



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 AM UTC

PDB ID : 5MBM / pdb_00005mbm
Title : Cathepsin B in complex with DARPin 8h6
Authors : Turk, D.; Kramer, L.; Renko, M.; Turk, B.
Deposited on : 2016-11-08
Resolution : 2.76 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

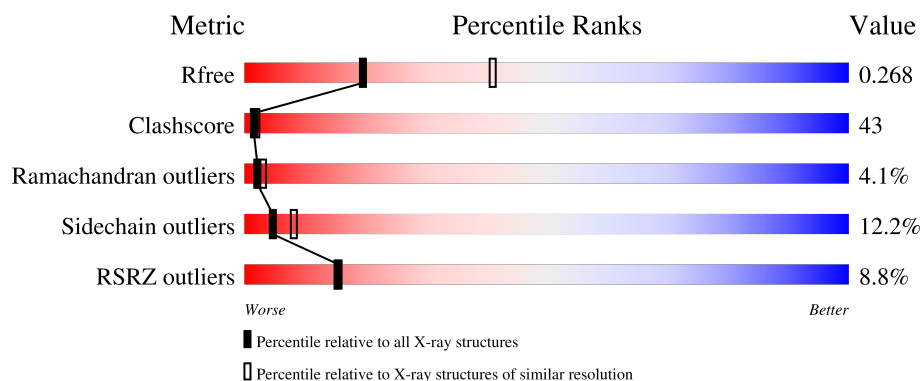
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	256	4% 29% 49% 21% .
1	B	256	16% 32% 40% 24% .
2	C	171	9% 25% 47% 19% 5%
2	D	171	4% 31% 42% 21% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCH	A	29	-	-	X	-
1	SCH	B	29	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6499 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 Cathepsin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	14	0	0
			1971	1235	337	380	19			
1	B	255	Total	C	N	O	S	15	0	0
			1963	1229	336	379	19			

- Molecule 2 is a protein called DARPin 8h6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	0	0	0
			1211	751	217	243			
2	D	163	Total	C	N	O	29	0	0
			1211	751	217	243			

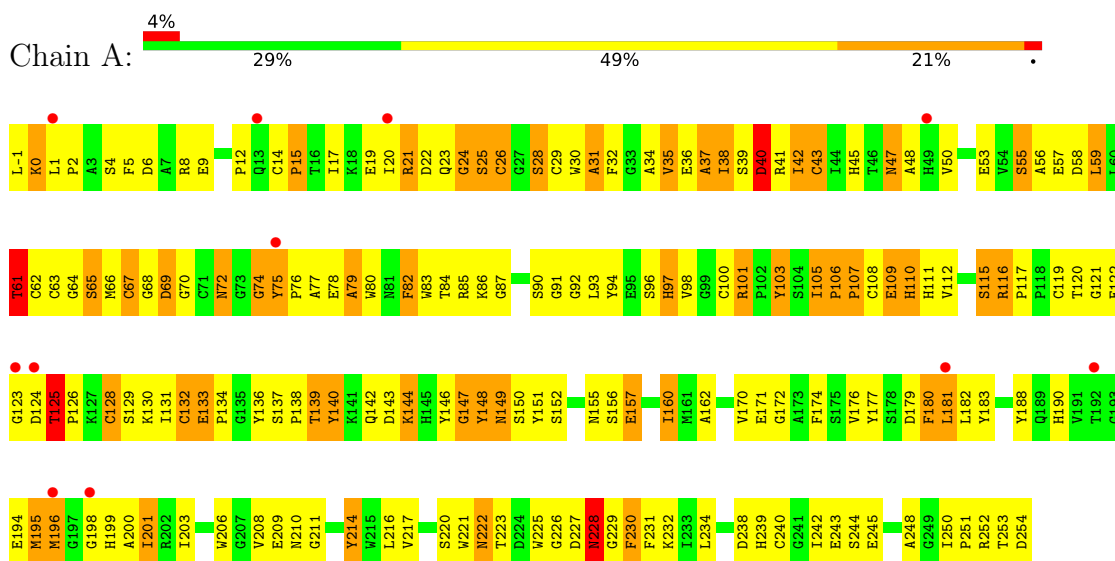
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	51	Total	O	0	0
			51	51		
3	C	22	Total	O	0	0
			22	22		
3	D	23	Total	O	0	0
			23	23		

