



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:08 AM UTC

PDB ID : 1SJA / pdb_00001sja
Title : X-ray structure of o-Succinylbenzoate Synthase complexed with N-acetylmethionine
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 : 2.30 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

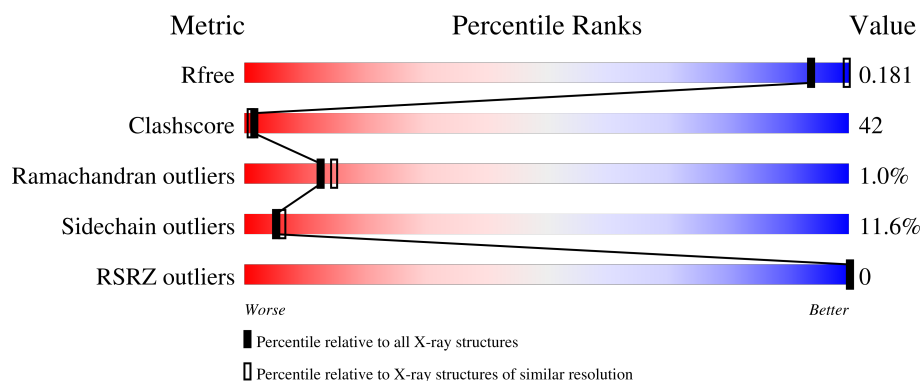
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

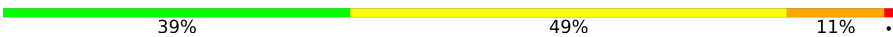
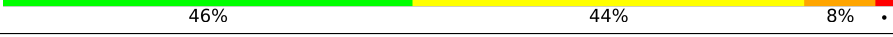
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	
1	C	368	
1	D	368	

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	AME	A	600	-	X	X	-
3	AME	B	700	-	X	X	-
3	AME	C	800	-	X	X	-
3	AME	D	900	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11704 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.

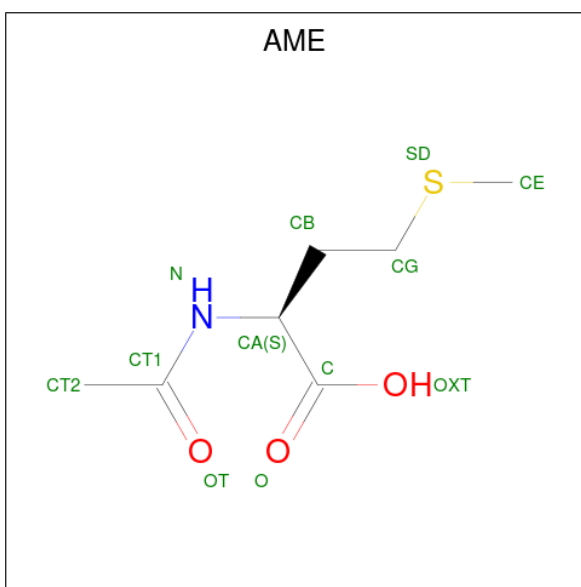
- Molecule 1 is a protein called N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	2	0
			2785	1769	487	517	12			
1	B	368	Total	C	N	O	S	0	3	0
			2796	1775	487	522	12			
1	C	368	Total	C	N	O	S	0	0	0
			2771	1761	481	517	12			
1	D	368	Total	C	N	O	S	0	1	0
			2778	1765	484	517	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-ACETYLMETHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 12	C 7	N 1	O 3	S 1	0	0
3	B	1	Total 12	C 7	N 1	O 3	S 1	0	0
3	C	1	Total 12	C 7	N 1	O 3	S 1	0	0
3	D	1	Total 12	C 7	N 1	O 3	S 1	0	0

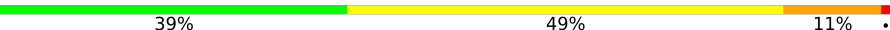
- Molecule 4 is water.

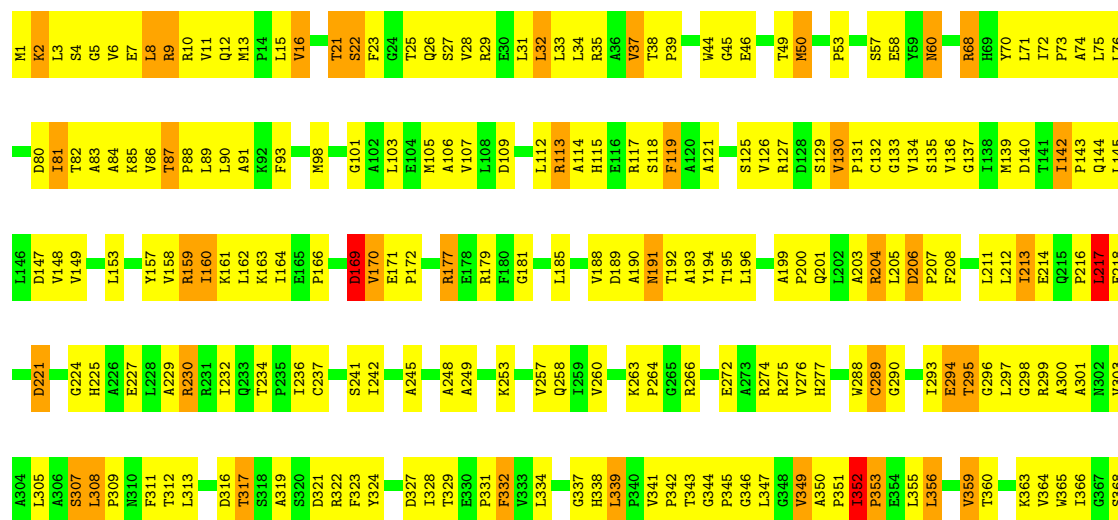
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	0	0
4	B	153	Total O 153 153	0	0
4	C	117	Total O 117 117	0	0
4	D	117	Total O 117 117	0	0

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.

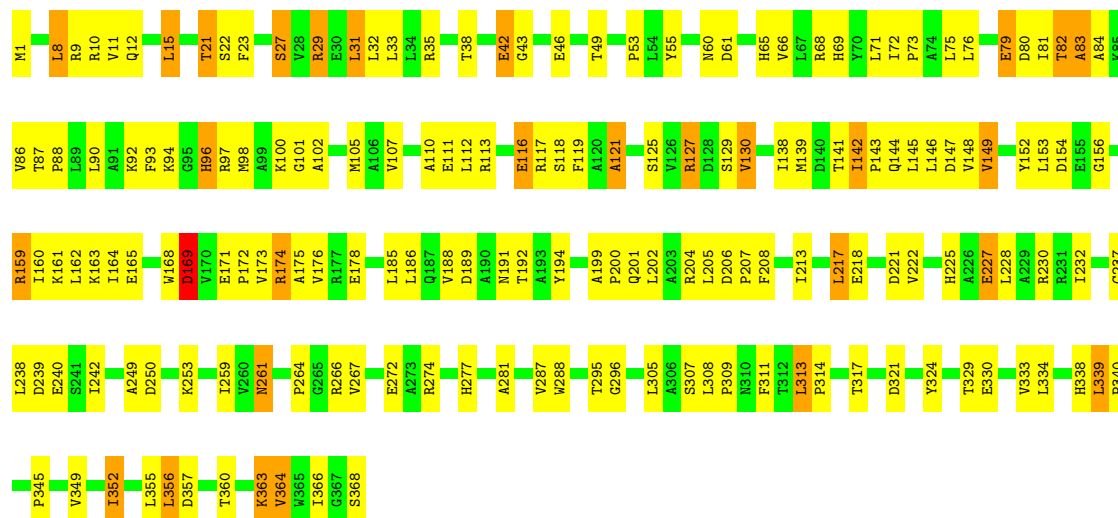
• Molecule 1: N-acylamino acid racemase

Chain A: 

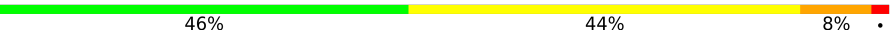


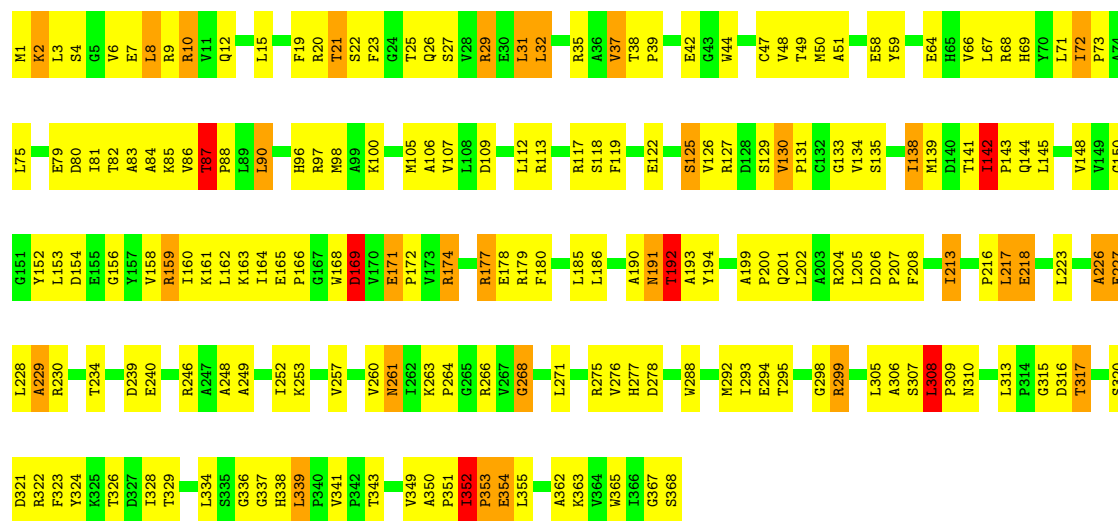
• Molecule 1: N-acylamino acid racemase

Chain B: 



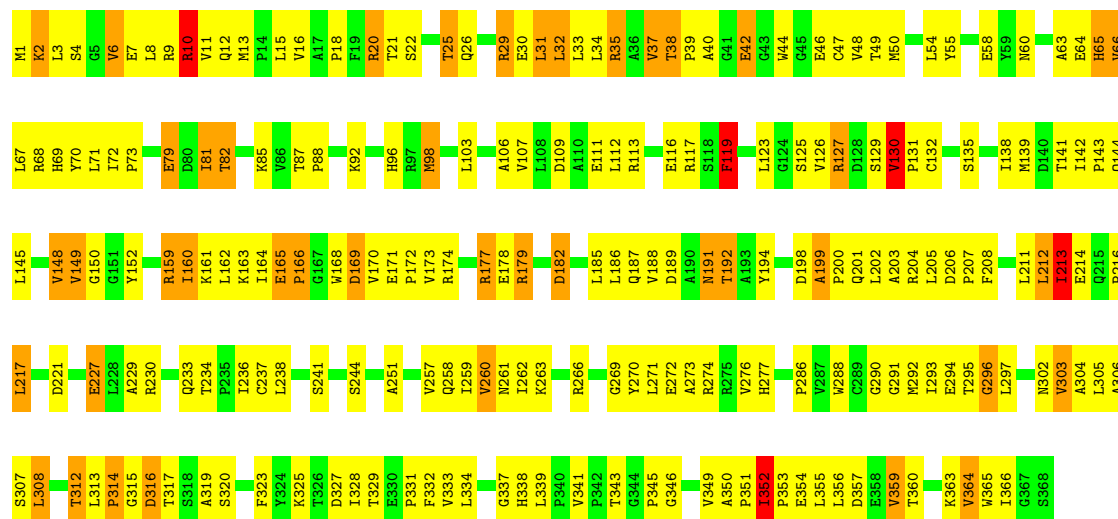
• Molecule 1: N-acylamino acid racemase

Chain C:  46% 44% 8% .



• Molecule 1: N-acylamino acid racemase

Chain D:  40% 47% 12% .



