



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:44 PM UTC

PDB ID : 6QZT / pdb_00006qzt
Title : Crystal structure of Csx1 from Sulfolobus islandicus orthorhombic form
Authors : Molina, R.; Montoya, G.; Sofos, N.; Stella, S.
Deposited on : 2019-03-12
Resolution : 2.93 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
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

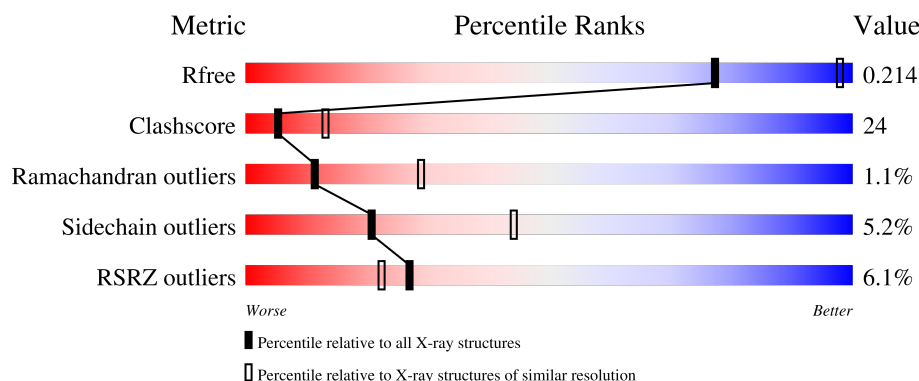
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	454	8% 61% 34% 5%
1	B	454	9% 61% 34% 5%
1	C	454	% 70% 26% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11190 atoms, of which 0 are hydrogens and 0 are deuteriums.

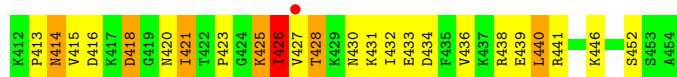
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-associated (Cas) DxTHG family.

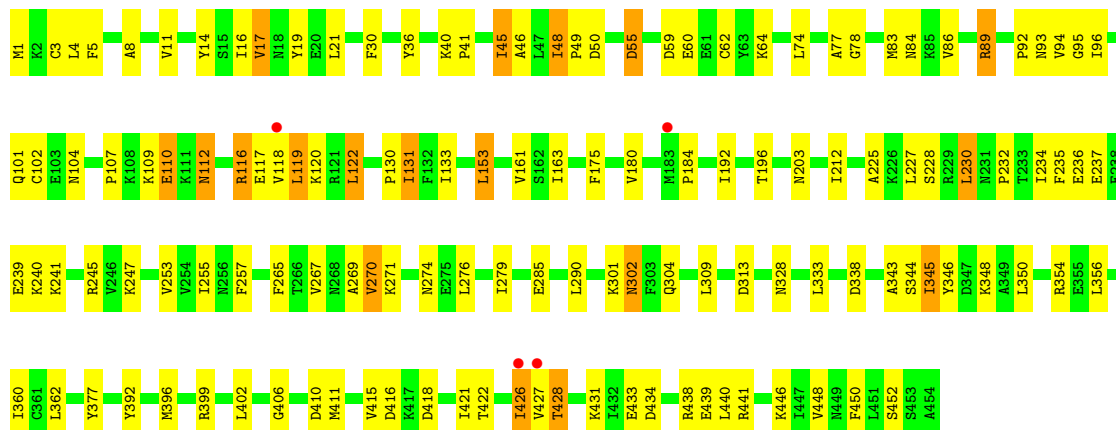
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			
1	B	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			
1	C	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	79	Total	O	0	0
			79	79		
2	B	69	Total	O	0	0
			69	69		
2	C	116	Total	O	0	0
			116	116		



• Molecule 1: CRISPR-associated (Cas) DxTHG family



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.23Å 118.68Å 356.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.32 – 2.93 39.32 – 2.93	Depositor EDS
% Data completeness (in resolution range)	68.5 (39.32-2.93) 68.7 (39.32-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.196 , 0.245 0.226 , 0.214	Depositor DCC
R_{free} test set	1691 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 105.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11190	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	0/3703	1.48	38/4990 (0.8%)
1	B	0.91	2/3703 (0.1%)	1.47	33/4990 (0.7%)
1	C	0.90	2/3703 (0.1%)	1.49	37/4990 (0.7%)
All	All	0.89	4/11109 (0.0%)	1.48	108/14970 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	LYS	CA-C	5.90	1.57	1.53
1	C	40	LYS	CA-C	5.82	1.57	1.53
1	B	40	LYS	CA-CB	5.56	1.56	1.52
1	C	55	ASP	CA-C	5.11	1.58	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	SER	N-CA-C	8.89	121.05	111.36
1	B	440	LEU	N-CA-C	8.60	120.66	111.28
1	C	448	VAL	N-CA-C	8.59	119.38	110.62
1	C	116	ARG	N-CA-C	8.53	123.09	110.46
1	A	432	ILE	N-CA-C	-8.41	102.51	110.42
1	A	300	HIS	N-CA-C	8.30	123.00	108.56
1	B	105	GLY	CA-C-O	-8.25	115.45	121.88
1	C	450	PHE	N-CA-C	-8.02	102.48	111.14
1	A	299	GLU	N-CA-C	-7.84	102.67	111.14
1	B	439	GLU	N-CA-C	7.83	122.60	112.89
1	B	20	GLU	N-CA-C	6.97	120.27	108.90
1	A	432	ILE	N-CA-CB	6.92	118.47	110.65
1	A	108	LYS	N-CA-C	-6.79	101.39	110.55
1	A	416	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	343	ALA	N-CA-C	-6.52	100.63	110.28
1	A	430	ASN	N-CA-C	6.48	120.39	112.23
1	C	236	GLU	N-CA-C	6.40	118.28	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CA-C-N	6.25	128.65	120.28
1	A	59	ASP	C-N-CA	6.25	128.65	120.28
1	C	343	ALA	N-CA-C	-6.23	101.06	110.28
1	B	416	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	393	SER	CA-C-N	6.16	126.78	119.94
1	A	393	SER	C-N-CA	6.16	126.78	119.94
1	A	49	PRO	N-CA-C	-6.14	102.20	111.41
1	B	345	ILE	CA-C-N	6.09	128.36	120.44
1	B	345	ILE	C-N-CA	6.09	128.36	120.44
1	B	182	GLY	CA-C-O	-6.08	117.72	122.52
1	C	265	PHE	CA-C-N	6.03	128.65	120.38
1	C	265	PHE	C-N-CA	6.03	128.65	120.38
1	A	328	ASN	CA-CB-CG	6.03	118.63	112.60
1	B	104	ASN	N-CA-C	6.01	118.18	109.71
1	A	343	ALA	N-CA-C	-5.97	101.44	110.28
1	A	345	ILE	CA-C-N	5.96	128.18	120.44
1	A	345	ILE	C-N-CA	5.96	128.18	120.44
1	B	452	SER	CA-C-N	5.93	128.23	120.28
1	B	452	SER	C-N-CA	5.93	128.23	120.28
1	B	102	CYS	N-CA-C	5.92	118.85	109.50
1	C	110	GLU	CA-C-N	5.92	130.60	120.72
1	C	110	GLU	C-N-CA	5.92	130.60	120.72
1	C	428	THR	CA-C-N	5.90	128.47	120.38
1	C	428	THR	C-N-CA	5.90	128.47	120.38
1	A	392	TYR	CA-C-N	5.88	129.65	120.82
1	A	392	TYR	C-N-CA	5.88	129.65	120.82
1	C	122	LEU	N-CA-C	-5.88	102.64	109.93
1	A	439	GLU	N-CA-C	5.86	117.67	111.28
1	C	30	PHE	CA-C-N	5.83	129.57	120.82
1	C	30	PHE	C-N-CA	5.83	129.57	120.82
1	A	343	ALA	CA-C-N	-5.78	113.41	122.08
1	A	343	ALA	C-N-CA	-5.78	113.41	122.08
1	B	265	PHE	CA-C-N	5.71	127.93	120.28
1	B	265	PHE	C-N-CA	5.71	127.93	120.28