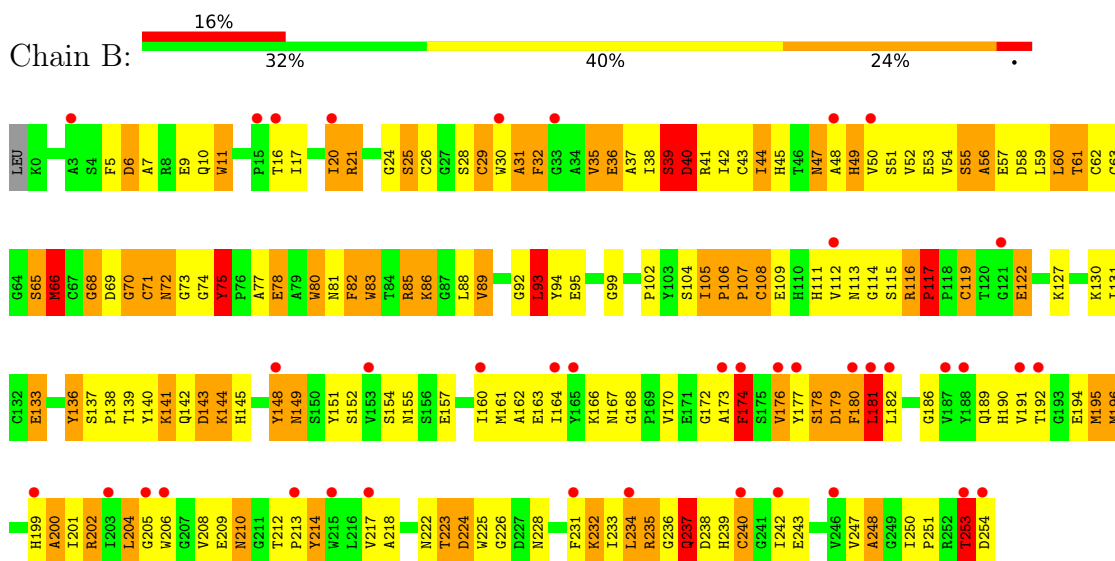
3 Residue-property plots [i](#)

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.