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	215.30Å 215.30Å 259.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 93.6 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.24Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.211 , 0.280 0.177 , 0.181	Depositor DCC
R_{free} test set	10587 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 164.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.217 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 0.210 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.206 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	0.90	EDS
Total number of atoms	11704	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 1.30% 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: AME, 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	1.12	0/2849	1.58	41/3878 (1.1%)
1	B	1.22	1/2868 (0.0%)	1.60	21/3902 (0.5%)
1	C	1.22	2/2827 (0.1%)	1.68	36/3850 (0.9%)
1	D	1.14	2/2838 (0.1%)	1.66	46/3864 (1.2%)
All	All	1.17	5/11382 (0.0%)	1.63	144/15494 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	ILE	CA-CB	-6.65	1.50	1.54
1	D	70	TYR	CA-C	-5.87	1.46	1.52
1	C	169	ASP	CA-C	-5.87	1.49	1.52
1	B	149	VAL	N-CA	-5.39	1.40	1.46
1	D	165	GLU	CD-OE2	5.25	1.35	1.25

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	ILE	N-CA-CB	12.80	118.56	110.50
1	B	314	PRO	CA-C-N	-8.97	114.44	122.43
1	B	314	PRO	C-N-CA	-8.97	114.44	122.43
1	A	294	GLU	N-CA-C	8.65	121.05	110.41
1	C	72	ILE	CA-C-O	8.35	124.28	118.69
1	B	96	HIS	CA-CB-CG	-8.20	105.60	113.80
1	A	169	ASP	CA-CB-CG	8.06	120.66	112.60
1	C	169	ASP	O-C-N	7.82	126.62	120.83
1	C	352	ILE	CA-C-N	7.78	129.56	119.84
1	C	352	ILE	C-N-CA	7.78	129.56	119.84
1	D	65	HIS	CA-CB-CG	-7.49	106.31	113.80
1	A	352	ILE	CA-C-N	7.47	129.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ILE	C-N-CA	7.47	129.18	119.84
1	D	208	PHE	N-CA-C	7.29	121.28	112.38
1	A	71	LEU	N-CA-C	7.12	118.94	111.03
1	C	80	ASP	CA-CB-CG	-7.12	105.48	112.60
1	D	259	ILE	CA-C-N	-7.10	113.13	122.99
1	D	259	ILE	C-N-CA	-7.10	113.13	122.99
1	D	316	ASP	CA-CB-CG	-7.03	105.58	112.60
1	B	169	ASP	CA-CB-CG	6.89	119.49	112.60
1	C	171	GLU	O-C-N	6.80	125.75	120.38
1	D	333	VAL	N-CA-C	6.69	117.50	107.80
1	D	130	VAL	CA-C-N	6.64	130.23	120.46
1	D	130	VAL	C-N-CA	6.64	130.23	120.46
1	B	121	ALA	CA-C-N	6.50	129.22	120.65
1	B	121	ALA	C-N-CA	6.50	129.22	120.65
1	D	160	ILE	N-CA-C	6.44	117.16	107.75
1	A	221	ASP	CA-CB-CG	-6.44	106.16	112.60
1	C	133	GLY	CA-C-N	-6.43	112.97	122.23
1	C	133	GLY	C-N-CA	-6.43	112.97	122.23
1	A	169	ASP	O-C-N	6.31	126.39	120.71
1	D	81	ILE	N-CA-C	6.27	117.05	107.77
1	C	164	ILE	CB-CA-C	6.27	119.93	110.90
1	C	37	VAL	N-CA-C	6.21	116.96	107.77
1	A	160	ILE	N-CA-C	6.20	116.85	108.17
1	A	308	LEU	CA-C-N	6.20	126.11	119.28
1	A	308	LEU	C-N-CA	6.20	126.11	119.28
1	D	221	ASP	N-CA-C	6.20	118.46	110.65
1	A	53	PRO	CB-CA-C	-6.18	104.79	112.89
1	B	221	ASP	N-CA-C	6.12	118.80	109.62
1	A	170	VAL	N-CA-C	6.09	116.76	110.36
1	C	29	ARG	N-CA-C	6.09	118.62	108.20
1	C	208	PHE	N-CA-C	6.09	120.44	113.19
1	A	130	VAL	CA-C-N	6.08	126.29	119.90
1	A	130	VAL	C-N-CA	6.08	126.29	119.90
1	B	208	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	193	ALA	N-CA-C	6.02	120.09	112.87
1	A	206	ASP	CA-C-N	6.00	125.55	119.19
1	A	206	ASP	C-N-CA	6.00	125.55	119.19
1	D	352	ILE	CA-C-N	5.99	127.32	119.84
1	D	352	ILE	C-N-CA	5.99	127.32	119.84
1	C	72	ILE	CA-CB-CG2	-5.98	100.33	110.50
1	B	165	GLU	N-CA-CB	-5.97	105.66	111.27
1	A	37	VAL	N-CA-C	5.96	116.44	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	PHE	CA-CB-CG	-5.89	107.91	113.80
1	D	162	LEU	CB-CA-C	-5.87	101.22	110.79
1	B	330	GLU	N-CA-C	-5.86	102.20	109.64
1	D	148	VAL	N-CA-CB	-5.84	104.49	110.62
1	D	308	LEU	CA-C-N	5.81	125.28	119.24
1	D	308	LEU	C-N-CA	5.81	125.28	119.24
1	A	93	PHE	CA-CB-CG	-5.80	108.00	113.80
1	D	37	VAL	N-CA-CB	5.79	119.20	111.90
1	D	20	ARG	N-CA-C	5.74	118.09	108.73
1	C	169	ASP	CA-CB-CG	5.74	118.34	112.60
1	D	25	THR	N-CA-CB	5.74	118.43	110.17
1	C	69	HIS	N-CA-C	5.73	118.47	111.82
1	D	312	THR	CA-CB-CG2	5.71	120.21	110.50
1	A	241	SER	CA-C-N	-5.68	116.34	122.59
1	A	241	SER	C-N-CA	-5.68	116.34	122.59
1	C	308	LEU	CA-C-N	5.67	125.52	119.28
1	C	308	LEU	C-N-CA	5.67	125.52	119.28
1	D	54	LEU	N-CA-C	5.67	120.21	113.12
1	C	260	VAL	N-CA-C	5.66	116.04	108.11
1	C	191	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	331	PRO	N-CA-CB	5.62	109.15	103.25
1	D	69	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	169	ASP	CA-C-N	5.59	127.81	120.60
1	A	169	ASP	C-N-CA	5.59	127.81	120.60
1	D	119	PHE	N-CA-C	-5.59	105.09	111.07
1	B	83	ALA	N-CA-C	-5.55	105.22	111.28
1	A	53	PRO	N-CA-CB	5.55	106.14	102.25
1	A	234	THR	CA-C-O	5.55	124.42	119.59
1	A	87	THR	CA-C-N	5.54	125.21	119.56
1	A	87	THR	C-N-CA	5.54	125.21	119.56
1	C	320	SER	N-CA-C	5.52	117.30	111.28
1	C	341	VAL	N-CA-CB	-5.50	103.51	111.21
1	C	107	VAL	N-CA-C	5.50	115.70	110.42
1	D	96	HIS	CA-CB-CG	-5.48	108.32	113.80
1	A	166	PRO	N-CA-CB	5.45	108.10	103.19
1	D	109	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	242	ILE	CB-CA-C	-5.45	105.70	112.45
1	B	71	LEU	N-CA-C	5.44	117.02	111.14
1	C	226	ALA	CA-C-N	5.44	127.51	120.44
1	C	226	ALA	C-N-CA	5.44	127.51	120.44
1	D	199	ALA	CA-C-O	5.41	123.61	118.63
1	A	260	VAL	N-CA-C	5.40	115.67	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	PHE	N-CA-C	5.39	119.48	113.01
1	A	217	LEU	N-CA-C	5.38	118.05	109.81
1	C	87	THR	O-C-N	5.38	124.63	120.38
1	D	213	ILE	CB-CA-C	5.36	118.39	110.77
1	A	81	ILE	N-CA-C	5.36	115.62	108.11
1	D	221	ASP	CA-CB-CG	-5.34	107.26	112.60
1	D	35	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	C	131	PRO	N-CA-CB	5.32	108.06	103.27
1	D	179	ARG	N-CA-C	5.32	117.16	111.36
1	C	71	LEU	N-CA-C	5.32	116.93	111.03
1	C	19	PHE	CA-CB-CG	-5.30	108.50	113.80
1	C	177	ARG	CA-C-O	5.30	126.17	120.55
1	B	333	VAL	N-CA-C	5.30	115.61	107.77
1	A	359	VAL	N-CA-CB	-5.28	102.51	111.23
1	D	345	PRO	N-CA-CB	5.28	107.94	103.35
1	D	166	PRO	N-CA-CB	5.27	107.93	103.19
1	D	38	THR	CA-C-N	5.27	124.45	118.97
1	D	38	THR	C-N-CA	5.27	124.45	118.97
1	B	352	ILE	CA-C-N	5.26	126.42	119.84
1	B	352	ILE	C-N-CA	5.26	126.42	119.84
1	A	303	VAL	N-CA-C	-5.23	105.44	110.72
1	C	268	GLY	CA-C-N	-5.22	115.50	122.54
1	C	268	GLY	C-N-CA	-5.22	115.50	122.54
1	A	332	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	242	ILE	N-CA-C	5.20	114.69	106.32
1	D	55	TYR	N-CA-C	-5.19	105.30	111.69
1	B	173	VAL	CB-CA-C	-5.18	105.30	112.24
1	C	229	ALA	CA-C-N	5.17	127.63	120.29
1	C	229	ALA	C-N-CA	5.17	127.63	120.29
1	C	72	ILE	O-C-N	5.15	123.72	120.42
1	D	10	ARG	N-CA-CB	5.15	119.79	110.83
1	A	60	ASN	CA-CB-CG	5.14	117.74	112.60
1	D	182	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	294	GLU	N-CA-C	5.11	118.09	110.52
1	B	191	ASN	N-CA-CB	5.09	119.23	111.70
1	A	157	TYR	CB-CA-C	5.07	117.45	109.84
1	A	208	PHE	N-CA-C	5.07	118.73	112.54
1	D	331	PRO	N-CA-CB	5.06	110.09	103.42
1	A	300	ALA	N-CA-C	5.05	116.59	111.14
1	D	6	VAL	CA-C-N	-5.04	116.07	122.77
1	D	6	VAL	C-N-CA	-5.04	116.07	122.77
1	D	296	GLY	N-CA-C	-5.04	109.07	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	PRO	N-CA-CB	5.03	107.78	103.36
1	B	130	VAL	CA-C-N	5.01	124.77	119.76
1	B	130	VAL	C-N-CA	5.01	124.77	119.76
1	D	262	ILE	N-CA-C	5.01	115.31	107.99
1	B	349	VAL	CB-CA-C	-5.01	101.72	110.38
1	D	38	THR	O-C-N	5.00	125.75	120.99

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	2785	0	2828	275	0
1	B	2796	0	2834	205	0
1	C	2771	0	2810	223	0
1	D	2778	0	2819	237	2
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	12	0	12	12	0
3	B	12	0	12	8	0
3	C	12	0	12	16	0
3	D	12	0	12	12	0
4	A	135	0	0	18	0
4	B	153	0	0	12	0
4	C	117	0	0	12	0
4	D	117	0	0	17	0
All	All	11704	0	11339	939	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 42.