1	C	84	ASN	CA-CB-CG	5.70	118.30	112.60
1	C	452	SER	CA-C-N	5.70	127.91	120.28
1	C	452	SER	C-N-CA	5.70	127.91	120.28
1	B	428	THR	CA-C-N	5.68	128.16	120.38
1	B	428	THR	C-N-CA	5.68	128.16	120.38
1	A	303	PHE	CA-C-N	5.68	129.34	120.82
1	A	303	PHE	C-N-CA	5.68	129.34	120.82
1	A	310	VAL	CA-C-N	5.68	128.20	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	VAL	C-N-CA	5.68	128.20	120.54
1	B	343	ALA	CA-C-N	-5.65	113.60	122.08
1	B	343	ALA	C-N-CA	-5.65	113.60	122.08
1	C	345	ILE	CA-C-N	5.60	128.10	120.54
1	C	345	ILE	C-N-CA	5.60	128.10	120.54
1	A	387	TYR	N-CA-C	-5.53	105.25	111.28
1	C	328	ASN	CA-CB-CG	5.50	118.10	112.60
1	C	343	ALA	CA-C-N	-5.49	114.09	122.21
1	C	343	ALA	C-N-CA	-5.49	114.09	122.21
1	C	112	ASN	CA-CB-CG	5.47	118.08	112.60
1	C	60	GLU	CB-CG-CD	5.46	121.89	112.60
1	B	313	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	452	SER	CA-C-N	5.44	127.57	120.28
1	A	452	SER	C-N-CA	5.44	127.57	120.28
1	C	153	LEU	N-CA-C	-5.37	105.18	112.26
1	C	313	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	96	ILE	N-CA-C	5.36	115.96	108.89
1	A	265	PHE	CA-C-N	5.34	127.44	120.28
1	A	265	PHE	C-N-CA	5.34	127.44	120.28
1	C	422	THR	CB-CA-C	5.34	117.61	110.13
1	A	346	TYR	N-CA-C	5.32	116.77	111.07
1	B	242	VAL	N-CA-CB	5.31	118.55	110.58
1	C	269	ALA	CA-C-N	5.31	129.01	120.30
1	C	269	ALA	C-N-CA	5.31	129.01	120.30
1	B	97	ALA	CA-C-N	5.30	131.67	121.54
1	B	97	ALA	C-N-CA	5.30	131.67	121.54
1	C	119	LEU	N-CA-C	5.29	118.43	109.76
1	C	84	ASN	N-CA-C	-5.28	105.11	112.45
1	B	328	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	156	GLY	CA-C-O	-5.24	118.62	122.23
1	C	228	SER	N-CA-C	5.23	117.39	111.11
1	A	313	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	117	GLU	CA-C-N	5.19	128.27	120.69
1	B	117	GLU	C-N-CA	5.19	128.27	120.69
1	A	74	LEU	N-CA-C	-5.18	106.92	114.12
1	B	225	ALA	CA-C-N	5.11	127.08	120.44
1	B	225	ALA	C-N-CA	5.11	127.08	120.44
1	B	52	LEU	N-CA-C	5.10	118.76	112.54
1	B	296	ASN	CA-C-N	5.09	127.61	120.28
1	B	296	ASN	C-N-CA	5.09	127.61	120.28
1	A	158	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	387	TYR	CA-C-N	5.09	129.22	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	TYR	C-N-CA	5.09	129.22	120.72
1	A	416	ASP	CA-C-N	5.09	127.35	120.38
1	A	416	ASP	C-N-CA	5.09	127.35	120.38
1	C	225	ALA	CA-C-N	5.08	127.05	120.44
1	C	225	ALA	C-N-CA	5.08	127.05	120.44
1	C	59	ASP	CA-C-N	5.07	127.03	120.44
1	C	59	ASP	C-N-CA	5.07	127.03	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3642	0	3675	213	0
1	B	3642	0	3677	248	0
1	C	3642	0	3675	113	0
2	A	79	0	0	3	0
2	B	69	0	0	1	0
2	C	116	0	0	1	0
All	All	11190	0	11027	529	0

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 24.

All (529) 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:28:THR:HG21	1:B:33:HIS:HB3	1.26	1.13
1:B:55:ASP:HB2	1:B:102:CYS:SG	1.88	1.13
1:C:118:VAL:HG22	1:C:119:LEU:H	1.11	1.11
1:A:48:ILE:HD11	1:A:90:LYS:CG	1.82	1.08
1:A:384:VAL:O	1:A:388:LEU:HB2	1.52	1.08
1:A:99:ALA:H	1:A:123:PRO:HG2	1.16	1.08
1:A:48:ILE:HD11	1:A:90:LYS:HG3	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:HB3	1:A:119:LEU:CD1	1.87	1.05
1:A:99:ALA:HB3	1:A:123:PRO:HB2	1.38	1.03
1:B:49:PRO:HG2	1:B:52:LEU:HD23	1.41	1.02
1:B:49:PRO:HG2	1:B:52:LEU:CD2	1.91	1.01
1:C:235:PHE:HE1	1:C:240:LYS:CA	1.74	1.01
1:A:48:ILE:HG13	1:A:90:LYS:HA	1.39	1.00
1:B:18:ASN:OD1	1:B:189:ILE:HA	1.62	1.00
1:A:253:VAL:HG12	1:A:276:LEU:HD11	1.44	0.99
1:A:154:THR:HG22	1:A:178:ALA:H	1.25	0.99
1:A:48:ILE:CD1	1:A:90:LYS:HG3	1.92	0.97
1:B:74:LEU:HD11	1:B:186:LYS:NZ	1.80	0.97
1:A:118:VAL:HG22	1:A:119:LEU:H	1.30	0.96
1:A:50:ASP:HB3	1:B:297:TRP:HH2	1.30	0.95
1:A:266:THR:O	1:A:270:VAL:HG23	1.69	0.93
1:B:94:VAL:HG12	1:B:95:GLY:N	1.84	0.91
1:C:235:PHE:HE1	1:C:240:LYS:CB	1.84	0.89
1:A:175:PHE:H	1:A:196:THR:HG22	1.38	0.89
1:A:330:LEU:HD12	1:B:421:ILE:HD11	1.54	0.89
1:C:16:ILE:HD11	1:C:74:LEU:HB3	1.55	0.89
1:A:99:ALA:H	1:A:123:PRO:CG	1.87	0.88
1:C:253:VAL:HG12	1:C:276:LEU:HD21	1.53	0.88
1:A:99:ALA:HB3	1:A:123:PRO:CB	2.04	0.87
1:B:28:THR:CG2	1:B:33:HIS:HB3	2.05	0.87
1:C:16:ILE:HD12	1:C:74:LEU:HD22	1.56	0.86
1:B:151:VAL:HG12	1:B:153:LEU:CD1	2.07	0.85
1:B:49:PRO:CG	1:B:52:LEU:HD23	2.07	0.85