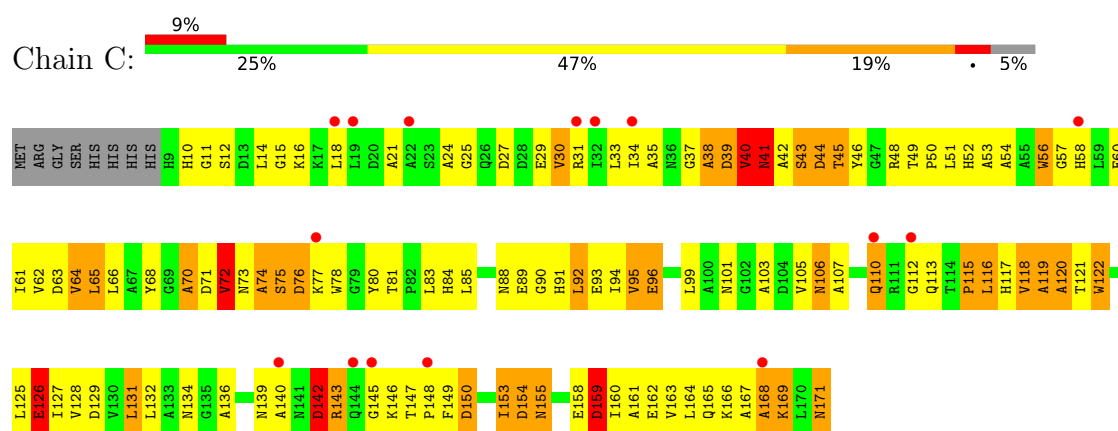
• Molecule 1: Cathepsin B



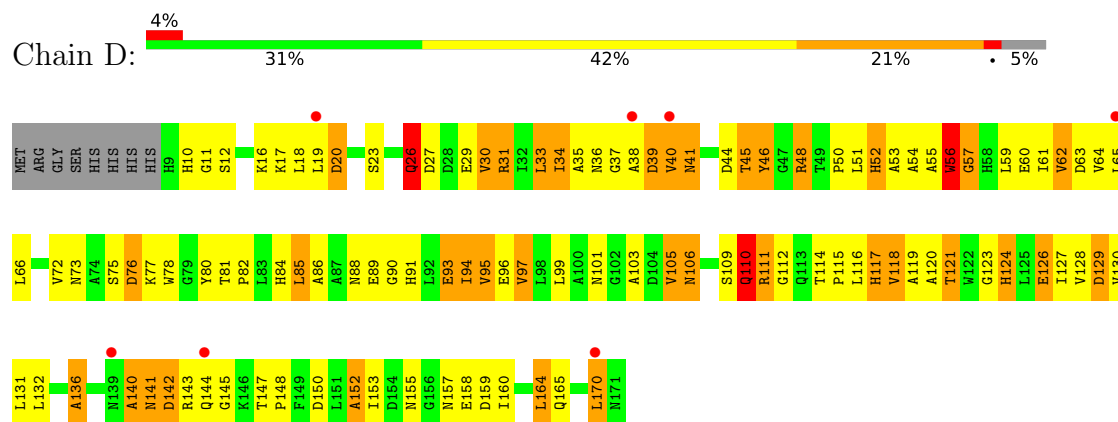
• Molecule 1: Cathepsin B



• Molecule 2: DARPin 8h6



• Molecule 2: DARPin 8h6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.45Å 201.52Å 46.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.76 46.70 – 2.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.70-2.76) 98.5 (46.70-2.76)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.77Å)	Xtriage
Refinement program	MAIN 2016	Depositor
R, R_{free}	0.256 , 0.281 0.258 , 0.268	Depositor DCC
R_{free} test set	1257 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: SCH

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	1.71	41/2021 (2.0%)	1.85	68/2744 (2.5%)
1	B	1.54	33/2013 (1.6%)	2.05	105/2733 (3.8%)
2	C	1.64	24/1232 (1.9%)	1.87	38/1682 (2.3%)
2	D	1.74	21/1232 (1.7%)	2.02	52/1682 (3.1%)
All	All	1.65	119/6498 (1.8%)	1.95	263/8841 (3.0%)