All (939) 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:117:ARG:NH1	1:A:121:ALA:HB1	1.41	1.34
1:A:58:GLU:HB2	1:A:98:MET:CE	1.67	1.23
1:C:38:THR:HB	1:C:39:PRO:HD2	1.17	1.15
1:C:35:ARG:NH1	1:C:42:GLU:OE2	1.80	1.14
1:C:141:THR:CG2	1:C:143:PRO:HD2	1.76	1.13
1:B:10:ARG:NH2	1:B:61:ASP:OD1	1.80	1.13
1:A:58:GLU:HB2	1:A:98:MET:HE2	1.27	1.09
1:B:127[A]:ARG:HG2	1:B:127[A]:ARG:HH11	1.17	1.08
1:C:141:THR:HG22	1:C:143:PRO:CD	1.83	1.07
1:C:49:THR:HG22	1:C:98:MET:HE3	1.10	1.07
1:A:117:ARG:HH11	1:A:121:ALA:CB	1.69	1.06
1:B:164:ILE:HD13	1:B:188:VAL:HG11	1.35	1.06
1:D:127[B]:ARG:NH2	1:D:308:LEU:O	1.87	1.06
1:C:67:LEU:O	1:C:72:ILE:HG13	1.54	1.05
1:D:29:ARG:HD3	1:D:31:LEU:HD23	1.35	1.05
1:A:21:THR:HG22	1:A:23:PHE:H	1.23	1.02
1:D:33:LEU:O	1:D:34:LEU:HD23	1.59	1.02
1:C:49:THR:HG22	1:C:98:MET:CE	1.89	1.02
1:D:163:LYS:NZ	3:D:900:AME:HN1	1.58	1.01
1:A:12:GLN:O	1:A:359:VAL:HG22	1.61	1.01
1:A:135:SER:CB	3:A:600:AME:HT23	1.91	1.01
1:C:135:SER:CB	3:C:800:AME:CT2	2.39	1.00
1:D:272:GLU:N	4:D:940:HOH:O	1.95	1.00
1:C:38:THR:HB	1:C:39:PRO:CD	1.92	1.00
1:C:58:GLU:HB2	1:C:98:MET:HE2	1.43	0.99
1:D:60:ASN:HB2	4:D:920:HOH:O	1.64	0.97
1:A:82:THR:HG22	1:A:84:ALA:H	1.26	0.97
1:C:135:SER:CB	3:C:800:AME:HT23	1.93	0.96
1:A:352:ILE:HG22	1:A:355:LEU:HG	1.48	0.95
1:A:117:ARG:NH1	1:A:121:ALA:CB	2.28	0.95
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.27	0.94
1:C:159:ARG:NH2	1:C:316:ASP:OD1	2.01	0.93
1:A:87:THR:HB	1:A:88:PRO:HD3	1.49	0.93
1:D:58:GLU:OE1	1:D:98:MET:HG3	1.68	0.93
1:A:21:THR:HG21	1:A:23:PHE:CE1	2.04	0.93
1:A:117:ARG:HH11	1:A:121:ALA:HB1	1.01	0.93
1:B:1:MET:HE2	1:B:38:THR:HG21	1.50	0.92
1:C:35:ARG:HD3	1:C:44:TRP:CZ2	2.03	0.92
1:D:206:ASP:HB2	1:D:207:PRO:HD3	1.48	0.92
1:A:1:MET:HE3	1:A:38:THR:HG21	1.51	0.92
1:B:82:THR:HG22	1:B:84:ALA:H	1.34	0.92
1:C:10:ARG:HG3	1:C:362:ALA:HB3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:38:THR:HG21	2.01	0.91
1:C:21:THR:HG21	1:C:23:PHE:CE1	2.06	0.91
1:C:205:LEU:C	1:C:207:PRO:HD2	1.97	0.90
1:B:49:THR:HG22	1:B:98:MET:CE	2.01	0.90
1:A:58:GLU:CB	1:A:98:MET:CE	2.49	0.90
1:D:29:ARG:HD3	1:D:31:LEU:CD2	2.02	0.89
1:A:21:THR:HG21	1:A:23:PHE:CD1	2.08	0.89
1:C:248:ALA:O	1:C:252:ILE:HG13	1.73	0.89
1:C:125:SER:HB2	1:C:307:SER:OG	1.73	0.89
1:D:216:PRO:C	1:D:217:LEU:HD23	1.98	0.89
1:A:329:THR:HG22	1:A:350:ALA:O	1.72	0.89
1:C:58:GLU:HB2	1:C:98:MET:CE	2.02	0.88
1:C:135:SER:HB3	3:C:800:AME:CT2	2.01	0.88
1:C:139:MET:HB2	1:C:168:TRP:CZ2	2.08	0.88
1:D:21:THR:HG22	1:D:22:SER:N	1.86	0.88
1:D:211:LEU:O	1:D:212:LEU:HB3	1.69	0.88
1:C:141:THR:HG22	1:C:143:PRO:HD2	0.91	0.88
1:C:352:ILE:HB	1:C:355:LEU:HD12	1.55	0.88
1:A:49:THR:HG22	1:A:98:MET:HE3	1.56	0.88
1:B:82:THR:HG22	1:B:84:ALA:N	1.89	0.88
1:C:49:THR:CG2	1:C:98:MET:HE3	2.00	0.88
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.53	0.87
1:A:204[A]:ARG:HG2	1:A:204[A]:ARG:HH11	1.37	0.87
1:B:15:LEU:HB2	1:B:27:SER:O	1.75	0.87
1:C:135:SER:OG	3:C:800:AME:HT23	1.75	0.87
1:B:49:THR:CG2	1:B:98:MET:CE	2.52	0.87
1:B:21:THR:HG22	1:B:23:PHE:H	1.39	0.86
1:D:159:ARG:HD2	4:D:963:HOH:O	1.74	0.86
1:D:206:ASP:N	1:D:207:PRO:HD2	1.89	0.86
1:A:68[A]:ARG:HG2	1:A:68[A]:ARG:HH11	1.39	0.85
1:C:213:ILE:HG22	1:C:234:THR:HG22	1.57	0.85
1:A:159:ARG:HD2	4:A:666:HOH:O	1.76	0.85
1:C:206:ASP:N	1:C:207:PRO:CD	2.40	0.84
1:A:135:SER:CB	3:A:600:AME:CT2	2.56	0.84
1:C:58:GLU:CB	1:C:98:MET:HE2	2.08	0.84
1:D:44:TRP:O	1:D:106:ALA:HA	1.77	0.84
1:D:21:THR:HG22	1:D:22:SER:H	1.43	0.83
1:A:206:ASP:HB2	1:A:207:PRO:HD3	1.58	0.83
1:B:21:THR:HG21	1:B:23:PHE:CE1	2.13	0.83
1:A:139:MET:HG3	1:A:145:LEU:HA	1.59	0.83
1:D:29:ARG:CD	1:D:31:LEU:HD23	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ILE:HG22	1:D:352:ILE:O	1.77	0.82
1:A:4:SER:HB2	1:A:37:VAL:HG12	1.57	0.82
1:B:127[A]:ARG:HG2	1:B:127[A]:ARG:NH1	1.82	0.82
1:A:10:ARG:NH2	1:A:60:ASN:HB3	1.94	0.82
1:C:87:THR:HG22	1:C:88:PRO:HD3	1.59	0.82
1:C:201:GLN:O	1:C:204:ARG:HB2	1.80	0.82
1:A:135:SER:HB2	3:A:600:AME:HT23	1.60	0.82
1:C:38:THR:CB	1:C:39:PRO:HD2	2.04	0.81
1:D:58:GLU:HB2	1:D:98:MET:HE3	1.60	0.81
1:D:135:SER:CB	3:D:900:AME:HT23	2.08	0.81
1:D:135:SER:OG	3:D:900:AME:HT23	1.79	0.81
1:A:73:PRO:HA	1:A:76:LEU:HD12	1.60	0.81
1:D:29:ARG:NH2	1:D:50:MET:HG2	1.96	0.81
1:A:169:ASP:OD1	1:A:194:TYR:OH	1.97	0.81
1:B:164:ILE:HD13	1:B:188:VAL:CG1	2.10	0.81
1:D:47:CYS:SG	1:D:49:THR:HG23	2.21	0.81
1:B:281:ALA:O	1:C:246:ARG:NH2	2.14	0.80
1:B:29:ARG:HD2	1:B:31:LEU:CD2	2.12	0.80
1:B:49:THR:HG22	1:B:98:MET:HE2	1.63	0.80
1:A:293:ILE:HG22	1:A:293:ILE:O	1.81	0.80
1:C:185:LEU:HA	4:C:870:HOH:O	1.81	0.79
1:D:29:ARG:HH21	1:D:50:MET:HG2	1.47	0.79
1:A:10:ARG:NH2	1:A:60:ASN:CB	2.46	0.79
1:C:118:SER:HB2	4:C:852:HOH:O	1.80	0.79
1:A:296:GLY:HA3	1:A:329:THR:OG1	1.82	0.79
1:D:164:ILE:HB	1:D:168:TRP:O	1.83	0.78
1:A:135:SER:HB2	3:A:600:AME:CT2	2.14	0.78
1:D:206:ASP:N	1:D:207:PRO:CD	2.45	0.78
1:B:169:ASP:OD1	1:B:194:TYR:OH	2.01	0.78
1:A:87:THR:CB	1:A:88:PRO:HD3	2.11	0.78
1:A:1:MET:HE3	1:A:38:THR:CG2	2.14	0.78
1:B:175:ALA:O	1:B:178:GLU:HB3	1.84	0.78
1:A:109:ASP:O	1:A:113:ARG:HG3	1.83	0.78
1:B:72:ILE:HB	1:B:73:PRO:HD3	1.66	0.78
1:B:164:ILE:HG23	1:B:188:VAL:HG13	1.66	0.78
1:B:139:MET:HG3	1:B:145:LEU:HA	1.67	0.77
1:B:87:THR:HB	1:B:88:PRO:HD3	1.65	0.77
1:D:16:VAL:HG23	1:D:323:PHE:O	1.83	0.77
1:D:163:LYS:HZ2	3:D:900:AME:HN1	1.32	0.77
1:D:159:ARG:NH2	1:D:316:ASP:OD1	2.15	0.77
1:D:13:MET:HE1	1:D:295:THR:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:THR:HA	1:B:98:MET:HE1	1.66	0.77
1:A:206:ASP:N	1:A:207:PRO:HD2	2.00	0.77
1:C:158:VAL:HG12	1:C:158:VAL:O	1.83	0.77
1:A:75:LEU:O	1:A:81:ILE:HD11	1.84	0.77
1:D:13:MET:HE2	1:D:31:LEU:HD11	1.67	0.77
1:C:3:LEU:HB2	1:C:81:ILE:HD12	1.67	0.77
1:D:188:VAL:O	4:D:964:HOH:O	2.02	0.77
1:C:87:THR:CG2	1:C:88:PRO:HD3	2.14	0.76
1:B:111:GLU:OE2	1:C:117:ARG:NH2	2.19	0.76
1:B:23:PHE:HZ	3:B:700:AME:HE1	1.50	0.76
1:C:206:ASP:N	1:C:207:PRO:HD2	2.01	0.76
1:B:10:ARG:NH1	1:B:60:ASN:HB3	2.00	0.76
1:D:58:GLU:CD	1:D:98:MET:HG3	2.11	0.76
1:A:58:GLU:CB	1:A:98:MET:HE2	2.10	0.76
1:D:328:ILE:HG13	1:D:329:THR:HG23	1.68	0.76
1:D:125:SER:HB2	1:D:307:SER:OG	1.87	0.75
1:C:87:THR:CB	1:C:88:PRO:HD3	2.16	0.75
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.69	0.75
1:A:334:LEU:HD12	1:A:339:LEU:HD13	1.68	0.75
1:A:117:ARG:HH12	1:A:121:ALA:HB1	1.46	0.75
1:D:327:ASP:O	1:D:355:LEU:HD13	1.87	0.75
1:D:263:LYS:HB2	1:D:266:ARG:NH1	2.01	0.75
1:B:127[A]:ARG:HH11	1:B:127[A]:ARG:CG	1.99	0.74
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.68	0.74
1:D:212:LEU:HD12	1:D:212:LEU:O	1.87	0.74
1:D:10:ARG:HD3	4:D:929:HOH:O	1.87	0.74
1:B:11:VAL:HG21	1:B:33:LEU:CD1	2.18	0.74
1:C:39:PRO:HG2	4:C:817:HOH:O	1.87	0.74
1:A:352:ILE:CG2	1:A:355:LEU:HG	2.17	0.73
1:D:213:ILE:HG22	1:D:234:THR:HG22	1.70	0.73
1:D:352:ILE:O	1:D:355:LEU:HB2	1.87	0.73
1:A:263:LYS:HB2	1:A:266:ARG:NH1	2.04	0.73
1:B:141:THR:HB	1:B:143:PRO:HD2	1.71	0.73
1:C:58:GLU:CB	1:C:98:MET:CE	2.65	0.73
1:A:82:THR:HG22	1:A:84:ALA:N	2.03	0.73
1:A:301:ALA:HB2	1:A:347:LEU:HD23	1.71	0.73
3:C:800:AME:OXT	4:C:895:HOH:O	2.06	0.73
1:D:48:VAL:HG22	4:D:916:HOH:O	1.87	0.73
1:B:146:LEU:C	4:B:765:HOH:O	2.32	0.72
1:B:11:VAL:HG21	1:B:33:LEU:HD12	1.71	0.72
1:C:135:SER:HB3	3:C:800:AME:HT21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:LYS:O	1:D:364:VAL:HB	1.88	0.72
1:A:113:ARG:HA	1:A:345:PRO:HB2	1.71	0.72
1:A:200:PRO:O	4:A:677:HOH:O	2.08	0.72
1:B:206:ASP:HB2	1:B:207:PRO:HD3	1.71	0.72
1:D:127[A]:ARG:HH11	1:D:127[A]:ARG:HB3	1.55	0.72
1:D:212:LEU:HD12	1:D:212:LEU:C	2.14	0.72
1:A:21:THR:CG2	1:A:23:PHE:CD1	2.73	0.71
1:C:82:THR:HG22	1:C:84:ALA:H	1.53	0.71
1:D:199:ALA:N	1:D:200:PRO:HD2	2.05	0.71
1:D:163:LYS:NZ	3:D:900:AME:N	2.35	0.71
1:C:263:LYS:HE2	4:C:895:HOH:O	1.91	0.71
1:B:113:ARG:HA	1:B:345:PRO:HB2	1.72	0.70
1:A:149:VAL:HG13	1:A:160:ILE:HD13	1.73	0.70
1:C:139:MET:HG3	1:C:145:LEU:HA	1.72	0.70
1:A:139:MET:HG3	1:A:145:LEU:CA	2.20	0.70
1:C:191:ASN:C	1:C:192:THR:HG23	2.17	0.70
1:A:58:GLU:HB2	1:A:98:MET:HE1	1.70	0.70
1:C:10:ARG:HD2	1:C:64:GLU:OE1	1.91	0.70
1:D:201:GLN:O	1:D:204:ARG:HB2	1.91	0.70
1:C:29:ARG:HG2	1:C:31:LEU:HD21	1.73	0.70
1:D:206:ASP:CB	1:D:207:PRO:HD3	2.18	0.70
1:D:130:VAL:HB	1:D:131:PRO:HD2	1.73	0.69
1:D:135:SER:CB	3:D:900:AME:CT2	2.69	0.69
1:C:21:THR:HG22	1:C:23:PHE:H	1.57	0.69
1:B:29:ARG:HD2	1:B:31:LEU:HD21	1.75	0.69
1:D:213:ILE:HG22	1:D:234:THR:CG2	2.22	0.69
1:C:217:LEU:HD21	1:C:228:LEU:HD22	1.72	0.69
1:A:12:GLN:O	1:A:359:VAL:CG2	2.37	0.69
1:B:23:PHE:CZ	3:B:700:AME:HE1	2.28	0.69
1:B:142:ILE:N	1:B:143:PRO:HD2	2.08	0.69
1:B:147:ASP:HA	4:B:765:HOH:O	1.92	0.69
1:D:13:MET:CE	1:D:295:THR:HG22	2.23	0.69
1:D:72:ILE:HB	1:D:73:PRO:HD3	1.75	0.69
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.74	0.69
1:B:206:ASP:N	1:B:207:PRO:CD	2.56	0.68
1:D:217:LEU:HD23	1:D:217:LEU:N	2.07	0.68
1:B:206:ASP:N	1:B:207:PRO:HD2	2.09	0.68
1:C:7:GLU:OE2	1:C:9:ARG:NH1	2.26	0.68
1:A:28:VAL:HG12	1:A:29:ARG:N	2.07	0.68
1:D:291:GLY:O	3:D:900:AME:OT	2.12	0.68
1:A:206:ASP:N	1:A:207:PRO:CD	2.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:CB	1:A:309:PRO:HD2	2.23	0.68
1:B:139:MET:HG3	1:B:145:LEU:CA	2.25	0.67
1:B:250:ASP:OD2	4:B:796:HOH:O	2.12	0.67
1:B:171:GLU:N	1:B:172:PRO:HD2	2.10	0.67
1:C:139:MET:HG3	1:C:145:LEU:CA	2.25	0.67
1:A:35:ARG:HG3	1:A:44:TRP:CE2	2.29	0.67
1:A:201:GLN:O	1:A:204[B]:ARG:HB2	1.95	0.67
1:B:49:THR:CG2	1:B:98:MET:HE2	2.22	0.67
1:D:205:LEU:C	1:D:207:PRO:HD2	2.18	0.67
1:B:261:ASN:C	1:B:261:ASN:OD1	2.37	0.67
1:A:105:MET:HE3	1:A:347:LEU:HD21	1.75	0.67
1:A:352:ILE:O	1:A:355:LEU:HB2	1.94	0.67
1:D:21:THR:CG2	1:D:22:SER:N	2.57	0.67
1:A:21:THR:CG2	1:A:23:PHE:H	2.04	0.67
1:D:9:ARG:HH21	1:D:363:LYS:HE2	1.59	0.67
1:C:10:ARG:CD	1:C:64:GLU:OE1	2.44	0.66
1:D:21:THR:CG2	1:D:22:SER:H	2.08	0.66
1:A:50:MET:HE1	3:A:600:AME:HE1	1.77	0.66
1:D:85:LYS:C	1:D:88:PRO:HD2	2.21	0.66
1:D:350:ALA:HB1	1:D:351:PRO:CD	2.25	0.66
1:D:244:SER:HB2	4:D:988:HOH:O	1.95	0.66
1:B:101:GLY:O	4:B:753:HOH:O	2.12	0.66
1:D:10:ARG:HG3	1:D:10:ARG:NH1	1.98	0.66
1:B:205:LEU:C	1:B:207:PRO:HD2	2.20	0.66
1:A:29:ARG:HD2	1:A:31:LEU:HD23	1.77	0.66
1:D:16:VAL:HG22	1:D:325:LYS:HG3	1.78	0.66
1:A:352:ILE:O	1:A:355:LEU:N	2.24	0.66
1:B:194:TYR:CE2	1:B:202:LEU:HD21	2.31	0.66
1:B:171:GLU:HB2	1:B:172:PRO:HD3	1.78	0.66
1:A:9:ARG:NE	1:A:360:THR:HG21	2.12	0.65
1:C:87:THR:HG22	1:C:88:PRO:CD	2.25	0.65
1:A:199:ALA:HB3	1:A:200:PRO:CD	2.25	0.65
1:B:159:ARG:C	1:B:159:ARG:HD2	2.21	0.65
1:C:87:THR:HB	1:C:88:PRO:HD3	1.77	0.65
1:A:288:TRP:HA	4:A:662:HOH:O	1.94	0.65
1:D:38:THR:HB	1:D:39:PRO:HD2	1.79	0.65
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.79	0.65
1:D:13:MET:CE	1:D:31:LEU:HD11	2.26	0.65
1:B:147:ASP:N	4:B:765:HOH:O	2.30	0.65
1:B:288:TRP:HB3	1:B:313:LEU:HB2	1.78	0.65
1:D:29:ARG:NH2	1:D:50:MET:CG	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASN:OD1	1:C:261:ASN:C	2.40	0.65
1:A:8:LEU:HD12	1:A:366:ILE:HD13	1.80	0.64
1:D:269:GLY:C	4:D:940:HOH:O	2.40	0.64
1:A:144:GLN:O	1:A:148:VAL:HG23	1.97	0.64
1:D:113:ARG:HG3	1:D:346:GLY:HA3	1.79	0.64
1:D:85:LYS:O	1:D:88:PRO:HD2	1.98	0.64
1:C:329:THR:HG21	1:C:349:VAL:HG11	1.79	0.64
1:A:352:ILE:HG22	1:A:352:ILE:O	1.97	0.64
1:A:290:GLY:HA2	4:A:695:HOH:O	1.96	0.64
1:A:319:ALA:HB1	1:A:332:PHE:O	1.97	0.64
1:A:352:ILE:HG22	1:A:355:LEU:CG	2.26	0.64
1:C:86:VAL:HG13	1:C:90:LEU:HD11	1.79	0.64
1:C:349:VAL:HG12	1:C:350:ALA:N	2.13	0.64
1:B:21:THR:CG2	1:B:22:SER:N	2.60	0.64
1:B:142:ILE:N	1:B:143:PRO:CD	2.61	0.64
1:D:328:ILE:O	1:D:351:PRO:HA	1.97	0.64
1:B:29:ARG:CD	1:B:31:LEU:CD2	2.76	0.63
1:B:29:ARG:CD	1:B:31:LEU:HD23	2.28	0.63
1:A:38:THR:HB	1:A:39:PRO:HD2	1.79	0.63
1:D:141:THR:OG1	1:D:144:GLN:HB2	1.98	0.63
1:A:277:HIS:HD2	1:A:311:PHE:CE1	2.17	0.63
1:A:33:LEU:HD23	1:A:45:GLY:O	1.98	0.63
1:B:277:HIS:HD2	1:B:311:PHE:CE1	2.16	0.63
1:A:50:MET:HE1	3:A:600:AME:CE	2.28	0.63
1:B:21:THR:HG23	1:B:22:SER:H	1.61	0.63
1:B:163:LYS:NZ	3:B:700:AME:HB2	2.13	0.63
1:C:352:ILE:CB	1:C:355:LEU:HD12	2.29	0.63
1:A:201:GLN:O	1:A:204[A]:ARG:HB2	1.99	0.62
1:C:135:SER:HB2	3:C:800:AME:CT2	2.28	0.62
1:B:82:THR:O	1:B:86:VAL:HG23	1.99	0.62
1:C:186:LEU:N	4:C:870:HOH:O	2.07	0.62
1:D:352:ILE:HG22	1:D:355:LEU:H	1.64	0.62
1:A:8:LEU:HD23	1:A:32:LEU:CD2	2.29	0.62
1:B:8:LEU:HD23	1:B:32:LEU:HD11	1.82	0.62
1:D:82:THR:HG22	1:D:85:LYS:H	1.64	0.62
1:D:169:ASP:OD1	1:D:194:TYR:OH	2.17	0.62
1:D:199:ALA:N	1:D:200:PRO:CD	2.62	0.62
1:A:87:THR:CB	1:A:88:PRO:CD	2.76	0.62
1:A:161:LYS:NZ	3:A:600:AME:OXT	2.28	0.62
1:A:6:VAL:HB	1:A:72:ILE:HD13	1.82	0.62
1:C:87:THR:CB	1:C:88:PRO:CD	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLU:N	1:C:172:PRO:HD2	2.14	0.62
1:C:334:LEU:HD21	1:C:337:GLY:HA2	1.80	0.62
1:A:119:PHE:CD2	1:A:301:ALA:HB1	2.35	0.61
1:A:159:ARG:NH2	1:A:316:ASP:OD1	2.20	0.61
1:C:59:TYR:OH	1:D:65:HIS:HD2	1.83	0.61
1:D:142:ILE:HB	1:D:143:PRO:CD	2.30	0.61
1:A:10:ARG:NH2	1:A:60:ASN:HB2	2.14	0.61
1:A:232:ILE:O	4:A:688:HOH:O	2.16	0.61
1:C:51:ALA:O	1:C:59:TYR:HB2	2.01	0.61
1:A:203:ALA:HA	1:A:232:ILE:HG22	1.83	0.61
1:C:191:ASN:O	1:C:192:THR:HG23	2.00	0.61
1:C:169:ASP:OD2	1:C:201:GLN:NE2	2.33	0.61
1:A:21:THR:HG22	1:A:23:PHE:N	2.06	0.61
1:D:191:ASN:C	1:D:192:THR:HG23	2.26	0.61
1:D:9:ARG:HH11	1:D:356:LEU:CD2	2.13	0.61
1:A:7:GLU:OE2	1:A:35:ARG:NH1	2.34	0.61
1:A:351:PRO:O	1:A:353:PRO:HD3	2.01	0.61
1:B:159:ARG:HB2	1:B:185:LEU:CB	2.31	0.61
1:D:144:GLN:O	1:D:148:VAL:HG23	2.00	0.61
1:A:171:GLU:HB2	1:A:172:PRO:HD3	1.83	0.60
1:B:75:LEU:O	1:B:81:ILE:HD11	2.00	0.60
1:C:139:MET:HB2	1:C:168:TRP:CH2	2.34	0.60
1:A:46:GLU:OE1	1:A:297:LEU:HB2	2.01	0.60