1:A:330:LEU:CD1	1:B:421:ILE:HD11	2.07	0.84
1:A:99:ALA:N	1:A:123:PRO:HG2	1.92	0.84
1:B:8:ALA:HB1	1:B:63:TYR:CZ	2.12	0.84
1:B:253:VAL:HG12	1:B:276:LEU:HD21	1.57	0.84
1:B:51:SER:HB3	1:B:124:TYR:CE2	2.12	0.84
1:C:428:THR:HG22	1:C:431:LYS:HG3	1.58	0.83
1:C:440:LEU:HD12	1:C:440:LEU:O	1.78	0.83
1:B:21:LEU:HD22	1:B:192:ILE:HD11	1.61	0.83
1:C:112:ASN:HD22	1:C:116:ARG:HB3	1.42	0.83
1:C:235:PHE:HE1	1:C:240:LYS:HA	1.41	0.83
1:B:151:VAL:HG12	1:B:153:LEU:HD12	1.59	0.83
1:C:101:GLN:HG3	1:C:120:LYS:CE	2.09	0.83
1:A:175:PHE:H	1:A:196:THR:CG2	1.92	0.82
1:B:52:LEU:HD12	1:B:53:VAL:N	1.95	0.82
1:B:8:ALA:HB1	1:B:63:TYR:CE1	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ASN:HB2	2:C:542:HOH:O	1.77	0.82
1:B:406:GLY:HA2	1:B:411:MET:HG3	1.61	0.81
1:A:273:MET:HE1	1:A:325:ILE:HG22	1.61	0.81
1:C:118:VAL:HG22	1:C:119:LEU:N	1.90	0.81
1:C:235:PHE:CE1	1:C:240:LYS:CA	2.63	0.81
1:C:235:PHE:CE1	1:C:240:LYS:HA	2.15	0.80
1:B:94:VAL:CG1	1:B:95:GLY:H	1.95	0.80
1:C:234:ILE:HD12	1:C:234:ILE:O	1.81	0.80
1:A:95:GLY:O	1:A:124:TYR:CE2	2.35	0.80
1:A:93:ASN:ND2	1:A:160:LEU:HD11	1.97	0.80
1:A:301:LYS:O	1:A:304:GLN:HB2	1.81	0.79
1:B:7:ILE:O	1:B:155:HIS:HB2	1.82	0.79
1:B:28:THR:HG21	1:B:33:HIS:CB	2.09	0.79
1:C:235:PHE:CE1	1:C:240:LYS:HB2	2.18	0.78
1:A:270:VAL:HG13	1:A:332:LYS:HB3	1.65	0.78
1:A:98:SER:HB2	1:A:120:LYS:HD2	1.64	0.77
1:A:174:LYS:HA	1:A:196:THR:CG2	2.14	0.76
1:C:235:PHE:CE1	1:C:240:LYS:CB	2.68	0.76
1:A:96:ILE:CD1	1:B:190:VAL:HG23	2.15	0.76
1:B:94:VAL:CG1	1:B:95:GLY:N	2.48	0.76
1:A:174:LYS:HA	1:A:196:THR:HG21	1.67	0.76
1:A:50:ASP:HB3	1:B:297:TRP:CH2	2.20	0.76
1:B:153:LEU:HD23	1:B:161:VAL:HG13	1.67	0.76
1:B:94:VAL:HG12	1:B:95:GLY:H	1.46	0.75
1:A:96:ILE:HD12	1:B:190:VAL:HG23	1.67	0.75
1:B:20:GLU:CG	1:B:191:ASN:HB3	2.16	0.75
1:B:49:PRO:CG	1:B:52:LEU:CD2	2.65	0.75
1:A:270:VAL:HG13	1:A:332:LYS:CB	2.17	0.75
1:A:28:THR:HG21	1:A:33:HIS:HB3	1.69	0.75
1:A:270:VAL:HG21	1:A:333:LEU:HG	1.68	0.75
1:B:5:PHE:CE1	1:B:45:ILE:HD13	2.21	0.74
1:B:60:GLU:O	1:B:64:LYS:HE3	1.86	0.73
1:B:61:GLU:HG3	1:B:64:LYS:HD2	1.69	0.73
1:C:267:VAL:O	1:C:271:LYS:HG2	1.89	0.73
1:A:212:ILE:HD13	1:A:319:LYS:HB3	1.70	0.73
1:B:61:GLU:HA	1:B:64:LYS:CD	2.19	0.73
1:A:28:THR:HA	1:A:76:PHE:CZ	2.24	0.72
1:B:20:GLU:HG3	1:B:191:ASN:HB3	1.71	0.72
1:B:52:LEU:HD12	1:B:52:LEU:C	2.14	0.72
1:B:61:GLU:HA	1:B:64:LYS:HB2	1.69	0.72
1:B:20:GLU:OE2	1:B:191:ASN:ND2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HD11	1:B:186:LYS:HZ1	1.49	0.72
1:A:184:PRO:HB2	1:A:188:SER:CB	2.20	0.72
1:C:101:GLN:HG3	1:C:120:LYS:HE3	1.70	0.72
1:B:19:TYR:CE2	1:B:28:THR:O	2.43	0.72
1:C:112:ASN:ND2	1:C:116:ARG:HB3	2.03	0.72
1:C:230:LEU:HD12	1:C:230:LEU:C	2.15	0.72
1:A:118:VAL:HG22	1:A:119:LEU:N	2.05	0.71
1:A:388:LEU:HD13	1:A:396:MET:HG2	1.72	0.71
1:B:61:GLU:HA	1:B:64:LYS:CG	2.21	0.71
1:C:234:ILE:HD12	1:C:234:ILE:C	2.16	0.71
1:A:48:ILE:HD11	1:A:90:LYS:CD	2.19	0.71
1:A:9:GLY:O	1:A:52:LEU:HD13	1.90	0.71
1:B:74:LEU:HD11	1:B:186:LYS:HZ2	1.55	0.71
1:A:55:ASP:HA	1:A:102:CYS:HB3	1.73	0.70
1:A:108:LYS:HB3	1:A:119:LEU:HD11	1.70	0.70
1:B:95:GLY:O	1:B:124:TYR:CD1	2.45	0.70
1:B:425:LYS:O	1:B:425:LYS:HG2	1.88	0.70
1:A:68:ILE:HG22	1:A:72:LYS:HE2	1.72	0.70
1:A:131:ILE:HG12	1:B:307:THR:HA	1.74	0.70
1:A:158:ASN:CG	1:B:161:VAL:HG21	2.16	0.70
1:A:354:ARG:HD3	1:A:396:MET:SD	2.32	0.70
1:A:388:LEU:CD1	1:A:396:MET:SD	2.79	0.70
1:B:61:GLU:O	1:B:64:LYS:HB2	1.91	0.69
1:C:45:ILE:N	1:C:45:ILE:HD12	2.07	0.69
1:A:388:LEU:HD13	1:A:396:MET:CG	2.22	0.69
1:C:232:PRO:HB2	1:C:235:PHE:HD2	1.57	0.69
1:C:301:LYS:O	1:C:304:GLN:HB2	1.92	0.69
1:B:18:ASN:OD1	1:B:189:ILE:CA	2.40	0.69
1:B:10:ASP:O	1:B:14:TYR:CZ	2.45	0.69
1:B:74:LEU:CD1	1:B:186:LYS:NZ	2.55	0.69
1:A:135:ASN:ND2	1:B:311:LEU:H	1.91	0.69
1:B:28:THR:HG23	1:B:30:PHE:O	1.92	0.68
1:B:101:GLN:NE2	1:B:121:ARG:HB2	2.08	0.68
1:A:99:ALA:HB3	1:A:123:PRO:CG	2.23	0.68
1:B:230:LEU:HD21	1:B:309:LEU:HD12	1.73	0.68
1:C:406:GLY:HA2	1:C:411:MET:HG3	1.76	0.68
1:B:14:TYR:CZ	1:B:155:HIS:CE1	2.82	0.67
1:C:16:ILE:CD1	1:C:74:LEU:HB3	2.24	0.67
1:A:93:ASN:O	1:A:128:ARG:HD3	1.94	0.67
1:B:51:SER:HB3	1:B:124:TYR:HE2	1.59	0.67
1:B:215:LEU:HD22	1:B:261:ILE:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLU:OE1	1:C:302:ASN:ND2	2.28	0.67