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	TYR	CA-C	11.99	1.68	1.52
2	C	63	ASP	CA-C	9.85	1.65	1.52
1	A	110	HIS	CA-C	-9.09	1.41	1.52
1	B	253	THR	CA-C	-9.04	1.40	1.52
1	A	107	PRO	CA-C	-8.87	1.42	1.52
2	D	95	VAL	CA-C	-8.49	1.42	1.52
1	A	38	ILE	CA-C	8.24	1.65	1.52
2	C	62	VAL	CA-C	8.06	1.63	1.52
2	D	119	ALA	CA-C	7.97	1.62	1.52
1	A	37	ALA	CA-C	-7.81	1.42	1.52
2	D	157	ASN	CA-C	-7.68	1.43	1.53
1	A	53	GLU	N-CA	-7.64	1.36	1.46
1	B	88	LEU	CA-C	-7.57	1.42	1.52
2	D	129	ASP	C-N	7.56	1.43	1.33
1	A	19	GLU	CA-C	7.43	1.62	1.52
1	A	75	TYR	CA-C	7.38	1.59	1.52
1	A	150	SER	CA-C	7.36	1.61	1.52
2	C	64	VAL	N-CA	-7.30	1.38	1.46
1	A	109	GLU	CA-C	-7.28	1.43	1.52
2	C	94	ILE	C-N	-7.27	1.24	1.33
2	D	121	THR	CA-C	7.26	1.62	1.52
1	B	66	MET	CA-C	-7.12	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	43	SER	CA-C	-7.09	1.44	1.52
2	D	164	LEU	C-N	7.05	1.43	1.33
1	A	21	ARG	CA-C	7.04	1.63	1.53
1	B	66	MET	SD-CE	-6.99	1.62	1.79
2	D	86	ALA	CA-C	6.99	1.61	1.52
1	A	105	ILE	N-CA	-6.91	1.40	1.46
2	C	64	VAL	C-N	6.90	1.42	1.33
2	D	97	VAL	CA-C	6.88	1.62	1.52
1	B	68	GLY	C-N	6.86	1.43	1.33
1	A	195	MET	SD-CE	-6.83	1.62	1.79
2	D	97	VAL	CA-CB	6.82	1.64	1.54
1	A	26	CYS	CA-C	-6.75	1.44	1.52
2	C	44	ASP	CA-C	-6.65	1.43	1.53
2	D	82	PRO	CA-C	-6.62	1.42	1.52
1	B	148	TYR	CA-C	-6.55	1.44	1.52
2	D	164	LEU	CA-C	6.52	1.61	1.52
1	B	35	VAL	CA-C	-6.45	1.45	1.52
2	C	92	LEU	CA-C	-6.39	1.44	1.52
1	A	131	ILE	C-N	6.36	1.44	1.33
1	B	56	ALA	C-N	6.36	1.42	1.33
1	B	131	ILE	CA-C	6.36	1.60	1.52
1	A	42	ILE	C-N	6.35	1.42	1.33
1	B	206	TRP	CA-C	-6.35	1.45	1.52
1	A	15	PRO	CA-C	6.30	1.61	1.52
1	B	36	GLU	CA-C	6.30	1.61	1.52
2	D	170	LEU	CA-C	6.26	1.61	1.52
1	B	61	THR	CA-C	-6.26	1.44	1.52
1	A	216	LEU	CA-C	6.20	1.61	1.52
1	B	63	CYS	CA-C	-6.19	1.44	1.52
1	A	101	ARG	N-CA	6.16	1.53	1.46
1	B	144	LYS	CA-C	6.16	1.61	1.52
2	C	95	VAL	CA-C	6.03	1.60	1.52
2	C	62	VAL	C-N	6.03	1.41	1.33
1	B	106	PRO	CA-C	6.03	1.56	1.52
2	C	168	ALA	C-O	-5.93	1.17	1.24
1	B	53	GLU	C-N	-5.91	1.26	1.33
1	B	235	ARG	CA-C	5.90	1.60	1.52