1:A:201:GLN:O	1:A:201:GLN:HG3	2.02	0.60
1:B:10:ARG:HD3	1:B:32:LEU:HD13	1.82	0.60
1:C:21:THR:HG21	1:C:23:PHE:CD1	2.37	0.60
1:D:295:THR:OG1	1:D:297:LEU:HB2	2.00	0.60
1:B:147:ASP:CA	4:B:765:HOH:O	2.49	0.60
1:B:228:LEU:HD12	1:B:228:LEU:O	2.02	0.60
1:B:11:VAL:CG2	1:B:33:LEU:HD12	2.32	0.60
1:B:159:ARG:HA	1:B:185:LEU:HB2	1.82	0.60
1:C:205:LEU:C	1:C:207:PRO:CD	2.71	0.60
1:D:159:ARG:HB2	1:D:185:LEU:HB2	1.84	0.60
1:B:164:ILE:CD1	1:B:188:VAL:CG1	2.79	0.60
1:A:274:ARG:O	1:A:277:HIS:HB3	2.02	0.60
1:C:223:LEU:O	1:C:226:ALA:HB3	2.01	0.59
1:D:60:ASN:O	1:D:63:ALA:HB3	2.02	0.59
1:A:9:ARG:HE	1:A:360:THR:HG21	1.67	0.59
1:A:35:ARG:HG3	1:A:44:TRP:CZ2	2.36	0.59
1:A:72:ILE:HG22	1:A:76:LEU:HD11	1.83	0.59
1:C:96:HIS:O	1:C:100:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.84	0.59
1:C:82:THR:HG22	1:C:84:ALA:N	2.16	0.59
1:A:171:GLU:N	1:A:172:PRO:HD2	2.17	0.59
1:B:87:THR:HB	1:B:88:PRO:CD	2.32	0.59
1:D:33:LEU:C	1:D:34:LEU:HD23	2.28	0.59
1:B:49:THR:HG23	1:B:98:MET:CE	2.31	0.59
1:C:29:ARG:CG	1:C:31:LEU:HD21	2.33	0.59
1:D:272:GLU:O	1:D:276:VAL:HG23	2.03	0.58
1:A:136:VAL:HB	1:A:162:LEU:HD23	1.84	0.58
1:B:227:GLU:HA	1:B:230:ARG:HH11	1.68	0.58
1:A:127:ARG:NH2	1:A:311:PHE:O	2.36	0.58
1:C:169:ASP:C	1:C:172:PRO:HD2	2.27	0.58
1:B:9:ARG:O	1:B:32:LEU:HD12	2.04	0.58
1:B:87:THR:CB	1:B:88:PRO:HD3	2.33	0.58
1:C:150:GLY:HA2	1:C:180:PHE:CE2	2.37	0.58
1:D:159:ARG:HG2	1:D:160:ILE:N	2.19	0.58
1:C:322:ARG:NH1	1:C:323:PHE:CE2	2.72	0.58
1:C:227:GLU:O	1:C:230:ARG:HB2	2.04	0.58
1:D:206:ASP:CB	1:D:207:PRO:CD	2.82	0.58
1:A:23:PHE:HZ	3:A:600:AME:SD	2.26	0.58
1:C:161:LYS:NZ	3:C:800:AME:OXT	2.36	0.58
1:D:169:ASP:OD2	1:D:201:GLN:NE2	2.37	0.58
1:C:158:VAL:O	1:C:158:VAL:CG1	2.51	0.58
1:A:169:ASP:OD2	1:A:201:GLN:NE2	2.32	0.57
1:B:29:ARG:HD2	1:B:31:LEU:HD23	1.84	0.57
1:C:1:MET:HE3	1:C:38:THR:HG21	1.86	0.57
1:B:21:THR:HG23	1:B:22:SER:N	2.18	0.57
1:A:301:ALA:HB2	1:A:347:LEU:CD2	2.34	0.57
1:C:20:ARG:HG2	1:C:138:ILE:HB	1.86	0.57
1:B:80:ASP:O	1:B:81:ILE:HG13	2.04	0.57
1:C:171:GLU:N	1:C:172:PRO:CD	2.67	0.57
1:D:29:ARG:CD	1:D:31:LEU:CD2	2.75	0.57
1:A:350:ALA:HB1	1:A:351:PRO:HD2	1.87	0.57
1:B:142:ILE:O	1:B:146:LEU:HG	2.05	0.57
1:B:143:PRO:O	1:B:146:LEU:N	2.38	0.57
1:C:129:SER:C	1:C:130:VAL:CG1	2.77	0.57
1:D:26:GLN:NE2	1:D:50:MET:SD	2.78	0.57
1:D:48:VAL:HG23	1:D:98:MET:SD	2.44	0.57
1:B:141:THR:CB	1:B:143:PRO:HD2	2.35	0.57
1:A:28:VAL:HG12	1:A:29:ARG:H	1.70	0.56
1:A:356:LEU:CD2	1:A:360:THR:OG1	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:TRP:C	1:D:366:ILE:HG13	2.29	0.56
1:A:135:SER:HB3	3:A:600:AME:CT2	2.33	0.56
1:A:327:ASP:OD1	1:A:328:ILE:N	2.39	0.56
1:C:159:ARG:HD2	4:C:864:HOH:O	2.03	0.56
1:D:35:ARG:NE	1:D:42:GLU:OE2	2.38	0.56
1:B:35:ARG:HD2	1:B:42:GLU:OE2	2.06	0.56
1:C:349:VAL:HG13	4:C:893:HOH:O	2.05	0.56
1:D:352:ILE:HG22	1:D:355:LEU:HB2	1.86	0.56
1:A:5:GLY:HA2	1:A:76:LEU:HD21	1.88	0.56
1:C:135:SER:HG	3:C:800:AME:HT23	1.70	0.56
1:D:103:LEU:O	1:D:107:VAL:HG23	2.05	0.56
1:A:70:TYR:C	1:A:73:PRO:HD2	2.31	0.56
1:B:159:ARG:HB2	1:B:185:LEU:HB2	1.87	0.56
1:A:212:LEU:C	1:A:212:LEU:HD12	2.31	0.56
1:D:365:TRP:O	1:D:366:ILE:HG13	2.06	0.56
1:D:159:ARG:HB2	1:D:185:LEU:CB	2.36	0.56
1:D:189:ASP:OD2	3:D:900:AME:OXT	2.24	0.56
1:A:212:LEU:HD12	1:A:212:LEU:O	2.06	0.55
1:A:21:THR:CG2	1:A:22:SER:N	2.69	0.55
1:B:21:THR:HG21	1:B:23:PHE:CZ	2.40	0.55
1:B:29:ARG:NE	1:B:31:LEU:CD2	2.69	0.55
1:B:49:THR:HA	1:B:98:MET:CE	2.34	0.55
1:B:97:ARG:HG3	4:B:751:HOH:O	2.06	0.55
1:B:201:GLN:O	1:B:204:ARG:HB2	2.06	0.55
1:B:334:LEU:HD12	1:B:338:HIS:O	2.07	0.55
1:A:68[A]:ARG:HH11	1:A:68[A]:ARG:CG	2.16	0.55
1:A:169:ASP:O	1:A:172:PRO:HD2	2.07	0.55
1:A:290:GLY:CA	4:A:695:HOH:O	2.52	0.55
1:C:8:LEU:CD2	1:C:32:LEU:HD22	2.35	0.55
1:D:171:GLU:N	1:D:172:PRO:HD2	2.20	0.55
1:C:21:THR:CG2	1:C:23:PHE:CD1	2.90	0.55
1:C:329:THR:HG21	1:C:349:VAL:CG1	2.36	0.55
1:D:274:ARG:O	1:D:277:HIS:HB3	2.07	0.55
1:A:11:VAL:HB	1:A:31:LEU:CD1	2.37	0.55
1:A:204[A]:ARG:HG2	1:A:204[A]:ARG:NH1	2.16	0.55
1:A:277:HIS:CD2	1:A:311:PHE:CE1	2.95	0.55
1:B:162:LEU:CD1	1:B:186:LEU:HD11	2.37	0.55
1:A:72:ILE:N	1:A:73:PRO:CD	2.69	0.55
1:B:127[B]:ARG:NH2	1:B:308:LEU:O	2.39	0.55
1:B:163:LYS:HZ1	3:B:700:AME:HB2	1.72	0.55
1:C:293:ILE:CD1	3:C:800:AME:HE2	2.37	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:HB3	2.07	0.55
1:B:148:VAL:HG13	1:B:152:TYR:CE1	2.42	0.55
1:C:127:ARG:HB2	1:C:307:SER:HB2	1.89	0.55
1:B:96:HIS:O	1:B:100:LYS:HG3	2.07	0.54
1:C:25:THR:CG2	1:C:26:GLN:N	2.69	0.54
1:C:169:ASP:O	1:C:172:PRO:HD2	2.07	0.54
1:D:11:VAL:HG22	1:D:360:THR:HA	1.89	0.54
1:A:338:HIS:O	1:A:339:LEU:HD12	2.08	0.54
1:B:35:ARG:NH1	1:B:42:GLU:OE2	2.39	0.54
1:B:81:ILE:CG2	1:B:82:THR:N	2.70	0.54
1:D:9:ARG:NH1	1:D:356:LEU:CD2	2.71	0.54
1:C:350:ALA:HB1	1:C:351:PRO:HD2	1.88	0.54
1:C:293:ILE:HD11	3:C:800:AME:CE	2.37	0.54
1:C:112:LEU:HB3	1:C:117:ARG:O	2.08	0.54
1:D:10:ARG:HH11	1:D:10:ARG:CG	2.13	0.54
1:A:8:LEU:HD12	1:A:366:ILE:CD1	2.38	0.54
1:A:33:LEU:HD21	1:A:297:LEU:HD12	1.90	0.54
1:A:204[A]:ARG:HH11	1:A:204[A]:ARG:CG	2.10	0.54
1:B:239:ASP:OD1	1:B:266:ARG:NH1	2.39	0.54
1:C:109:ASP:O	1:C:113:ARG:HG3	2.07	0.54
1:D:46:GLU:OE2	1:D:295:THR:HG23	2.07	0.54
1:D:206:ASP:HB2	1:D:207:PRO:CD	2.31	0.54
1:A:229:ALA:HB2	1:A:236:ILE:HG13	1.90	0.54
1:D:194:TYR:CG	1:D:202:LEU:HD11	2.43	0.54
1:A:8:LEU:CD2	1:A:32:LEU:HD21	2.37	0.54
1:B:145:LEU:O	1:B:145:LEU:HG	2.01	0.54
1:B:149:VAL:HG12	1:B:153:LEU:HD12	1.89	0.54
1:C:293:ILE:HD12	3:C:800:AME:HE2	1.89	0.54
1:D:160:ILE:O	1:D:186:LEU:HD12	2.08	0.54
1:A:329:THR:HG22	1:A:350:ALA:C	2.31	0.54
1:B:199:ALA:N	1:B:200:PRO:HD2	2.22	0.54
1:D:214:GLU:HA	1:D:237:CYS:HB3	1.89	0.54
1:A:272:GLU:O	1:A:276:VAL:HG23	2.08	0.53
1:B:81:ILE:HG22	1:B:82:THR:N	2.22	0.53
1:B:227:GLU:HA	1:B:230:ARG:NH1	2.22	0.53
1:D:139:MET:HE3	1:D:148:VAL:HG21	1.90	0.53
1:C:194:TYR:CE2	1:C:202:LEU:HD21	2.44	0.53
1:A:135:SER:OG	3:A:600:AME:HT23	2.09	0.53
1:B:49:THR:HG22	1:B:98:MET:HE1	1.87	0.53
1:C:321:ASP:HA	1:C:324:TYR:O	2.08	0.53
1:D:58:GLU:OE1	1:D:98:MET:CG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLY:HA3	1:B:110:ALA:HB2	1.91	0.53
1:C:329:THR:CG2	1:C:349:VAL:CG1	2.86	0.53
1:D:2:LYS:HD2	1:D:3:LEU:N	2.24	0.53
1:A:2:LYS:HD2	1:A:39:PRO:HG3	1.90	0.53
1:A:177:ARG:HD2	1:A:181:GLY:O	2.09	0.53
1:B:21:THR:HG21	1:B:23:PHE:CD1	2.44	0.53
1:C:352:ILE:HG22	1:C:352:ILE:O	2.08	0.53
1:A:164:ILE:HG12	1:A:188:VAL:HB	1.89	0.53
1:A:199:ALA:CB	1:A:200:PRO:HD3	2.34	0.53
1:B:81:ILE:CD1	4:B:716:HOH:O	2.56	0.53
1:B:138:ILE:HG23	1:B:168:TRP:CD1	2.43	0.53
1:A:159:ARG:HG2	1:A:160:ILE:N	2.23	0.53
1:A:199:ALA:N	1:A:200:PRO:HD2	2.23	0.53
1:D:258:GLN:O	1:D:286:PRO:HD2	2.09	0.53
1:A:33:LEU:CD2	1:A:297:LEU:HD12	2.40	0.53
1:C:292:MET:O	1:C:293:ILE:HB	2.09	0.53
1:A:200:PRO:O	1:A:203:ALA:HB3	2.09	0.52
1:B:11:VAL:HG21	1:B:33:LEU:HD11	1.90	0.52
1:C:50:MET:HE2	4:C:830:HOH:O	2.10	0.52
1:C:293:ILE:CD1	3:C:800:AME:CE	2.88	0.52
1:B:72:ILE:N	1:B:73:PRO:HD2	2.25	0.52
1:D:64:GLU:O	1:D:67:LEU:HB2	2.08	0.52
1:D:191:ASN:O	1:D:192:THR:HG23	2.08	0.52
1:D:261:ASN:ND2	1:D:288:TRP:CH2	2.78	0.52
1:A:13:MET:HG2	1:A:359:VAL:HG21	1.91	0.52
1:A:33:LEU:CD2	1:A:45:GLY:O	2.56	0.52
1:A:9:ARG:NE	1:A:356:LEU:HD22	2.25	0.52
1:A:135:SER:OG	1:A:161:LYS:HE2	2.10	0.52
1:A:28:VAL:CG1	1:A:29:ARG:N	2.72	0.52
1:A:149:VAL:HG13	1:A:160:ILE:CD1	2.39	0.52
1:B:33:LEU:HD23	1:B:46:GLU:HG3	1.91	0.52
1:C:293:ILE:O	1:C:293:ILE:HG22	2.09	0.52
1:C:315:GLY:C	1:C:317:THR:H	2.16	0.52
1:D:11:VAL:HG13	1:D:359:VAL:HB	1.91	0.52
1:D:163:LYS:HE3	1:D:191:ASN:OD1	2.10	0.52
1:A:293:ILE:O	1:A:293:ILE:CG2	2.52	0.52
1:D:271:LEU:N	4:D:940:HOH:O	2.42	0.52
1:B:87:THR:CB	1:B:88:PRO:CD	2.88	0.52
1:C:29:ARG:CG	1:C:31:LEU:CD2	2.89	0.52
1:C:329:THR:HB	1:C:349:VAL:CG1	2.40	0.52
1:D:1:MET:SD	1:D:38:THR:HG21	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PRO:HA	1:D:26:GLN:O	2.09	0.52
1:A:212:LEU:HD11	4:A:667:HOH:O	2.10	0.51
1:B:1:MET:HE3	1:B:38:THR:HG21	1.90	0.51
1:D:174:ARG:O	1:D:178:GLU:HB2	2.11	0.51
1:B:29:ARG:NE	1:B:31:LEU:HD23	2.25	0.51
1:C:349:VAL:CG1	1:C:350:ALA:N	2.72	0.51
1:C:352:ILE:O	1:C:355:LEU:N	2.44	0.51
1:D:139:MET:HG3	1:D:145:LEU:HA	1.93	0.51
1:A:9:ARG:HE	1:A:356:LEU:HD22	1.74	0.51
1:A:308:LEU:HB3	1:A:309:PRO:HD2	1.90	0.51
1:A:356:LEU:O	1:A:359:VAL:HG12	2.11	0.51
1:B:72:ILE:N	1:B:73:PRO:CD	2.73	0.51
1:B:125:SER:HB2	1:B:307:SER:OG	2.10	0.51
1:C:159:ARG:HG2	1:C:160:ILE:N	2.23	0.51
1:D:60:ASN:CB	4:D:920:HOH:O	2.38	0.51
1:A:125:SER:CB	1:A:307:SER:OG	2.58	0.51
1:A:356:LEU:HD23	1:A:360:THR:OG1	2.10	0.51
1:B:163:LYS:NZ	3:B:700:AME:CB	2.73	0.51
1:C:308:LEU:CB	1:C:309:PRO:CD	2.89	0.51
1:C:143:PRO:O	1:C:144:GLN:C	2.53	0.51
1:C:129:SER:C	1:C:130:VAL:HG13	2.34	0.51
1:C:171:GLU:OE1	1:C:171:GLU:HA	2.11	0.51
1:C:367:GLY:O	1:C:368:SER:O	2.29	0.51
1:D:270:TYR:O	1:D:273:ALA:HB3	2.11	0.51
1:A:21:THR:HG23	1:A:22:SER:N	2.24	0.51
1:A:308:LEU:CB	1:A:309:PRO:CD	2.88	0.51
1:B:164:ILE:CG2	1:B:188:VAL:HG13	2.38	0.51
1:C:199:ALA:O	1:C:200:PRO:C	2.54	0.51
1:B:277:HIS:CD2	1:B:311:PHE:CE1	2.98	0.50
1:D:30:GLU:O	1:D:60:ASN:ND2	2.37	0.50
1:A:112:LEU:HB3	1:A:117:ARG:O	2.11	0.50
1:B:274:ARG:O	1:B:277:HIS:HB3	2.10	0.50
1:C:148:VAL:CG1	1:C:152:TYR:CE1	2.95	0.50
1:A:8:LEU:CD2	1:A:32:LEU:CD2	2.89	0.50
1:B:49:THR:HG23	1:B:98:MET:HE3	1.94	0.50
1:C:277:HIS:CD2	1:C:310:ASN:HB3	2.47	0.50
1:C:334:LEU:HD12	1:C:339:LEU:HD13	1.94	0.50
1:A:171:GLU:N	1:A:172:PRO:CD	2.75	0.50
1:C:83:ALA:O	1:C:86:VAL:HB	2.11	0.50
1:C:59:TYR:OH	1:D:65:HIS:CD2	2.64	0.50
1:C:329:THR:CG2	1:C:349:VAL:HG11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HB	1:A:31:LEU:HD12	1.93	0.50
1:A:334:LEU:HD21	1:A:337:GLY:HA2	1.92	0.50
1:B:171:GLU:N	1:B:172:PRO:CD	2.75	0.50
1:D:60:ASN:CA	4:D:920:HOH:O	2.60	0.50
1:B:308:LEU:HB3	1:B:309:PRO:HD2	1.94	0.50
1:C:352:ILE:O	1:C:355:LEU:HB2	2.11	0.50
1:C:21:THR:HG21	1:C:23:PHE:CZ	2.46	0.50
1:C:119:PHE:HB2	4:C:853:HOH:O	2.12	0.50
1:C:213:ILE:HG22	1:C:234:THR:CG2	2.34	0.50
1:D:79:GLU:OE1	1:D:79:GLU:HA	2.10	0.50
1:A:118:SER:HB2	4:A:654:HOH:O	2.11	0.50
1:C:35:ARG:HD3	1:C:44:TRP:CH2	2.45	0.50
1:C:275:ARG:O	1:C:276:VAL:C	2.53	0.50
1:A:125:SER:HB2	1:A:307:SER:OG	2.11	0.49
1:A:113:ARG:HG2	1:A:346:GLY:HA3	1.93	0.49
1:C:148:VAL:HG13	1:C:152:TYR:CE1	2.46	0.49
1:C:161:LYS:HE2	1:C:163:LYS:HE2	1.95	0.49
1:C:328:ILE:O	1:C:351:PRO:HA	2.12	0.49
1:A:87:THR:N	1:A:88:PRO:HD2	2.26	0.49
1:A:288:TRP:CE3	1:A:289:CYS:O	2.65	0.49
1:B:10:ARG:HH12	1:B:60:ASN:HB3	1.74	0.49
1:A:10:ARG:CZ	1:A:60:ASN:HB3	2.42	0.49
1:A:28:VAL:CG1	1:A:29:ARG:H	2.26	0.49
1:C:298:GLY:O	1:C:299:ARG:C	2.53	0.49
1:D:135:SER:HB3	3:D:900:AME:CT2	2.41	0.49
1:A:163:LYS:HZ1	3:A:600:AME:HB2	1.78	0.49
1:A:205:LEU:C	1:A:207:PRO:HD2	2.36	0.49
1:B:80:ASP:C	1:B:81:ILE:HG13	2.37	0.49
1:B:92:LYS:HD2	1:B:93:PHE:CZ	2.47	0.49
1:C:72:ILE:N	1:C:73:PRO:HD2	2.27	0.49
1:D:169:ASP:HB2	1:D:170:VAL:HG23	1.95	0.49
1:D:194:TYR:N	1:D:194:TYR:CD1	2.79	0.49
1:D:227:GLU:O	1:D:230:ARG:HB2	2.13	0.49
1:B:164:ILE:CG2	1:B:188:VAL:CG1	2.91	0.49
1:B:249:ALA:O	1:B:253:LYS:HG3	2.12	0.49
1:D:25:THR:HG22	1:D:26:GLN:N	2.26	0.49
1:A:91:ALA:O	4:A:646:HOH:O	2.19	0.49
1:A:199:ALA:CB	1:A:200:PRO:CD	2.88	0.49
1:D:9:ARG:NH1	1:D:356:LEU:HG	2.27	0.49
1:D:212:LEU:C	1:D:212:LEU:CD1	2.85	0.49
1:A:134:VAL:HG13	1:A:134:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:O	1:A:148:VAL:HB	2.12	0.49
1:A:190:ALA:O	1:A:191:ASN:C	2.53	0.49
1:A:221:ASP:O	1:A:225:HIS:ND1	2.39	0.49
1:A:328:ILE:O	1:A:351:PRO:HA	2.12	0.49
1:B:86:VAL:O	1:B:90:LEU:HG	2.12	0.49
1:C:153:LEU:HD12	1:C:180:PHE:CD2	2.47	0.49
1:A:46:GLU:OE2	1:A:294:GLU:HB3	2.13	0.49
1:B:55:TYR:CZ	1:B:240:GLU:HG3	2.48	0.49
1:D:4:SER:HB2	1:D:37:VAL:HG12	1.94	0.49
1:B:11:VAL:HG12	1:B:12:GLN:N	2.28	0.49
1:D:169:ASP:HB2	1:D:170:VAL:H	1.37	0.48
3:D:900:AME:CT1	3:D:900:AME:SD	3.01	0.48
1:A:85:LYS:C	1:A:88:PRO:HD2	2.38	0.48
1:B:171:GLU:HB2	1:B:172:PRO:CD	2.43	0.48
1:C:87:THR:HB	1:C:88:PRO:CD	2.41	0.48
1:B:321:ASP:HA	1:B:324:TYR:O	2.13	0.48
1:C:139:MET:HG3	1:C:145:LEU:HB2	1.95	0.48
1:A:142:ILE:N	1:A:143:PRO:HD2	2.28	0.48
1:A:308:LEU:HG	1:A:309:PRO:HD2	1.95	0.48
1:C:25:THR:HG22	1:C:26:GLN:N	2.28	0.48
1:C:47:CYS:SG	1:C:49:THR:HG23	2.53	0.48
1:D:4:SER:HB2	1:D:37:VAL:O	2.13	0.48
1:D:171:GLU:HA	1:D:171:GLU:OE1	2.12	0.48
1:B:8:LEU:O	1:B:363:LYS:HA	2.13	0.48
1:C:21:THR:CG2	1:C:22:SER:N	2.76	0.48
1:D:165:GLU:O	1:D:166:PRO:C	2.56	0.48
1:B:21:THR:CG2	1:B:23:PHE:CD1	2.96	0.48
1:A:352:ILE:O	1:A:355:LEU:CB	2.61	0.48
1:A:364:VAL:HG22	1:A:365:TRP:N	2.29	0.48
1:B:75:LEU:CD2	1:B:90:LEU:HD21	2.44	0.48
1:D:15:LEU:HD21	1:D:29:ARG:HB2	1.95	0.48
1:D:67:LEU:HD23	1:D:71:LEU:HB2	1.95	0.48
1:D:11:VAL:HG12	1:D:12:GLN:N	2.29	0.48
1:A:161:LYS:NZ	1:A:316:ASP:OD2	2.47	0.48
1:A:321:ASP:HA	1:A:324:TYR:O	2.13	0.48
1:D:199:ALA:HB3	1:D:200:PRO:CD	2.43	0.48
1:A:8:LEU:HB2	1:A:364:VAL:CG1	2.44	0.47
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.72	0.47
1:B:159:ARG:C	1:B:159:ARG:CD	2.86	0.47
1:D:130:VAL:O	1:D:338:HIS:HA	2.13	0.47
1:D:303:VAL:HG23	1:D:317:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:N	1:A:323:PHE:O	2.45	0.47
1:D:20:ARG:HD3	1:D:138:ILE:HB	1.96	0.47
1:B:29:ARG:CD	1:B:31:LEU:HD21	2.41	0.47
1:B:81:ILE:HD12	4:B:716:HOH:O	2.12	0.47
1:D:127[A]:ARG:NH1	1:D:129:SER:O	2.47	0.47
1:B:225:HIS:CD2	1:B:238:LEU:HD21	2.50	0.47
1:D:170:VAL:HG22	1:D:205:LEU:HD23	1.96	0.47
1:B:217:LEU:HB2	1:B:225:HIS:CE1	2.50	0.47
1:A:87:THR:N	1:A:88:PRO:CD	2.77	0.47
1:A:216:PRO:C	1:A:217:LEU:HD23	2.40	0.47
1:A:334:LEU:HD12	1:A:339:LEU:CD1	2.41	0.47
1:B:194:TYR:CD2	1:B:202:LEU:HD21	2.50	0.47