1:C:180:VAL:HG11	1:C:184:PRO:HG3	1.77	0.67
1:A:108:LYS:HB3	1:A:119:LEU:HD13	1.74	0.66
1:A:141:PHE:HB3	1:A:171:PHE:CE2	2.30	0.66
1:A:253:VAL:HG12	1:A:276:LEU:CD1	2.21	0.66
1:B:414:ASN:HB2	2:B:502:HOH:O	1.96	0.66
1:C:232:PRO:HB2	1:C:235:PHE:CD2	2.30	0.66
1:B:67:VAL:HG12	1:B:79:MET:HE1	1.77	0.66
1:B:235:PHE:HE2	1:B:240:LYS:HG3	1.59	0.66
1:A:18:ASN:HB2	1:A:189:ILE:HA	1.77	0.66
1:A:217:GLU:HB3	1:A:258:LEU:HB2	1.77	0.66
1:A:132:PHE:CD1	1:B:304:GLN:HA	2.30	0.66
1:A:96:ILE:CD1	1:B:190:VAL:CG2	2.74	0.65
1:B:60:GLU:C	1:B:64:LYS:HE3	2.22	0.65
1:A:28:THR:HG22	1:A:29:PHE:H	1.62	0.65
1:A:154:THR:HG22	1:A:178:ALA:N	2.06	0.65
1:A:153:LEU:HD21	1:A:175:PHE:HD2	1.61	0.64
1:B:95:GLY:O	1:B:124:TYR:HD1	1.78	0.64
1:C:153:LEU:HD11	1:C:175:PHE:HD2	1.62	0.64
1:A:108:LYS:HD3	1:A:119:LEU:HD11	1.80	0.64
1:C:48:ILE:HG13	1:C:48:ILE:O	1.97	0.64
1:B:28:THR:HB	1:B:33:HIS:CD2	2.32	0.64
1:B:121:ARG:HG2	1:B:123:PRO:HD2	1.79	0.64
1:B:14:TYR:HB3	1:B:29:PHE:HB2	1.79	0.64
1:B:38:LEU:HD11	1:B:39:PHE:CE2	2.33	0.63
1:B:29:PHE:H	1:B:29:PHE:HD2	1.47	0.63
1:A:7:ILE:HG21	1:A:156:GLY:HA3	1.81	0.63
1:B:62:CYS:HG	1:B:102:CYS:CB	2.10	0.63
1:A:99:ALA:HB3	1:A:123:PRO:HG2	1.82	0.62
1:C:392:TYR:OH	1:C:446:LYS:HB3	1.99	0.62
1:A:99:ALA:N	1:A:123:PRO:CG	2.56	0.62
1:A:94:VAL:HG11	1:B:193:VAL:HG11	1.81	0.61
1:C:118:VAL:CG2	1:C:119:LEU:H	1.96	0.61
1:B:61:GLU:HA	1:B:64:LYS:CB	2.29	0.61
1:A:311:LEU:H	1:B:135:ASN:ND2	1.98	0.61
1:B:61:GLU:HA	1:B:64:LYS:HD2	1.81	0.61
1:A:132:PHE:CG	1:B:304:GLN:HA	2.35	0.61
1:B:427:VAL:HG23	1:B:431:LYS:HD2	1.81	0.61
1:B:51:SER:CB	1:B:124:TYR:CE2	2.83	0.61
1:A:270:VAL:CG1	1:A:332:LYS:HB2	2.31	0.61
1:B:24:GLN:OE1	1:B:38:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:CD1	1:B:186:LYS:HZ2	2.14	0.60
1:B:8:ALA:CB	1:B:63:TYR:CZ	2.84	0.60
1:B:10:ASP:OD1	1:B:12:SER:N	2.35	0.60
1:A:175:PHE:N	1:A:196:THR:CG2	2.65	0.60
1:B:61:GLU:CA	1:B:64:LYS:HB2	2.32	0.59
1:A:100:ILE:HA	1:A:119:LEU:O	2.03	0.59
1:A:95:GLY:O	1:A:124:TYR:HE2	1.86	0.59
1:B:235:PHE:CE2	1:B:240:LYS:HG3	2.36	0.59
1:C:130:PRO:HB3	1:C:163:ILE:HD11	1.83	0.59
1:A:253:VAL:CG1	1:A:276:LEU:HD11	2.26	0.59
1:C:354:ARG:HD3	1:C:396:MET:SD	2.43	0.59
1:B:270:VAL:HA	1:B:273:MET:HG3	1.84	0.58
1:C:116:ARG:HG2	1:C:117:GLU:N	2.18	0.58
1:A:297:TRP:HE1	1:B:90:LYS:HG3	1.67	0.58
1:C:227:LEU:O	1:C:230:LEU:HB3	2.02	0.58
1:C:257:PHE:HB2	1:C:276:LEU:HD11	1.85	0.58
1:A:94:VAL:HG13	1:B:179:PRO:HG2	1.83	0.58
1:A:96:ILE:HD11	1:B:190:VAL:HB	1.86	0.58
1:A:158:ASN:HB3	1:B:161:VAL:HG11	1.85	0.58
1:B:31:ALA:HB3	1:B:154:THR:HG21	1.86	0.58
1:A:130:PRO:HB3	1:A:163:ILE:HD11	1.84	0.58
1:A:439:GLU:OE2	1:A:439:GLU:HA	2.02	0.58
1:B:4:LEU:HB2	1:B:41:PRO:HG3	1.86	0.58
1:B:62:CYS:CB	1:B:102:CYS:HG	2.15	0.58
1:A:16:ILE:HG13	1:A:74:LEU:HD13	1.86	0.58
1:A:175:PHE:N	1:A:196:THR:HG22	2.14	0.58
1:A:49:PRO:HA	1:A:91:ILE:O	2.04	0.57
1:B:130:PRO:HB3	1:B:163:ILE:HD11	1.86	0.57
1:A:93:ASN:HD22	1:A:160:LEU:HD11	1.68	0.57
1:C:8:ALA:HB3	1:C:48:ILE:HA	1.86	0.57
1:B:151:VAL:CG1	1:B:153:LEU:CD1	2.80	0.57
1:B:346:TYR:OH	1:B:433:GLU:HG2	2.03	0.57
1:C:253:VAL:HG12	1:C:276:LEU:CD2	2.32	0.57
1:C:350:LEU:HD12	1:C:402:LEU:HD12	1.87	0.57
1:B:25:THR:HG22	1:B:25:THR:O	2.03	0.57
1:B:350:LEU:HD12	1:B:402:LEU:HD12	1.87	0.57
1:A:118:VAL:CG2	1:A:119:LEU:H	2.13	0.57
1:A:6:TYR:OH	1:A:63:TYR:CE2	2.58	0.57
1:A:350:LEU:HD12	1:A:402:LEU:HD12	1.87	0.57
1:B:38:LEU:HD11	1:B:39:PHE:CD2	2.39	0.57
1:A:91:ILE:HD11	1:A:140:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HD2	1:B:52:LEU:HD21	1.87	0.56
1:B:38:LEU:HD12	1:B:39:PHE:N	2.20	0.56
1:B:235:PHE:CD1	1:B:235:PHE:N	2.72	0.56
1:A:176:TYR:HE1	1:A:194:GLU:OE1	1.88	0.56
1:B:93:ASN:HB3	1:B:124:TYR:OH	2.06	0.56
1:C:45:ILE:HG23	1:C:89:ARG:HG3	1.87	0.56
1:A:99:ALA:CB	1:A:123:PRO:HG2	2.35	0.56
1:C:239:GLU:CD	1:C:302:ASN:ND2	2.64	0.56
1:C:16:ILE:CD1	1:C:74:LEU:HD22	2.34	0.56
1:B:14:TYR:OH	1:B:155:HIS:CE1	2.58	0.56
1:A:21:LEU:CD1	1:A:192:ILE:HG13	2.36	0.55
1:A:48:ILE:HD12	1:A:48:ILE:O	2.06	0.55
1:B:157:THR:HG22	1:B:158:ASN:N	2.21	0.55
1:B:60:GLU:O	1:B:64:LYS:HG3	2.07	0.55
1:C:230:LEU:HD21	1:C:309:LEU:HB2	1.89	0.55
1:A:28:THR:HA	1:A:76:PHE:HZ	1.67	0.55