1	B	85	ARG	CA-C	5.90	1.60	1.52
1	B	21	ARG	CA-C	5.85	1.59	1.52
1	B	39	SER	CA-C	5.85	1.60	1.52
1	A	137	SER	CA-C	-5.84	1.46	1.52
1	A	160	ILE	CA-C	5.83	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	MET	SD-CE	-5.82	1.65	1.79
1	A	106	PRO	CA-C	5.81	1.57	1.52
2	C	89	GLU	C-O	-5.81	1.17	1.24
2	D	150	ASP	CA-C	-5.74	1.45	1.52
1	A	22	ASP	C-N	5.73	1.42	1.33
1	A	220	SER	C-N	5.72	1.41	1.33
1	B	82	PHE	N-CA	-5.71	1.39	1.46
1	A	149	ASN	C-N	5.71	1.41	1.33
2	C	139	ASN	CA-C	-5.70	1.45	1.52
1	A	93	LEU	CB-CG	-5.69	1.42	1.53
2	D	132	LEU	C-N	5.69	1.42	1.33
2	C	121	THR	C-N	5.66	1.41	1.33
2	C	116	LEU	C-N	5.65	1.40	1.33
1	A	43	CYS	C-N	5.63	1.41	1.33
2	C	76	ASP	C-N	5.60	1.41	1.33
1	A	59	LEU	CA-CB	-5.55	1.44	1.53
1	B	60	LEU	CA-C	5.53	1.59	1.52
2	D	84	HIS	C-N	5.50	1.40	1.33
1	A	162	ALA	CA-C	5.48	1.59	1.52
2	D	75	SER	CA-C	5.47	1.60	1.53
2	D	153	ILE	CA-CB	5.47	1.60	1.54
2	D	91	HIS	CA-C	-5.45	1.46	1.52
1	A	149	ASN	CA-CB	-5.45	1.44	1.53
2	C	65	LEU	CA-C	5.45	1.60	1.52
1	A	74	GLY	C-N	5.42	1.41	1.33
1	A	188	TYR	CA-C	5.40	1.60	1.52
1	A	35	VAL	C-O	5.38	1.30	1.24
1	A	157	GLU	CA-C	5.37	1.59	1.52
1	B	6	ASP	C-N	5.35	1.41	1.34
1	A	31	ALA	C-O	-5.33	1.17	1.24
2	C	96	GLU	CA-C	5.33	1.59	1.52
1	A	140	TYR	CA-C	5.32	1.60	1.52
1	B	20	ILE	CA-C	5.31	1.60	1.53
2	C	120	ALA	CA-C	5.31	1.60	1.52
1	A	79	ALA	CA-C	5.26	1.59	1.52
2	C	116	LEU	CA-C	5.26	1.59	1.52
1	B	180	PHE	CA-C	-5.24	1.48	1.53
1	B	140	TYR	CA-C	-5.24	1.45	1.52
2	D	30	VAL	C-N	-5.24	1.26	1.33
1	B	235	ARG	C-N	5.23	1.39	1.34
1	B	130	LYS	C-O	5.23	1.30	1.24
1	A	148	TYR	C-N	5.22	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	SER	N-CA	5.21	1.52	1.46
1	B	240	CYS	CA-C	5.20	1.59	1.52
1	A	206	TRP	CA-C	-5.13	1.46	1.52
2	C	74	ALA	CA-C	5.11	1.59	1.52
1	B	151	TYR	CA-C	5.09	1.58	1.52
2	C	42	ALA	CA-C	-5.09	1.46	1.52
1	B	54	VAL	CA-C	-5.06	1.46	1.52
2	D	62	VAL	CA-C	5.05	1.59	1.52
2	C	143	ARG	CA-C	-5.05	1.45	1.52
1	B	61	THR	N-CA	-5.05	1.40	1.46
1	A	98	VAL	C-O	-5.05	1.17	1.24
2	C	72	VAL	CA-C	5.05	1.59	1.52
2	D	170	LEU	C-N	5.03	1.40	1.33