1:B:237:CYS:HA	1:B:259:ILE:O	2.15	0.47
1:B:267:VAL:O	1:B:272:GLU:HG2	2.14	0.47
1:C:150:GLY:CA	1:C:180:PHE:CZ	2.98	0.47
1:D:48:VAL:HG12	1:D:292:MET:HB2	1.96	0.47
1:D:143:PRO:O	1:D:144:GLN:C	2.58	0.47
1:A:21:THR:CG2	1:A:23:PHE:CG	2.97	0.47
1:A:170:VAL:HA	1:A:205:LEU:HD21	1.96	0.47
1:C:48:VAL:HG22	4:C:827:HOH:O	2.15	0.47
1:C:162:LEU:HG	1:C:186:LEU:HD11	1.96	0.47
1:B:116:GLU:HA	1:B:345:PRO:HB3	1.97	0.47
1:B:296:GLY:HA3	1:B:329:THR:OG1	2.15	0.47
1:C:271:LEU:HD23	1:C:271:LEU:HA	1.55	0.47
1:D:6:VAL:HA	1:D:35:ARG:O	2.15	0.47
1:D:40:ALA:CB	4:D:906:HOH:O	2.63	0.47
1:A:236:ILE:HG22	1:A:237:CYS:N	2.30	0.46
1:B:55:TYR:OH	1:B:239:ASP:OD1	2.33	0.46
1:B:72:ILE:HB	1:B:73:PRO:CD	2.43	0.46
1:B:127[B]:ARG:HB2	1:B:307:SER:HB2	1.98	0.46
1:C:6:VAL:HG12	1:C:7:GLU:N	2.30	0.46
1:C:165:GLU:O	1:C:166:PRO:C	2.57	0.46
1:D:251:ALA:HB2	4:D:987:HOH:O	2.15	0.46
1:A:213:ILE:HG12	1:A:216:PRO:HG3	1.97	0.46
1:C:308:LEU:HB3	1:C:309:PRO:HD2	1.97	0.46
1:A:322:ARG:NH1	1:A:323:PHE:CE2	2.82	0.46
1:B:356:LEU:C	1:B:356:LEU:CD2	2.88	0.46
1:D:319:ALA:HB1	1:D:332:PHE:O	2.15	0.46
1:A:112:LEU:HD22	1:A:117:ARG:HB3	1.96	0.46
1:B:75:LEU:HD21	1:B:90:LEU:HD21	1.97	0.46
1:C:3:LEU:HB2	1:C:81:ILE:CD1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:CYS:HB2	1:D:334:LEU:HD11	1.96	0.46
1:D:238:LEU:HD13	1:D:241:SER:HB2	1.96	0.46
1:A:191:ASN:C	1:A:192:THR:HG23	2.41	0.46
1:B:72:ILE:CB	1:B:73:PRO:HD3	2.43	0.46
1:C:105:MET:O	1:C:106:ALA:C	2.58	0.46
1:A:113:ARG:HA	1:A:345:PRO:CB	2.41	0.46
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.71	0.46
1:B:143:PRO:O	1:B:144:GLN:C	2.59	0.46
1:D:315:GLY:C	1:D:317:THR:H	2.23	0.46
1:D:352:ILE:O	1:D:355:LEU:N	2.49	0.46
1:D:353:PRO:O	1:D:354:GLU:C	2.59	0.46
1:B:161:LYS:NZ	3:B:700:AME:C	2.79	0.46
1:D:60:ASN:N	4:D:920:HOH:O	2.48	0.46
1:D:185:LEU:HD23	1:D:185:LEU:HA	1.68	0.46
1:B:340:PRO:HG2	4:B:852:HOH:O	2.14	0.46
1:C:109:ASP:HA	1:C:119:PHE:HE1	1.81	0.46
1:C:352:ILE:HA	1:C:353:PRO:HD3	1.75	0.46
1:C:68:ARG:O	1:C:73:PRO:CD	2.64	0.46
1:C:249:ALA:O	1:C:253:LYS:HG3	2.16	0.46
1:D:295:THR:C	1:D:297:LEU:H	2.22	0.46
1:A:316:ASP:OD2	4:A:695:HOH:O	2.20	0.46
1:B:264:PRO:HG3	1:B:305:LEU:HD22	1.98	0.46
1:C:217:LEU:O	1:C:218:GLU:C	2.59	0.46
1:D:142:ILE:N	1:D:143:PRO:HD2	2.30	0.46
1:B:146:LEU:HD23	1:B:176:VAL:HG22	1.98	0.45
1:D:290:GLY:HA2	4:D:1000:HOH:O	2.15	0.45
1:A:87:THR:HG22	1:A:88:PRO:N	2.31	0.45
1:A:206:ASP:HB2	1:A:207:PRO:CD	2.39	0.45
1:A:288:TRP:CA	4:A:662:HOH:O	2.57	0.45
1:B:159:ARG:HB2	1:B:185:LEU:HB3	1.98	0.45
1:C:32:LEU:HD23	1:C:32:LEU:HA	1.67	0.45
1:A:329:THR:HG21	1:A:349:VAL:HG23	1.98	0.45
1:A:199:ALA:N	1:A:200:PRO:CD	2.79	0.45
1:C:125:SER:HA	1:C:308:LEU:HD12	1.98	0.45
1:C:135:SER:HB2	3:C:800:AME:HT22	1.97	0.45
1:C:139:MET:HG3	1:C:145:LEU:CB	2.47	0.45
1:C:171:GLU:HB2	1:C:172:PRO:HD3	1.98	0.45
1:A:15:LEU:HD12	1:A:26:GLN:O	2.16	0.45
1:A:185:LEU:HD22	1:A:211:LEU:HD11	1.98	0.45
1:A:356:LEU:HD22	1:A:360:THR:OG1	2.17	0.45
1:B:10:ARG:HH12	1:B:60:ASN:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:THR:HB	1:B:218:GLU:HA	1.97	0.45
1:C:67:LEU:C	1:C:72:ILE:HG13	2.35	0.45
1:C:75:LEU:O	1:C:81:ILE:HD11	2.17	0.45
1:C:141:THR:HG22	1:C:142:ILE:N	2.31	0.45
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.72	0.45
1:A:103:LEU:O	1:A:107:VAL:HG23	2.16	0.45
1:B:222:VAL:O	1:B:225:HIS:N	2.50	0.45
1:D:159:ARG:HB3	1:D:314:PRO:HG2	1.98	0.45
1:A:2:LYS:C	1:A:2:LYS:HD3	2.42	0.45
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.66	0.45
1:B:154:ASP:C	1:B:156:GLY:N	2.75	0.45
1:B:267:VAL:HG23	1:B:272:GLU:HB3	1.98	0.45
1:C:38:THR:CB	1:C:39:PRO:CD	2.65	0.45
1:C:264:PRO:HG3	1:C:305:LEU:HD22	1.98	0.45
1:D:72:ILE:HB	1:D:73:PRO:CD	2.44	0.45
1:A:112:LEU:O	1:A:115:HIS:N	2.43	0.45
1:B:87:THR:N	1:B:88:PRO:HD2	2.32	0.45
1:A:68[A]:ARG:HG2	1:A:68[A]:ARG:NH1	2.17	0.45
1:B:68:ARG:HG3	1:B:366:ILE:CD1	2.47	0.45
1:C:29:ARG:HG3	1:C:31:LEU:CD2	2.46	0.45
1:C:31:LEU:HD13	1:C:295:THR:HG23	1.98	0.45
1:C:135:SER:CB	3:C:800:AME:HT22	2.43	0.45
1:C:308:LEU:HD12	1:C:308:LEU:HA	1.62	0.45
1:C:352:ILE:HG22	1:C:355:LEU:HG	1.97	0.45
1:D:16:VAL:HG23	1:D:323:PHE:C	2.41	0.45
1:B:8:LEU:HB2	1:B:364:VAL:HG12	1.98	0.44
1:A:44:TRP:O	1:A:106:ALA:HA	2.16	0.44
1:A:203:ALA:CA	1:A:232:ILE:HG22	2.48	0.44
1:C:87:THR:N	1:C:88:PRO:HD2	2.32	0.44
1:A:1:MET:HB2	1:A:81:ILE:O	2.17	0.44
1:C:365:TRP:HE1	1:C:367:GLY:HA3	1.81	0.44
1:A:5:GLY:HA2	1:A:76:LEU:CD2	2.47	0.44
1:A:257:VAL:HG22	1:A:258:GLN:N	2.31	0.44
1:D:29:ARG:NH1	1:D:292:MET:O	2.51	0.44
1:A:328:ILE:O	1:A:352:ILE:N	2.38	0.44
1:B:10:ARG:HH22	1:B:61:ASP:CG	2.17	0.44
1:B:102:ALA:O	1:B:105:MET:HB3	2.17	0.44
1:A:57:SER:HA	1:B:94:LYS:O	2.18	0.44
1:A:249:ALA:O	1:A:253:LYS:HB2	2.17	0.44
1:A:298:GLY:O	1:A:299:ARG:C	2.59	0.44
1:C:148:VAL:CG1	1:C:152:TYR:HE1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:HG12	1:D:150:GLY:N	2.32	0.44
1:D:339:LEU:HA	1:D:339:LEU:HD23	1.53	0.44
1:A:288:TRP:HE3	1:A:289:CYS:O	2.00	0.44
1:B:339:LEU:HA	1:B:339:LEU:HD12	1.49	0.44
1:C:288:TRP:HB3	1:C:313:LEU:HB2	1.99	0.44
1:C:293:ILE:HD11	3:C:800:AME:HE3	1.99	0.44
1:D:11:VAL:CG1	1:D:12:GLN:N	2.80	0.44
1:C:68:ARG:O	1:C:73:PRO:CG	2.66	0.44
1:C:72:ILE:N	1:C:73:PRO:CD	2.81	0.44
1:C:129:SER:HA	1:C:339:LEU:O	2.17	0.44
1:D:130:VAL:CB	1:D:131:PRO:HD2	2.39	0.44
1:A:70:TYR:O	1:A:73:PRO:HD2	2.18	0.44
1:A:126:VAL:HG22	1:A:309:PRO:HD3	2.00	0.44
1:A:350:ALA:HB1	1:A:351:PRO:CD	2.48	0.43
1:B:159:ARG:CB	1:B:185:LEU:HB2	2.48	0.43
1:B:163:LYS:HZ3	3:B:700:AME:CB	2.30	0.43
1:B:164:ILE:HG23	1:B:188:VAL:CG1	2.42	0.43
1:D:229:ALA:HB2	1:D:236:ILE:HG13	1.99	0.43
1:B:272:GLU:HB2	4:B:747:HOH:O	2.16	0.43
1:C:97:ARG:O	1:C:268:GLY:HA2	2.18	0.43
1:D:9:ARG:HH11	1:D:356:LEU:HD21	1.82	0.43
3:D:900:AME:N	3:D:900:AME:SD	2.91	0.43
1:A:9:ARG:HD3	1:A:360:THR:HG23	2.00	0.43
1:A:147:ASP:HA	4:A:663:HOH:O	2.18	0.43
1:A:169:ASP:HB2	1:A:170:VAL:H	1.46	0.43
1:A:217:LEU:O	1:A:218:GLU:C	2.59	0.43
1:B:153:LEU:HG	1:B:160:ILE:HD11	1.99	0.43
1:C:166:PRO:HD3	1:C:193:ALA:HB1	2.00	0.43
1:C:336:GLY:O	1:C:338:HIS:HD2	2.01	0.43
1:D:302:ASN:O	1:D:305:LEU:HB3	2.18	0.43
1:D:305:LEU:C	1:D:307:SER:H	2.26	0.43
1:D:329:THR:HG22	1:D:351:PRO:HA	2.01	0.43
1:A:129:SER:HA	1:A:339:LEU:O	2.18	0.43
1:B:308:LEU:CB	1:B:309:PRO:HD2	2.48	0.43
1:A:16:VAL:HG23	1:A:323:PHE:O	2.19	0.43
1:A:86:VAL:O	1:A:90:LEU:HG	2.19	0.43
1:C:20:ARG:HD3	1:C:138:ILE:HG22	1.99	0.43
1:A:118:SER:HB3	1:A:344:GLY:O	2.18	0.43
1:A:127:ARG:NH1	1:A:307:SER:C	2.77	0.43
1:C:58:GLU:HB2	1:C:98:MET:HE1	1.93	0.43
1:C:206:ASP:N	1:C:207:PRO:HD3	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ARG:NH2	1:D:357:ASP:OD1	2.51	0.43
1:D:142:ILE:CB	1:D:143:PRO:CD	2.95	0.43
1:C:294:GLU:O	1:C:299:ARG:NH2	2.46	0.43
1:D:295:THR:HG23	1:D:295:THR:H	1.48	0.43
1:A:169:ASP:O	1:A:172:PRO:HG2	2.19	0.43
1:B:171:GLU:O	1:B:174:ARG:N	2.52	0.43
1:C:21:THR:HG23	1:C:22:SER:N	2.33	0.43
1:C:169:ASP:OD1	1:C:194:TYR:OH	2.27	0.43
1:C:174:ARG:O	1:C:178:GLU:HB2	2.18	0.43
1:D:66:VAL:CG1	1:D:67:LEU:N	2.81	0.43
1:D:177:ARG:HD2	1:D:182:ASP:HA	2.00	0.43
1:A:23:PHE:CZ	3:A:600:AME:SD	3.09	0.43
1:A:112:LEU:C	1:A:114:ALA:N	2.76	0.43
1:B:49:THR:CA	1:B:98:MET:CE	2.97	0.43
1:B:83:ALA:O	1:B:86:VAL:HB	2.18	0.43
1:C:7:GLU:HB3	1:C:35:ARG:HB3	2.00	0.43
1:C:122:GLU:OE1	1:C:122:GLU:HA	2.18	0.43
1:C:305:LEU:O	1:C:307:SER:N	2.52	0.43
1:D:13:MET:HE1	1:D:295:THR:CG2	2.44	0.43
1:D:49:THR:OG1	1:D:60:ASN:OD1	2.37	0.43
1:D:119:PHE:HB2	4:D:951:HOH:O	2.19	0.43
1:D:189:ASP:OD1	1:D:189:ASP:C	2.62	0.43
1:B:31:LEU:HD13	1:B:295:THR:HG23	2.00	0.43
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.69	0.43
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.67	0.43
1:C:190:ALA:HB3	1:C:216:PRO:HA	2.01	0.43
1:C:257:VAL:O	1:C:257:VAL:HG13	2.18	0.43
1:D:72:ILE:N	1:D:73:PRO:HD2	2.33	0.43
1:D:139:MET:HB2	1:D:168:TRP:CH2	2.53	0.43
1:D:199:ALA:O	1:D:203:ALA:N	2.49	0.43
1:D:305:LEU:C	1:D:307:SER:N	2.77	0.43
1:B:145:LEU:O	1:B:149:VAL:HG23	2.19	0.42
1:A:140:ASP:HB2	1:A:144:GLN:OE1	2.19	0.42
1:A:163:LYS:HE3	1:A:191:ASN:OD1	2.19	0.42
1:B:33:LEU:CD2	1:B:46:GLU:HG3	2.48	0.42
1:C:15:LEU:HD12	1:C:26:GLN:O	2.18	0.42
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.75	0.42
1:A:171:GLU:HB2	1:A:172:PRO:CD	2.48	0.42
1:C:3:LEU:HD12	1:C:3:LEU:HA	1.59	0.42
1:C:82:THR:HB	1:C:85:LYS:HG3	2.00	0.42
1:C:226:ALA:O	1:C:229:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ARG:HG2	1:D:32:LEU:HD21	2.01	0.42
1:A:129:SER:C	1:A:130:VAL:HG13	2.43	0.42
1:A:211:LEU:O	1:A:212:LEU:HB3	2.19	0.42
1:D:9:ARG:NH1	1:D:356:LEU:HD23	2.34	0.42
1:D:320:SER:HB2	1:D:332:PHE:H	1.85	0.42
1:A:133:GLY:HA2	1:A:159:ARG:H	1.85	0.42
1:A:177:ARG:O	1:A:181:GLY:O	2.37	0.42
1:A:245:ALA:O	1:A:248:ALA:HB3	2.20	0.42
1:B:49:THR:CG2	1:B:98:MET:HE3	2.43	0.42
1:B:118:SER:O	1:B:119:PHE:C	2.62	0.42
1:A:119:PHE:CD2	1:A:301:ALA:CB	3.03	0.42
1:A:227:GLU:O	1:A:230:ARG:HB2	2.20	0.42
1:D:304:ALA:O	1:D:305:LEU:C	2.60	0.42
1:A:264:PRO:HG3	1:A:305:LEU:CD2	2.49	0.42
1:C:86:VAL:HG13	1:C:90:LEU:CD1	2.47	0.42
1:D:206:ASP:CG	1:D:233:GLN:HB2	2.45	0.42
1:D:7:GLU:HB3	1:D:35:ARG:HB3	2.01	0.42
1:A:21:THR:HG21	1:A:23:PHE:CG	2.53	0.42
1:A:312:THR:O	1:A:313:LEU:HG	2.20	0.42
1:B:32:LEU:HD12	1:B:32:LEU:HA	1.79	0.42
1:D:127[A]:ARG:HH11	1:D:127[A]:ARG:CB	2.29	0.42
1:D:161:LYS:NZ	3:D:900:AME:C	2.82	0.42
1:D:257:VAL:HG21	1:D:260:VAL:HG23	2.02	0.42
1:A:341:VAL:HA	1:A:342:PRO:HD2	1.88	0.42
1:B:112:LEU:HD22	1:B:117:ARG:HB3	2.02	0.42
1:C:4:SER:HB2	1:C:37:VAL:O	2.19	0.42
1:C:350:ALA:HB1	1:C:351:PRO:CD	2.50	0.42
1:C:352:ILE:CG2	1:C:355:LEU:HG	2.50	0.42
1:D:149:VAL:O	1:D:152:TYR:N	2.53	0.42
1:D:296:GLY:O	1:D:349:VAL:HG21	2.20	0.42
1:D:297:LEU:HD23	1:D:297:LEU:HA	1.83	0.42
1:D:303:VAL:CG1	1:D:341:VAL:HA	2.50	0.42
1:A:275:ARG:NH2	4:A:727:HOH:O	2.52	0.41
1:A:295:THR:OG1	1:A:328:ILE:HD11	2.20	0.41
1:D:270:TYR:C	4:D:940:HOH:O	2.62	0.41
1:D:288:TRP:HB3	1:D:313:LEU:HB2	2.02	0.41
1:A:74:ALA:HB2	4:A:640:HOH:O	2.19	0.41
1:A:82:THR:O	1:A:83:ALA:C	2.61	0.41
1:A:132:CYS:O	1:A:158:VAL:HG23	2.20	0.41
1:B:127[A]:ARG:NH1	1:B:129:SER:O	2.54	0.41
1:B:163:LYS:NZ	1:B:189:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:HD22	1:B:360:THR:OG1	2.20	0.41
1:D:145:LEU:O	1:D:148:VAL:HB	2.20	0.41
1:C:239:ASP:HB3	1:C:240:GLU:OE1	2.20	0.41
1:D:9:ARG:HH21	1:D:363:LYS:CE	2.31	0.41
1:A:25:THR:HG22	1:A:26:GLN:N	2.35	0.41
1:A:204[A]:ARG:NH1	1:A:204[A]:ARG:CG	2.72	0.41
1:A:214:GLU:HB2	4:A:667:HOH:O	2.20	0.41
1:D:198:ASP:C	1:D:200:PRO:HD2	2.44	0.41
1:A:8:LEU:HG	1:A:34:LEU:HD23	2.03	0.41
1:A:101:GLY:C	4:A:652:HOH:O	2.63	0.41
1:C:239:ASP:O	1:C:240:GLU:C	2.64	0.41
1:C:353:PRO:O	1:C:354:GLU:C	2.63	0.41
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.88	0.41
1:B:129:SER:C	1:B:130:VAL:CG1	2.93	0.41
1:B:242:ILE:HD12	1:B:242:ILE:HG23	1.83	0.41
1:D:173:VAL:O	1:D:174:ARG:C	2.61	0.41
1:A:68[A]:ARG:CG	1:A:68[A]:ARG:NH1	2.77	0.41
1:A:130:VAL:HA	1:A:131:PRO:HD3	1.67	0.41
1:A:159:ARG:CD	4:A:666:HOH:O	2.50	0.41
1:A:196:LEU:HD12	1:A:196:LEU:O	2.21	0.41
1:B:161:LYS:HZ1	3:B:700:AME:C	2.34	0.41
1:B:199:ALA:N	1:B:200:PRO:CD	2.84	0.41
1:C:58:GLU:HB3	1:C:98:MET:CE	2.47	0.41
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.79	0.41
1:C:154:ASP:C	1:C:156:GLY:N	2.79	0.41
1:D:87:THR:N	1:D:88:PRO:HD2	2.35	0.41
1:A:129:SER:C	1:A:130:VAL:CG1	2.93	0.41
1:A:163:LYS:HD2	1:A:189:ASP:HB3	2.03	0.41
1:B:9:ARG:NH2	1:B:357:ASP:OD1	2.53	0.41
1:B:118:SER:O	1:B:121:ALA:N	2.53	0.41
1:B:153:LEU:CG	1:B:160:ILE:HD11	2.51	0.41
1:B:171:GLU:O	1:B:172:PRO:C	2.64	0.41
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.78	0.41
1:D:149:VAL:O	1:D:150:GLY:C	2.64	0.41
1:D:149:VAL:HG13	1:D:160:ILE:HD13	2.03	0.41
1:D:161:LYS:HA	1:D:187:GLN:O	2.21	0.41
1:D:171:GLU:N	1:D:172:PRO:CD	2.82	0.41
1:D:296:GLY:HA3	1:D:329:THR:OG1	2.21	0.41
1:A:13:MET:HE1	1:A:324:TYR:CD1	2.56	0.41
1:C:20:ARG:HD3	1:C:138:ILE:CG2	2.51	0.41
1:C:239:ASP:OD1	1:C:266:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ARG:NH2	1:D:49:THR:O	2.54	0.41
1:D:141:THR:HB	1:D:143:PRO:HD2	2.02	0.41
1:B:82:THR:CG2	1:B:83:ALA:N	2.84	0.40
1:C:72:ILE:HB	1:C:73:PRO:CD	2.49	0.40
1:C:87:THR:N	1:C:88:PRO:CD	2.83	0.40
1:D:163:LYS:HD2	1:D:189:ASP:HB3	2.03	0.40
1:D:334:LEU:HD21	1:D:337:GLY:HA2	2.03	0.40
1:A:169:ASP:C	1:A:172:PRO:HD2	2.46	0.40
1:A:221:ASP:OD2	1:A:224:GLY:HA3	2.20	0.40
1:A:308:LEU:CG	1:A:309:PRO:HD2	2.50	0.40
1:B:65:HIS:CD2	1:B:69:HIS:HD2	2.39	0.40
1:B:148:VAL:CG1	1:B:152:TYR:CE1	3.04	0.40
1:D:123:LEU:HD23	1:D:123:LEU:HA	1.91	0.40
1:D:163:LYS:HD2	1:D:163:LYS:HA	1.89	0.40
1:D:216:PRO:O	1:D:217:LEU:HD23	2.20	0.40
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.38	0.40
1:A:21:THR:HG22	1:A:23:PHE:CG	2.57	0.40
1:A:142:ILE:H	1:A:143:PRO:HD2	1.86	0.40
1:B:148:VAL:O	1:B:149:VAL:C	2.62	0.40
1:C:2:LYS:HD3	4:C:818:HOH:O	2.20	0.40
1:C:217:LEU:O	1:C:218:GLU:O	2.39	0.40
1:C:338:HIS:O	1:C:339:LEU:HD12	2.21	0.40
1:A:339:LEU:HD12	1:A:339:LEU:HA	1.78	0.40
1:B:83:ALA:HA	1:B:107:VAL:HG11	2.03	0.40
1:B:240:GLU:OE2	4:B:732:HOH:O	2.22	0.40
1:B:352:ILE:O	1:B:355:LEU:N	2.55	0.40
1:C:275:ARG:O	1:C:278:ASP:N	2.54	0.40
1:D:159:ARG:HH21	1:D:161:LYS:CB	2.34	0.40
1:A:8:LEU:HD23	1:A:32:LEU:HD21	1.99	0.40
1:C:20:ARG:CG	1:C:138:ILE:HB	2.52	0.40
1:D:25:THR:CG2	1:D:26:GLN:N	2.84	0.40
1:D:46:GLU:CD	1:D:295:THR:HG23	2.46	0.40
1:D:85:LYS:O	1:D:88:PRO:CD	2.69	0.40
1:D:191:ASN:C	1:D:192:THR:CG2	2.94	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)
1:D:325:LYS:CD	1:D:325:LYS:CD[6_556]	1.08	1.12
1:D:325:LYS:CD	1:D:325:LYS:CE[6_556]	1.84	0.36