1:A:79:MET:O	1:A:83:MET:HG2	2.08	0.54
1:A:174:LYS:HA	1:A:196:THR:HG22	1.88	0.54
1:A:243:LEU:HD11	1:A:303:PHE:HE2	1.73	0.54
1:B:53:VAL:CG2	1:B:62:CYS:SG	2.95	0.54
1:B:97:ALA:H	1:B:124:TYR:HB3	1.71	0.54
1:C:62:CYS:SG	1:C:107:PRO:HD3	2.47	0.54
1:A:135:ASN:HD21	1:B:311:LEU:H	1.56	0.54
1:B:7:ILE:O	1:B:155:HIS:CB	2.54	0.54
1:B:97:ALA:H	1:B:124:TYR:CB	2.21	0.54
1:B:315:ASP:HA	1:B:318:LEU:HD23	1.90	0.54
1:C:11:VAL:HG23	1:C:14:TYR:CD2	2.43	0.54
1:A:101:GLN:HG2	1:A:102:CYS:H	1.72	0.54
1:A:101:GLN:HG2	1:A:102:CYS:N	2.22	0.54
1:B:131:ILE:HD12	1:B:131:ILE:H	1.73	0.54
1:A:5:PHE:CD1	1:A:45:ILE:HB	2.43	0.54
1:B:70:ARG:HH12	1:B:74:LEU:HD11	1.73	0.54
1:A:28:THR:HG22	1:A:29:PHE:N	2.23	0.54
1:A:184:PRO:HB2	1:A:188:SER:HB2	1.90	0.54
1:C:346:TYR:OH	1:C:433:GLU:HG2	2.07	0.54
1:A:9:GLY:O	1:A:52:LEU:CD1	2.56	0.53
1:A:47:LEU:HG	1:A:91:ILE:HD13	1.89	0.53
1:B:19:TYR:HE2	1:B:28:THR:O	1.89	0.53
1:C:239:GLU:OE2	1:C:302:ASN:ND2	2.41	0.53
1:B:434:ASP:O	1:B:438:ARG:HB2	2.08	0.53
1:B:61:GLU:CG	1:B:64:LYS:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLU:HG3	1:B:20:GLU:O	2.08	0.53
1:B:253:VAL:HG12	1:B:276:LEU:CD2	2.34	0.53
1:B:74:LEU:CD1	1:B:186:LYS:HZ1	2.20	0.53
1:C:118:VAL:CG2	1:C:119:LEU:N	2.62	0.53
1:A:50:ASP:OD2	1:A:128:ARG:NH1	2.41	0.53
1:A:370:PHE:HB2	1:B:413:PRO:HD2	1.90	0.53
1:B:151:VAL:CG1	1:B:153:LEU:HD11	2.38	0.53
1:A:387:TYR:HE1	1:A:391:ARG:HG3	1.74	0.53
1:A:48:ILE:HD12	1:A:48:ILE:C	2.33	0.53
1:B:235:PHE:CE2	1:B:240:LYS:HE2	2.44	0.53
1:A:48:ILE:HG13	1:A:90:LYS:CA	2.27	0.53
1:B:30:PHE:CZ	1:B:33:HIS:HB2	2.44	0.52
1:B:233:THR:O	1:B:235:PHE:CD1	2.62	0.52
1:A:108:LYS:CG	1:A:119:LEU:HD11	2.40	0.52
1:B:96:ILE:HA	1:B:124:TYR:HD1	1.74	0.52
1:B:257:PHE:HB2	1:B:276:LEU:HD11	1.90	0.52
1:A:179:PRO:HG3	1:B:159:VAL:HG21	1.91	0.52
1:B:436:VAL:HA	1:B:440:LEU:HB2	1.91	0.52
1:A:96:ILE:HD11	1:B:190:VAL:CB	2.40	0.52
1:A:124:TYR:CE1	1:A:126:GLU:CG	2.93	0.52
1:C:8:ALA:HB2	1:C:48:ILE:HG22	1.91	0.52
1:C:153:LEU:HD11	1:C:175:PHE:CD2	2.43	0.52
1:A:270:VAL:HG13	1:A:332:LYS:HB2	1.90	0.52
1:B:28:THR:HG21	1:B:34:ALA:N	2.25	0.52
1:B:428:THR:HG22	1:B:430:ASN:H	1.74	0.52
1:C:101:GLN:HG3	1:C:120:LYS:HE2	1.92	0.52
1:C:239:GLU:CD	1:C:302:ASN:HD22	2.17	0.52
1:A:392:TYR:OH	1:A:446:LYS:HE2	2.10	0.52
1:B:6:TYR:CB	1:B:152:ASP:HB3	2.39	0.52
1:B:52:LEU:C	1:B:52:LEU:CD1	2.82	0.52
1:B:101:GLN:HE21	1:B:121:ARG:HD3	1.75	0.52
1:B:46:ALA:HB3	1:B:88:ILE:HG13	1.92	0.52
1:B:62:CYS:SG	1:B:102:CYS:CB	2.97	0.52
1:A:346:TYR:OH	1:A:433:GLU:HG2	2.11	0.51
1:B:19:TYR:CE1	1:B:190:VAL:HG13	2.45	0.51
1:A:389:ARG:O	1:A:389:ARG:HG3	2.09	0.51
1:A:133:ILE:HG22	1:A:163:ILE:HG21	1.93	0.51
1:A:304:GLN:HG2	1:B:128:ARG:HB3	1.93	0.51
1:B:28:THR:CB	1:B:33:HIS:CD2	2.93	0.51
1:B:29:PHE:CE2	1:B:76:PHE:CE2	2.98	0.51
1:B:340:TYR:HD1	1:B:345:ILE:CG2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:TYR:HB3	1:C:192:ILE:HD11	1.92	0.51
1:C:112:ASN:HD22	1:C:116:ARG:CB	2.20	0.51
1:B:5:PHE:CD2	1:B:141:PHE:CZ	2.99	0.51
1:C:55:ASP:HA	1:C:102:CYS:HB2	1.90	0.51
1:C:64:LYS:HA	1:C:83:MET:CE	2.40	0.51
1:A:388:LEU:HD12	1:A:396:MET:SD	2.51	0.51
1:B:10:ASP:O	1:B:14:TYR:CE1	2.64	0.51
1:A:108:LYS:CB	1:A:119:LEU:HD11	2.37	0.51
1:B:48:ILE:CD1	1:B:48:ILE:N	2.73	0.51
1:C:110:GLU:CD	1:C:120:LYS:HG3	2.36	0.50
1:C:131:ILE:HD12	1:C:131:ILE:H	1.76	0.50
1:B:178:ALA:HB2	1:B:192:ILE:HG22	1.93	0.50
1:A:116:ARG:HB3	2:A:541:HOH:O	2.10	0.50
1:B:233:THR:O	1:B:235:PHE:CE1	2.65	0.50
1:B:423:PRO:HB2	1:B:426:ILE:HG22	1.93	0.50
1:B:19:TYR:CD1	1:B:190:VAL:HG13	2.47	0.50
1:A:273:MET:HE3	1:A:324:LEU:HA	1.93	0.50
1:B:48:ILE:HD13	1:B:88:ILE:HG23	1.94	0.50
1:C:8:ALA:CB	1:C:48:ILE:HG22	2.41	0.49
1:A:129:SER:N	1:B:304:GLN:O	2.37	0.49
1:B:29:PHE:CD2	1:B:76:PHE:HE2	2.29	0.49
1:A:413:PRO:HD2	1:B:370:PHE:HB2	1.94	0.49
1:C:270:VAL:HG21	1:C:333:LEU:HD22	1.94	0.49
1:C:440:LEU:HD12	1:C:440:LEU:C	2.32	0.49
1:A:273:MET:HE2	1:A:325:ILE:H	1.77	0.49
1:B:19:TYR:HA	1:B:190:VAL:O	2.12	0.49
1:B:133:ILE:HG22	1:B:163:ILE:HG21	1.94	0.49
1:A:21:LEU:HD12	1:A:192:ILE:HG13	1.95	0.49
1:C:232:PRO:HD2	1:C:235:PHE:CE2	2.47	0.49
1:A:29:PHE:HD2	2:A:510:HOH:O	1.95	0.49
1:A:47:LEU:HG	1:A:91:ILE:CD1	2.43	0.49
