	C	12	GLN
1	C	26	GLN
1	D	69	HIS
1	D	191	ASN
1	D	258	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	SMG	C	1200	2	15,15,15	1.16	1 (6%)	18,18,18	2.44	6 (33%)
3	SMG	A	1000	2	15,15,15	1.12	1 (6%)	18,18,18	1.41	2 (11%)
3	SMG	B	1100	2	15,15,15	1.10	1 (6%)	18,18,18	1.69	3 (16%)
3	SMG	D	1300	2	15,15,15	1.18	1 (6%)	18,18,18	2.08	3 (16%)

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	SMG	C	1200	2	-	4/17/17/17	-
3	SMG	A	1000	2	-	6/17/17/17	-
3	SMG	B	1100	2	-	4/17/17/17	-
3	SMG	D	1300	2	-	6/17/17/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1200	SMG	C4-C3	-2.90	1.45	1.51
3	D	1300	SMG	C4-C3	-2.83	1.45	1.51
3	A	1000	SMG	C4-C3	-2.65	1.46	1.51
3	B	1100	SMG	C4-C3	-2.64	1.46	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1200	SMG	CB-C1-N1	-7.42	96.21	110.91
3	D	1300	SMG	CB-C1-N1	-6.98	97.10	110.91
3	B	1100	SMG	C4-C3-N1	3.95	122.83	115.86
3	C	1200	SMG	CB-C1-C2	-3.89	101.11	110.35
3	C	1200	SMG	C4-C5-C6	-3.68	103.92	113.67
3	A	1000	SMG	CE-SD-CG	2.78	114.72	100.32
3	C	1200	SMG	O12-C2-O11	-2.75	117.84	124.08
3	D	1300	SMG	C4-C5-C6	-2.69	106.52	113.67
3	B	1100	SMG	O31-C3-N1	-2.68	118.42	122.95
3	A	1000	SMG	C4-C3-N1	2.56	120.37	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1100	SMG	C1-N1-C3	-2.45	115.54	121.68
3	D	1300	SMG	CG-CB-C1	-2.32	105.61	112.83
3	C	1200	SMG	O31-C3-N1	-2.06	119.46	122.95
3	C	1200	SMG	CB-CG-SD	-2.00	100.60	113.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	SMG	N1-C1-CB-CG
3	C	1200	SMG	N1-C1-CB-CG
3	C	1200	SMG	C2-C1-CB-CG
3	D	1300	SMG	N1-C1-CB-CG
3	B	1100	SMG	C1-CB-CG-SD
3	A	1000	SMG	C1-CB-CG-SD
3	D	1300	SMG	C1-CB-CG-SD
3	A	1000	SMG	CB-CG-SD-CE
3	A	1000	SMG	C2-C1-CB-CG
3	D	1300	SMG	C2-C1-CB-CG
3	B	1100	SMG	CB-CG-SD-CE
3	D	1300	SMG	CB-CG-SD-CE
3	D	1300	SMG	C4-C5-C6-O62
3	D	1300	SMG	C4-C5-C6-O61
3	A	1000	SMG	C4-C5-C6-O62
3	B	1100	SMG	C4-C5-C6-O61
3	B	1100	SMG	C4-C5-C6-O62
3	A	1000	SMG	C4-C5-C6-O61
3	C	1200	SMG	C4-C5-C6-O62
3	C	1200	SMG	C4-C5-C6-O61

There are no ring outliers.

4 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1200	SMG	13	0
3	A	1000	SMG	9	0
3	B	1100	SMG	9	0
3	D	1300	SMG	11	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	367/368 (99%)	-0.12	1 (0%) 90 91	23, 51, 84, 98	5 (1%)
1	B	368/368 (100%)	-0.56	3 (0%) 82 84	22, 38, 67, 100	3 (0%)
1	C	367/368 (99%)	-0.18	3 (0%) 82 84	27, 47, 80, 100	2 (0%)
1	D	368/368 (100%)	0.30	12 (3%) 49 51	27, 58, 91, 100	1 (0%)
All	All	1470/1472 (99%)	-0.14	19 (1%) 75 77	22, 48, 84, 100	11 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	367	GLY	3.2
1	D	184	VAL	2.8
1	B	1	MET	2.8
1	D	39	PRO	2.5
1	C	23	PHE	2.5
1	D	44	TRP	2.4
1	B	23	PHE	2.3
1	D	1	MET	2.3
1	D	324	TYR	2.3
1	B	220[A]	GLU	2.2
1	C	41	GLY	2.1
1	D	362	ALA	2.1
1	D	368	SER	2.1
1	A	274[A]	ARG	2.1
1	D	21	THR	2.1
1	D	68[A]	ARG	2.1
1	D	352	ILE	2.1
1	D	126	VAL	2.0
1	D	354	GLU	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 [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($\text{\AA}^2$)	Q<0.9
3	SMG	D	1300	16/16	0.90	0.14	37,78,100,100	0
3	SMG	C	1200	16/16	0.92	0.12	23,54,100,100	0
3	SMG	A	1000	16/16	0.94	0.10	38,57,85,100	0
2	MG	A	1001	1/1	0.94	0.06	47,47,47,47	0
2	MG	D	1301	1/1	0.94	0.06	66,66,66,66	0
3	SMG	B	1100	16/16	0.95	0.10	31,50,100,100	0
2	MG	C	1201	1/1	0.97	0.05	47,47,47,47	0
2	MG	B	1101	1/1	0.98	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.