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	368/368 (100%)	334 (91%)	29 (8%)	5 (1%)	9	9
1	B	370/368 (100%)	343 (93%)	26 (7%)	1 (0%)	36	46
1	C	366/368 (100%)	337 (92%)	25 (7%)	4 (1%)	11	13
1	D	367/368 (100%)	315 (86%)	47 (13%)	5 (1%)	9	9
All	All	1471/1472 (100%)	1329 (90%)	127 (9%)	15 (1%)	12	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	THR
1	C	218	GLU
1	A	191	ASN
1	C	306	ALA
1	D	212	LEU
1	A	113	ARG
1	B	53	PRO
1	C	192	THR
1	D	306	ALA
1	A	353	PRO
1	D	364	VAL
1	D	191	ASN
1	D	149	VAL
1	A	137	GLY
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	293/291 (101%)	258 (88%)	35 (12%)	5	6
1	B	295/291 (101%)	263 (89%)	32 (11%)	6	7
1	C	291/291 (100%)	254 (87%)	37 (13%)	4	5
1	D	292/291 (100%)	255 (87%)	37 (13%)	4	5
All	All	1171/1164 (101%)	1030 (88%)	141 (12%)	5	5

All (141) 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	16	VAL
1	A	21	THR
1	A	22	SER
1	A	27	SER
1	A	32	LEU
1	A	50	MET
1	A	68[A]	ARG
1	A	68[B]	ARG
1	A	80	ASP
1	A	119	PHE
1	A	142	ILE
1	A	159	ARG
1	A	169	ASP
1	A	177	ARG
1	A	179	ARG
1	A	195	THR
1	A	204[A]	ARG
1	A	204[B]	ARG
1	A	213	ILE
1	A	217	LEU
1	A	230	ARG
1	A	289	CYS
1	A	295	THR
1	A	307	SER
1	A	317	THR
1	A	339	LEU
1	A	343	THR
1	A	349	VAL