1:A:152:ASP:OD1	1:A:154:THR:HG23	2.13	0.49
1:C:439:GLU:OE2	1:C:439:GLU:HA	2.12	0.48
1:B:18:ASN:OD1	1:B:188:SER:O	2.31	0.48
1:A:96:ILE:CD1	1:B:190:VAL:HB	2.44	0.48
1:A:99:ALA:O	1:A:123:PRO:HG3	2.13	0.48
1:A:108:LYS:CD	1:A:119:LEU:HD11	2.42	0.48
1:B:29:PHE:HE2	1:B:76:PHE:CD2	2.30	0.48
1:B:96:ILE:HA	1:B:124:TYR:CD1	2.48	0.48
1:A:52:LEU:HD23	1:A:53:VAL:HG23	1.95	0.48
1:A:98:SER:HB2	1:A:120:LYS:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TYR:CE1	1:A:391:ARG:HG3	2.49	0.48
1:C:227:LEU:HD22	1:C:247:LYS:HA	1.96	0.48
1:A:18:ASN:HB2	1:A:189:ILE:HG22	1.95	0.48
1:A:20:GLU:HB2	1:A:25:THR:HB	1.96	0.48
1:A:329:ASP:HB2	1:B:421:ILE:HG13	1.96	0.48
1:B:154:THR:HB	1:B:178:ALA:H	1.78	0.48
1:A:128:ARG:HG3	1:B:304:GLN:HB2	1.95	0.48
1:C:133:ILE:HG22	1:C:163:ILE:HG21	1.96	0.48
1:C:356:LEU:HG	1:C:360:ILE:HD11	1.95	0.48
1:C:427:VAL:HG23	1:C:431:LYS:HD2	1.96	0.48
1:B:95:GLY:O	1:B:124:TYR:CE1	2.67	0.48
1:C:55:ASP:CA	1:C:102:CYS:HB2	2.43	0.48
1:A:101:GLN:CG	1:A:102:CYS:H	2.25	0.48
1:B:29:PHE:HE2	1:B:76:PHE:CE2	2.32	0.48
1:C:3:CYS:HB3	1:C:5:PHE:CE1	2.49	0.48
1:B:30:PHE:CE1	1:B:33:HIS:HB2	2.49	0.47
1:A:297:TRP:NE1	1:B:90:LYS:HG3	2.29	0.47
1:A:406:GLY:HA2	1:A:411:MET:HG3	1.96	0.47
1:A:235:PHE:CE1	1:A:240:LYS:HD2	2.48	0.47
1:A:403:MET:O	1:B:403:MET:HE2	2.14	0.47
1:B:384:VAL:O	1:B:388:LEU:HD13	2.14	0.47
1:A:97:ALA:HB3	1:A:124:TYR:CD2	2.50	0.47
1:B:71:ALA:HB2	1:B:79:MET:HE2	1.96	0.47
1:B:235:PHE:N	1:B:235:PHE:HD1	2.11	0.47
1:B:49:PRO:CG	1:B:52:LEU:HD21	2.44	0.47
1:A:307:THR:HG22	1:B:131:ILE:HD13	1.97	0.47
1:B:38:LEU:CD1	1:B:39:PHE:CD2	2.97	0.47
1:B:53:VAL:HG21	1:B:62:CYS:SG	2.55	0.47
1:B:55:ASP:HB3	1:B:59:ASP:HB3	1.96	0.47
1:B:55:ASP:CB	1:B:102:CYS:SG	2.81	0.47
1:B:415:VAL:HG22	1:B:421:ILE:HD13	1.97	0.47
1:C:338:ASP:OD1	1:C:441:ARG:HD3	2.15	0.47
1:A:46:ALA:C	1:A:47:LEU:HD12	2.40	0.47
1:A:96:ILE:HD12	1:B:190:VAL:CG2	2.39	0.47
1:B:344:SER:HB3	1:B:346:TYR:CZ	2.50	0.47
1:A:122:LEU:N	1:A:123:PRO:HD3	2.30	0.47
1:B:98:SER:HB2	1:B:121:ARG:HB3	1.97	0.47
1:A:415:VAL:HG22	1:A:421:ILE:HG12	1.96	0.47
1:B:51:SER:CB	1:B:124:TYR:HE2	2.26	0.47
1:A:124:TYR:CE1	1:A:126:GLU:HG2	2.50	0.46
1:B:48:ILE:N	1:B:89:ARG:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:CB	1:B:64:LYS:HD2	2.45	0.46
1:A:178:ALA:HB2	1:A:192:ILE:HG22	1.97	0.46
1:B:18:ASN:OD1	1:B:188:SER:C	2.58	0.46
1:B:61:GLU:C	1:B:64:LYS:HB2	2.39	0.46
1:A:344:SER:HB3	1:A:346:TYR:CZ	2.51	0.46
1:B:436:VAL:O	1:B:440:LEU:HB3	2.16	0.46
1:C:116:ARG:CG	1:C:117:GLU:N	2.78	0.46
1:A:298:GLU:CD	1:B:90:LYS:HD2	2.40	0.46
1:B:111:LYS:HB2	1:B:116:ARG:NH2	2.30	0.46
1:C:101:GLN:OE1	1:C:122:LEU:HB3	2.14	0.46
1:C:237:GLU:O	1:C:241:LYS:HG3	2.16	0.46
1:A:273:MET:CE	1:A:325:ILE:H	2.28	0.46
1:C:301:LYS:HD2	1:C:304:GLN:OE1	2.15	0.46
1:A:392:TYR:OH	1:A:446:LYS:CE	2.63	0.46
1:B:406:GLY:O	1:B:411:MET:HB2	2.15	0.46
1:B:423:PRO:HB2	1:B:426:ILE:CG2	2.46	0.46
1:C:94:VAL:HG12	1:C:95:GLY:N	2.30	0.46
1:C:101:GLN:CB	1:C:120:LYS:HE2	2.45	0.46
1:A:96:ILE:O	1:B:180:VAL:O	2.34	0.46
1:C:50:ASP:N	1:C:50:ASP:OD1	2.47	0.46
1:A:309:LEU:C	1:A:309:LEU:HD23	2.41	0.46
1:A:347:ASP:OD1	1:A:347:ASP:N	2.36	0.46
1:B:48:ILE:N	1:B:48:ILE:HD12	2.31	0.46
1:B:276:LEU:HD23	1:B:279:ILE:HD12	1.98	0.46
1:A:21:LEU:HB2	1:A:192:ILE:CG1	2.46	0.45
1:B:29:PHE:CD2	1:B:29:PHE:N	2.72	0.45
1:C:415:VAL:HG22	1:C:421:ILE:HG12	1.97	0.45
1:B:427:VAL:CG2	1:B:431:LYS:HD2	2.46	0.45
1:C:45:ILE:N	1:C:45:ILE:CD1	2.75	0.45
1:A:253:VAL:CG1	1:A:276:LEU:CD1	2.92	0.45
1:B:55:ASP:HB3	1:B:59:ASP:HA	1.97	0.45
1:C:253:VAL:CG1	1:C:276:LEU:HD21	2.38	0.45
1:A:112:ASN:CG	1:A:117:GLU:OE1	2.59	0.45
1:B:314:LEU:O	1:B:318:LEU:HD22	2.16	0.45
1:C:428:THR:CG2	1:C:431:LYS:HG3	2.38	0.45
1:A:340:TYR:HD1	1:A:345:ILE:HG23	1.81	0.45
1:B:428:THR:HB	1:B:431:LYS:HG3	1.98	0.45
1:C:110:GLU:O	1:C:117:GLU:HA	2.16	0.45
1:C:17:VAL:HG23	1:C:19:TYR:CE2	2.51	0.45
1:C:64:LYS:HG3	1:C:83:MET:HE3	1.97	0.45
1:A:230:LEU:O	1:A:247:LYS:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD12	1:B:38:LEU:C	2.42	0.45
1:A:48:ILE:HD12	1:A:90:LYS:HG3	1.91	0.44
1:A:124:TYR:CZ	1:A:126:GLU:HB2	2.52	0.44
1:A:174:LYS:CA	1:A:196:THR:CG2	2.92	0.44
1:A:409:THR:HA	1:B:370:PHE:O	2.16	0.44
1:B:36:TYR:CD1	1:B:36:TYR:C	2.95	0.44
1:B:230:LEU:O	1:B:247:LYS:HD2	2.17	0.44
1:C:101:GLN:HB2	1:C:120:LYS:HB3	1.98	0.44
1:A:112:ASN:HB2	1:A:117:GLU:OE1	2.17	0.44
1:A:176:TYR:CE1	1:A:194:GLU:OE1	2.68	0.44
1:C:344:SER:HB3	1:C:346:TYR:CZ	2.52	0.44
1:B:157:THR:CG2	1:B:158:ASN:N	2.80	0.44
1:C:153:LEU:HB3	1:C:161:VAL:HG13	1.98	0.44
1:A:9:GLY:HA3	1:A:155:HIS:HB3	2.00	0.44
1:A:28:THR:CG2	1:A:29:PHE:H	2.29	0.44
1:A:184:PRO:HB2	1:A:188:SER:HB3	2.00	0.44
1:B:340:TYR:HD1	1:B:345:ILE:HG23	1.81	0.44
1:C:49:PRO:HB2	1:C:93:ASN:HD22	1.81	0.44
1:A:31:ALA:HB1	1:A:154:THR:HG21	2.00	0.44
1:C:234:ILE:C	1:C:234:ILE:CD1	2.86	0.44
1:C:276:LEU:HD23	1:C:279:ILE:HD12	2.00	0.44
1:A:101:GLN:CG	1:A:102:CYS:N	2.81	0.44
1:B:19:TYR:HD2	1:B:34:ALA:HB2	1.82	0.44
1:B:28:THR:HG21	1:B:34:ALA:H	1.82	0.44
1:B:124:TYR:CD1	1:B:124:TYR:O	2.70	0.44
1:A:162:SER:O	1:A:165:MET:HB3	2.18	0.43
1:A:311:LEU:H	1:B:135:ASN:HD21	1.66	0.43
1:A:249:THR:HA	2:A:533:HOH:O	2.17	0.43
1:A:301:LYS:HB2	1:A:304:GLN:OE1	2.19	0.43
1:A:340:TYR:HD1	1:A:345:ILE:CG2	2.31	0.43
1:A:28:THR:HG22	1:A:30:PHE:H	1.83	0.43
1:A:403:MET:HE3	1:B:403:MET:HB3	2.00	0.43
1:B:100:ILE:HD12	1:B:100:ILE:H	1.83	0.43
1:A:99:ALA:CA	1:A:123:PRO:HG2	2.48	0.43
1:B:6:TYR:HB2	1:B:152:ASP:HB3	2.00	0.43
1:C:416:ASP:OD1	1:C:418:ASP:N	2.49	0.43
1:A:101:GLN:HB3	1:A:119:LEU:HB2	2.01	0.43
1:A:217:GLU:HG2	1:A:259:TRP:CA	2.49	0.43
1:A:131:ILE:CG1	1:B:307:THR:HA	2.46	0.43
1:A:158:ASN:ND2	1:B:154:THR:O	2.51	0.43
1:A:184:PRO:CB	1:A:188:SER:CB	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:HD11	1:C:309:LEU:HD21	2.01	0.43
1:A:96:ILE:HD11	1:B:190:VAL:HG23	1.94	0.43
1:C:362:LEU:HD11	1:C:377:TYR:HB2	2.00	0.42
1:B:72:LYS:O	1:B:72:LYS:HG2	2.18	0.42
1:A:310:VAL:HA	1:B:135:ASN:HD21	1.83	0.42
1:B:93:ASN:H	1:B:128:ARG:HH11	1.67	0.42
1:B:235:PHE:CD2	1:B:240:LYS:HB2	2.54	0.42
1:C:290:LEU:CD1	1:C:309:LEU:HD21	2.49	0.42
1:C:36:TYR:CD1	1:C:41:PRO:HD2	2.55	0.42
1:B:227:LEU:O	1:B:247:LYS:HG2	2.18	0.42
1:C:270:VAL:HG11	1:C:333:LEU:HD22	2.01	0.42
1:B:19:TYR:CD2	1:B:34:ALA:HB2	2.54	0.42
1:B:55:ASP:HB3	1:B:59:ASP:CA	2.49	0.42
1:B:61:GLU:CA	1:B:64:LYS:HD2	2.49	0.42
1:B:217:GLU:HB3	1:B:258:LEU:HB2	2.01	0.42
1:B:101:GLN:NE2	1:B:121:ARG:HD3	2.35	0.42
1:B:283:LEU:HD11	1:B:314:LEU:HD22	2.01	0.42
1:A:96:ILE:HD11	1:B:190:VAL:CG2	2.48	0.42
1:A:158:ASN:ND2	1:B:161:VAL:HG21	2.34	0.42
1:A:227:LEU:O	1:A:247:LYS:HG2	2.19	0.42
1:B:19:TYR:O	1:B:25:THR:HA	2.19	0.42
1:C:345:ILE:HG22	1:C:348:LYS:HB2	2.02	0.42
1:A:90:LYS:HG2	1:B:297:TRP:HZ2	1.85	0.42
1:A:124:TYR:OH	1:A:126:GLU:HB2	2.20	0.42
1:C:46:ALA:HB2	1:C:86:VAL:CG1	2.49	0.41
1:A:94:VAL:HG23	1:A:128:ARG:H	1.85	0.41
1:B:49:PRO:CD	1:B:52:LEU:HD21	2.49	0.41
1:B:59:ASP:O	1:B:62:CYS:N	2.51	0.41
1:A:16:ILE:CD1	1:A:74:LEU:HD13	2.50	0.41
1:C:434:ASP:O	1:C:438:ARG:HB2	2.20	0.41
1:A:217:GLU:HG2	1:A:259:TRP:HA	2.01	0.41
1:C:11:VAL:HA	1:C:14:TYR:CD2	2.55	0.41
1:C:109:LYS:HG2	1:C:119:LEU:HD23	2.02	0.41
1:A:92:PRO:HG2	1:A:133:ILE:HA	2.03	0.41
1:A:272:SER:O	1:A:275:GLU:N	2.53	0.41
1:B:6:TYR:O	1:B:47:LEU:HD12	2.21	0.41
1:C:301:LYS:O	1:C:304:GLN:CB	2.64	0.41
1:A:48:ILE:CG1	1:A:90:LYS:HA	2.28	0.41
1:A:93:ASN:ND2	1:A:160:LEU:CD1	2.79	0.41
1:B:29:PHE:CE2	1:B:76:PHE:CD2	3.08	0.41
1:B:151:VAL:HG11	1:B:153:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:SER:HA	1:B:399:ARG:HE	1.86	0.41
1:B:48:ILE:CD1	1:B:88:ILE:HG23	2.50	0.41
1:B:114:GLU:O	1:B:114:GLU:HG2	2.20	0.41
1:C:17:VAL:HG11	1:C:184:PRO:HG2	2.03	0.41
1:A:48:ILE:HD11	1:A:90:LYS:CB	2.46	0.41
1:A:99:ALA:CB	1:A:123:PRO:CG	2.95	0.41
1:A:232:PRO:HG3	1:A:306:GLU:OE1	2.21	0.41
1:B:19:TYR:CE1	1:B:190:VAL:CG1	3.03	0.41
1:B:418:ASP:OD1	1:B:418:ASP:N	2.54	0.41
1:C:4:LEU:HB2	1:C:41:PRO:HG3	2.03	0.41
1:B:4:LEU:HD23	1:B:5:PHE:N	2.36	0.41
1:B:152:ASP:OD1	1:B:154:THR:HG22	2.20	0.41
1:C:235:PHE:HB2	1:C:239:GLU:OE1	2.21	0.41
1:A:174:LYS:CA	1:A:196:THR:HG21	2.44	0.40
1:C:92:PRO:HG2	1:C:133:ILE:HA	2.03	0.40
1:A:254:VAL:HG13	1:A:320:VAL:HG21	2.02	0.40
1:B:29:PHE:HD2	1:B:76:PHE:HE2	1.69	0.40
1:B:157:THR:HG22	1:B:158:ASN:H	1.86	0.40
1:A:283:LEU:HD11	1:A:314:LEU:HD22	2.03	0.40
1:B:26:GLN:HG3	1:B:37:ASN:HB2	2.02	0.40
1:B:55:ASP:HB3	1:B:59:ASP:CB	2.51	0.40
1:C:1:MET:O	1:C:1:MET:HG2	2.21	0.40