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Mol	Chain	Res	Type
1	A	352	ILE
1	A	356	LEU
1	A	363	LYS
1	A	368	SER
1	B	8	LEU
1	B	15	LEU
1	B	21	THR
1	B	27	SER
1	B	29	ARG
1	B	31	LEU
1	B	42	GLU
1	B	66	VAL
1	B	79[A]	GLU
1	B	79[B]	GLU
1	B	79[C]	GLU
1	B	82	THR
1	B	116	GLU
1	B	127[A]	ARG
1	B	127[B]	ARG
1	B	142	ILE
1	B	159	ARG
1	B	169	ASP
1	B	174	ARG
1	B	213	ILE
1	B	217	LEU
1	B	227	GLU
1	B	232	ILE
1	B	261	ASN
1	B	287	VAL
1	B	313	LEU
1	B	317	THR
1	B	339	LEU
1	B	356	LEU
1	B	363	LYS
1	B	364	VAL
1	B	368	SER
1	C	2	LYS
1	C	8	LEU
1	C	10	ARG
1	C	12	GLN
1	C	21	THR
1	C	27	SER

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Mol	Chain	Res	Type
1	C	31	LEU
1	C	32	LEU
1	C	66	VAL
1	C	79	GLU
1	C	87	THR
1	C	90	LEU
1	C	125	SER
1	C	126	VAL
1	C	130	VAL
1	C	134	VAL
1	C	138	ILE
1	C	142	ILE
1	C	159	ARG
1	C	169	ASP
1	C	174	ARG
1	C	177	ARG
1	C	179	ARG
1	C	192	THR
1	C	213	ILE
1	C	217	LEU
1	C	227	GLU
1	C	261	ASN
1	C	299	ARG
1	C	308	LEU
1	C	317	THR
1	C	326	THR
1	C	339	LEU
1	C	343	THR
1	C	352	ILE
1	C	354	GLU
1	C	363	LYS
1	D	2	LYS
1	D	8	LEU
1	D	10	ARG
1	D	29	ARG
1	D	31	LEU
1	D	32	LEU
1	D	42	GLU
1	D	66	VAL
1	D	68	ARG
1	D	79	GLU
1	D	81	ILE