1:C:245:ARG:HH22	1:C:285:GLU:CD	2.29	0.40
1:A:120:LYS:HB3	1:A:120:LYS:HE3	1.93	0.40
1:A:153:LEU:HB3	1:A:161:VAL:HG13	2.03	0.40
1:A:297:TRP:NE1	1:B:90:LYS:O	2.48	0.40
1:B:53:VAL:HG23	1:B:62:CYS:SG	2.61	0.40
1:A:232:PRO:HG3	1:A:306:GLU:CD	2.47	0.40
1:B:20:GLU:CG	1:B:20:GLU:O	2.69	0.40
1:C:354:ARG:HG2	1:C:399:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

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	452/454 (100%)	416 (92%)	30 (7%)	6 (1%)	9	25
1	B	452/454 (100%)	411 (91%)	35 (8%)	6 (1%)	9	25
1	C	452/454 (100%)	423 (94%)	26 (6%)	3 (1%)	18	40
All	All	1356/1362 (100%)	1250 (92%)	91 (7%)	15 (1%)	11	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	426	ILE
1	C	77	ALA
1	C	78	GLY
1	A	115	GLY
1	A	273	MET
1	B	60	GLU
1	B	103	GLU
1	B	425	LYS
1	A	53	VAL
1	B	98	SER
1	A	110	GLU
1	A	51	SER
1	A	105	GLY
1	B	106	ALA
1	C	426	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/407 (100%)	385 (95%)	22 (5%)	20	42
1	B	407/407 (100%)	381 (94%)	26 (6%)	16	36
1	C	407/407 (100%)	391 (96%)	16 (4%)	28	53
All	All	1221/1221 (100%)	1157 (95%)	64 (5%)	21	44

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	37	ASN
1	A	48	ILE
1	A	75	ASN
1	A	91	ILE
1	A	100	ILE
1	A	110	GLU
1	A	122	LEU
1	A	131	ILE
1	A	183	MET
1	A	191	ASN
1	A	234	ILE
1	A	241	LYS
1	A	255	ILE
1	A	310	VAL
1	A	347	ASP
1	A	354	ARG
1	A	388	LEU
1	A	391	ARG
1	A	426	ILE
1	A	432	ILE
1	A	438	ARG
1	B	25	THR
1	B	29	PHE
1	B	48	ILE
1	B	87	GLU
1	B	88	ILE
1	B	127	LYS
1	B	131	ILE
1	B	180	VAL
1	B	191	ASN
1	B	196	THR
1	B	227	LEU
1	B	235	PHE
1	B	255	ILE
1	B	267	VAL
1	B	270	VAL
1	B	274	ASN
1	B	400	ASN
1	B	409	THR
1	B	414	ASN
1	B	418	ASP

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Mol	Chain	Res	Type
1	B	420	ASN
1	B	421	ILE
1	B	426	ILE
1	B	432	ILE
1	B	441	ARG
1	B	446	LYS
1	C	17	VAL
1	C	21	LEU
1	C	45	ILE
1	C	48	ILE
1	C	89	ARG
1	C	104	ASN
1	C	131	ILE
1	C	196	THR
1	C	212	ILE
1	C	230	LEU
1	C	255	ILE
1	C	270	VAL
1	C	274	ASN
1	C	302	ASN
1	C	410	ASP
1	C	426	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	200	GLN
1	A	203	ASN
1	A	252	ASN
1	A	260	ASN
1	A	263	ASN
1	A	420	ASN
1	B	33	HIS
1	B	56	ASN
1	B	65	ASN
1	B	101	GLN
1	B	135	ASN
1	B	200	GLN
1	B	302	ASN
1	B	379	HIS
1	C	26	GLN

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Mol	Chain	Res	Type
1	C	27	ASN
1	C	112	ASN
1	C	135	ASN
1	C	155	HIS
1	C	200	GLN
1	C	214	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	454/454 (100%)	0.60	38 (8%)	17 15	54, 108, 168, 186	0
1	B	454/454 (100%)	0.57	41 (9%)	15 13	48, 100, 168, 191	0
1	C	454/454 (100%)	-0.03	4 (0%)	81 75	38, 74, 116, 143	0
All	All	1362/1362 (100%)	0.38	83 (6%)	27 22	38, 91, 165, 191	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	GLU	6.0
1	B	9	GLY	4.7
1	A	63	TYR	4.4
1	B	51	SER	4.4
1	A	67	VAL	4.3
1	A	195	LEU	4.0
1	A	51	SER	4.0
1	A	52	LEU	4.0
1	A	9	GLY	3.9
1	B	16	ILE	3.9
1	B	117	GLU	3.8
1	B	189	ILE	3.8
1	B	47	LEU	3.7
1	A	180	VAL	3.6
1	B	28	THR	3.6
1	B	179	PRO	3.6
1	A	100	ILE	3.5
1	B	63	TYR	3.4
1	A	8	ALA	3.4
1	A	122	LEU	3.3
1	B	186	LYS	3.2
1	C	118	VAL	3.1
1	B	181	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	7	ILE	3.0
1	A	303	PHE	3.0
1	B	67	VAL	3.0
1	A	17	VAL	2.9
1	B	7	ILE	2.9
1	B	188	SER	2.9
1	B	427	VAL	2.9
1	B	160	LEU	2.8
1	A	30	PHE	2.8
1	A	82	PHE	2.8
1	A	34	ALA	2.7
1	A	74	LEU	2.7
1	B	32	ALA	2.7
1	B	74	LEU	2.7
1	B	235	PHE	2.6
1	B	406	GLY	2.6
1	A	254	VAL	2.6
1	B	44	VAL	2.6
1	A	88	ILE	2.6
1	A	187	ASP	2.6
1	A	188	SER	2.5
1	A	53	VAL	2.5
1	B	100	ILE	2.5
1	C	426	ILE	2.5
1	A	118	VAL	2.5
1	B	107	PRO	2.5
1	A	105	GLY	2.5
1	B	96	ILE	2.5
1	A	123	PRO	2.5
1	B	180	VAL	2.5
1	B	106	ALA	2.4
1	B	93	ASN	2.4
1	B	29	PHE	2.4
1	B	52	LEU	2.4
1	B	17	VAL	2.4
1	A	112	ASN	2.4
1	A	181	MET	2.3
1	A	108	LYS	2.3
1	B	304	GLN	2.3
1	A	77	ALA	2.2
1	A	191	ASN	2.2
1	B	234	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	117	GLU	2.2
1	B	8	ALA	2.2
1	C	427	VAL	2.2
1	A	14	TYR	2.2
1	B	30	PHE	2.2
1	A	121	ARG	2.2
1	B	68	ILE	2.2
1	B	178	ALA	2.2
1	B	48	ILE	2.1
1	C	183	MET	2.1
1	B	49	PRO	2.1
1	B	66	LEU	2.1
1	B	31	ALA	2.1
1	A	314	LEU	2.1
1	A	76	PHE	2.1
1	A	4	LEU	2.0
1	A	66	LEU	2.0
1	A	198	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.