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Mol	Chain	Res	Type
1	D	82	THR
1	D	92	LYS
1	D	98	MET
1	D	111	GLU
1	D	116	GLU
1	D	117	ARG
1	D	119	PHE
1	D	126	VAL
1	D	127[A]	ARG
1	D	127[B]	ARG
1	D	130	VAL
1	D	159	ARG
1	D	169	ASP
1	D	177	ARG
1	D	179	ARG
1	D	192	THR
1	D	213	ILE
1	D	217	LEU
1	D	227	GLU
1	D	260	VAL
1	D	293	ILE
1	D	303	VAL
1	D	312	THR
1	D	343	THR
1	D	352	ILE
1	D	359	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	258	GLN
1	A	283	HIS
1	B	65	HIS
1	B	69	HIS
1	B	96	HIS
1	C	12	GLN
1	C	65	HIS
1	C	258	GLN
1	C	338	HIS
1	D	65	HIS
1	D	258	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	AME	C	800	2	11,11,11	1.83	3 (27%)	13,13,13	1.88	3 (23%)
3	AME	A	600	2	11,11,11	1.83	3 (27%)	13,13,13	2.10	7 (53%)
3	AME	B	700	2	11,11,11	1.83	3 (27%)	13,13,13	2.35	5 (38%)
3	AME	D	900	2	11,11,11	1.80	3 (27%)	13,13,13	2.04	4 (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
3	AME	C	800	2	-	9/12/12/12	-
3	AME	A	600	2	-	5/12/12/12	-
3	AME	B	700	2	-	9/12/12/12	-
3	AME	D	900	2	-	6/12/12/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	AME	CT1-N	3.83	1.46	1.34
3	A	600	AME	CT1-N	3.75	1.46	1.34
3	B	700	AME	CT1-N	3.74	1.46	1.34
3	D	900	AME	CT1-N	3.71	1.46	1.34
3	C	800	AME	OT-CT1	3.37	1.30	1.23
3	B	700	AME	OT-CT1	3.34	1.30	1.23
3	A	600	AME	OT-CT1	3.27	1.30	1.23
3	D	900	AME	OT-CT1	3.25	1.30	1.23
3	A	600	AME	O-C	3.00	1.31	1.22
3	C	800	AME	O-C	2.86	1.30	1.22
3	B	700	AME	O-C	2.81	1.30	1.22
3	D	900	AME	O-C	2.74	1.30	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	900	AME	CB-CA-N	5.08	120.96	110.91
3	B	700	AME	CB-CA-N	4.86	120.52	110.91
3	C	800	AME	CB-CA-N	4.73	120.27	110.91
3	A	600	AME	CB-CA-N	3.99	118.81	110.91
3	B	700	AME	CT2-CT1-N	3.97	122.70	116.12
3	A	600	AME	CB-CA-C	-3.47	102.13	110.35
3	B	700	AME	CB-CA-C	-3.21	102.74	110.35
3	A	600	AME	OXT-C-CA	2.78	122.93	113.51
3	B	700	AME	OXT-C-CA	2.77	122.87	113.51
3	D	900	AME	CT2-CT1-N	2.50	120.26	116.12
3	D	900	AME	OT-CT1-CT2	-2.34	117.88	122.05
3	A	600	AME	OT-CT1-CT2	-2.31	117.94	122.05
3	A	600	AME	CT2-CT1-N	2.27	119.88	116.12
3	D	900	AME	OXT-C-CA	2.24	121.08	113.51
3	B	700	AME	OT-CT1-CT2	-2.14	118.24	122.05
3	A	600	AME	OXT-C-O	-2.04	119.45	124.08
3	A	600	AME	CA-N-CT1	2.02	127.24	121.58
3	C	800	AME	OT-CT1-CT2	-2.02	118.46	122.05
3	C	800	AME	CB-CA-C	-2.01	105.58	110.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	700	AME	CT2-CT1-N-CA

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Mol	Chain	Res	Type	Atoms
3	B	700	AME	OT-CT1-N-CA
3	B	700	AME	C-CA-CB-CG
3	B	700	AME	N-CA-CB-CG
3	C	800	AME	CT2-CT1-N-CA
3	C	800	AME	CA-CB-CG-SD
3	C	800	AME	OT-CT1-N-CA
3	D	900	AME	O-C-CA-N
3	D	900	AME	OXT-C-CA-N
3	B	700	AME	CA-CB-CG-SD
3	D	900	AME	CA-CB-CG-SD
3	A	600	AME	OXT-C-CA-CB
3	A	600	AME	CT2-CT1-N-CA
3	A	600	AME	CA-CB-CG-SD
3	B	700	AME	OXT-C-CA-N
3	D	900	AME	CB-CG-SD-CE
3	A	600	AME	OT-CT1-N-CA
3	C	800	AME	C-CA-CB-CG
3	D	900	AME	C-CA-CB-CG
3	A	600	AME	O-C-CA-CB
3	B	700	AME	O-C-CA-N
3	C	800	AME	O-C-CA-N
3	C	800	AME	OXT-C-CA-N
3	C	800	AME	N-CA-CB-CG
3	B	700	AME	O-C-CA-CB
3	C	800	AME	OXT-C-CA-CB
3	D	900	AME	OXT-C-CA-CB
3	C	800	AME	O-C-CA-CB
3	B	700	AME	OXT-C-CA-CB

There are no ring outliers.

4 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	800	AME	16	0
3	A	600	AME	12	0
3	B	700	AME	8	0
3	D	900	AME	12	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/368 (100%)	-1.30	0 100 100	23, 55, 88, 100	2 (0%)
1	B	368/368 (100%)	-1.45	0 100 100	20, 39, 77, 100	3 (0%)
1	C	368/368 (100%)	-1.34	0 100 100	24, 48, 84, 100	0
1	D	368/368 (100%)	-1.25	0 100 100	24, 58, 93, 100	1 (0%)
All	All	1472/1472 (100%)	-1.33	0 100 100	20, 49, 87, 100	6 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	AME	A	600	12/12	0.99	0.06	62,88,100,100	0
3	AME	B	700	12/12	0.99	0.06	36,63,80,97	0
3	AME	C	800	12/12	0.99	0.06	26,97,100,100	0
3	AME	D	900	12/12	0.99	0.05	40,83,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	601	1/1	1.00	0.01	41,41,41,41	0
2	MG	B	701	1/1	1.00	0.01	35,35,35,35	0
2	MG	C	801	1/1	1.00	0.03	49,49,49,49	0
2	MG	D	901	1/1	1.00	0.01	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.