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	MET	N-CA-C	-13.75	94.78	111.69
1	B	55	SER	CA-C-N	-10.60	104.20	120.31
1	B	55	SER	C-N-CA	-10.60	104.20	120.31
1	B	80	TRP	N-CA-C	-10.23	99.33	112.23
2	C	171	ASN	CA-CB-CG	9.89	122.50	112.60
2	C	41	ASN	CA-CB-CG	9.49	122.09	112.60
1	B	116	ARG	CA-C-N	9.44	130.11	120.38
1	B	116	ARG	C-N-CA	9.44	130.11	120.38
1	B	75	TYR	CA-C-N	-9.31	109.98	120.04
1	B	75	TYR	C-N-CA	-9.31	109.98	120.04
1	B	145	HIS	CA-C-N	-9.21	106.98	122.64
1	B	145	HIS	C-N-CA	-9.21	106.98	122.64
2	D	91	HIS	CA-CB-CG	-9.12	104.68	113.80
1	B	70	GLY	CA-C-N	-8.65	109.05	122.37
1	B	70	GLY	C-N-CA	-8.65	109.05	122.37
1	A	238	ASP	N-CA-C	-8.61	99.24	111.56
2	D	127	ILE	N-CA-C	-8.58	102.93	110.74
1	B	130	LYS	CA-C-N	-8.53	110.42	122.71
1	B	130	LYS	C-N-CA	-8.53	110.42	122.71
2	D	56	TRP	N-CA-C	-8.44	99.27	110.24
1	A	222	ASN	CA-CB-CG	8.36	120.96	112.60
1	A	111	HIS	CA-CB-CG	-8.32	105.48	113.80
1	B	116	ARG	CB-CA-C	8.23	122.33	109.15
2	D	142	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	97	HIS	N-CA-CB	-8.11	100.37	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	136	ALA	CA-C-N	-8.10	110.10	122.09
2	D	136	ALA	C-N-CA	-8.10	110.10	122.09
2	D	95	VAL	N-CA-C	-8.07	102.67	110.42
1	B	204	LEU	N-CA-C	8.07	122.91	112.26
2	D	90	GLY	CA-C-N	-7.99	111.79	122.42
2	D	90	GLY	C-N-CA	-7.99	111.79	122.42
2	C	63	ASP	CA-C-N	7.83	130.43	120.56
2	C	63	ASP	C-N-CA	7.83	130.43	120.56
2	C	64	VAL	CA-C-N	-7.77	110.05	120.54
2	C	64	VAL	C-N-CA	-7.77	110.05	120.54
2	C	30	VAL	N-CA-C	-7.73	103.71	110.74
1	B	21	ARG	N-CA-C	7.68	121.04	108.99
1	A	151	TYR	N-CA-C	7.53	119.59	108.60
1	B	253	THR	N-CA-C	-7.53	94.77	110.80
2	D	143	ARG	N-CA-C	-7.50	103.23	112.38
2	C	112	GLY	N-CA-C	-7.50	104.40	115.72
2	C	168	ALA	CA-C-O	-7.45	112.88	121.07
2	D	140	ALA	CA-C-N	-7.41	112.19	122.93
2	D	140	ALA	C-N-CA	-7.41	112.19	122.93
1	B	174	PHE	CA-CB-CG	7.40	121.20	113.80
1	A	75	TYR	CA-C-N	7.38	126.92	119.24
1	A	75	TYR	C-N-CA	7.38	126.92	119.24
1	A	116	ARG	CA-C-N	7.34	125.02	119.66
1	A	116	ARG	C-N-CA	7.34	125.02	119.66
1	B	47	ASN	CA-CB-CG	7.29	119.89	112.60
2	D	164	LEU	CA-C-N	-7.24	110.58	120.28
2	D	164	LEU	C-N-CA	-7.24	110.58	120.28
1	A	35	VAL	CA-C-N	-7.23	110.02	120.29
1	A	35	VAL	C-N-CA	-7.23	110.02	120.29
2	D	153	ILE	N-CA-C	-7.19	103.52	110.42
1	A	62	CYS	CA-C-N	-7.16	107.87	121.54
1	A	62	CYS	C-N-CA	-7.16	107.87	121.54
2	C	41	ASN	N-CA-C	-7.14	95.60	110.80
1	B	86	LYS	CA-C-O	-7.13	111.73	119.08
1	B	143	ASP	CA-C-N	-7.09	111.02	120.95
1	B	143	ASP	C-N-CA	-7.09	111.02	120.95
2	D	34	ILE	N-CA-C	-7.09	104.29	110.74
2	C	142	ASP	CA-CB-CG	7.05	119.65	112.60
1	A	82	PHE	N-CA-C	-7.01	103.56	111.14
1	B	179	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	149	ASN	CA-CB-CG	6.99	119.59	112.60
1	A	55	SER	N-CA-C	6.95	119.44	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	CYS	CA-C-N	6.92	134.94	123.25
1	B	71	CYS	C-N-CA	6.92	134.94	123.25
2	D	170	LEU	N-CA-C	-6.84	103.45	112.34
1	A	125	THR	CA-C-N	-6.83	113.68	120.98
1	A	125	THR	C-N-CA	-6.83	113.68	120.98
1	A	214	TYR	N-CA-C	6.81	118.91	108.42
1	B	66	MET	N-CA-CB	6.77	120.28	110.20
1	B	78	GLU	CA-C-N	-6.75	110.70	120.29
1	B	78	GLU	C-N-CA	-6.75	110.70	120.29
1	B	234	LEU	N-CA-C	6.69	119.34	108.63
1	A	196	MET	N-CA-CB	-6.66	100.62	111.01
2	C	39	ASP	CA-C-O	-6.65	113.50	120.55
1	B	117	PRO	N-CA-C	6.65	118.81	110.70
2	D	93	GLU	CA-C-N	-6.65	111.35	120.46
2	D	93	GLU	C-N-CA	-6.65	111.35	120.46
2	C	140	ALA	CA-C-N	-6.63	112.58	122.39
2	C	140	ALA	C-N-CA	-6.63	112.58	122.39
2	D	85	LEU	CA-C-N	-6.62	111.41	120.28
2	D	85	LEU	C-N-CA	-6.62	111.41	120.28
2	D	52	HIS	CA-C-N	-6.61	108.69	121.58
2	D	52	HIS	C-N-CA	-6.61	108.69	121.58
1	B	253	THR	N-CA-CB	6.59	121.63	110.49
1	B	53	GLU	N-CA-C	-6.58	102.32	110.41
1	B	62	CYS	N-CA-C	6.56	121.45	113.38
1	A	47	ASN	CA-CB-CG	-6.53	106.07	112.60
1	B	40	ASP	CB-CA-C	-6.52	100.10	110.86
1	B	104	SER	N-CA-C	6.51	121.22	113.28
2	D	152	ALA	CA-C-N	6.49	128.74	120.56
2	D	152	ALA	C-N-CA	6.49	128.74	120.56
1	A	35	VAL	N-CA-C	-6.47	102.97	111.05
1	A	139	THR	N-CA-C	6.46	118.90	110.43
1	B	11	TRP	CA-C-N	6.45	126.14	119.56
1	B	11	TRP	C-N-CA	6.45	126.14	119.56
1	B	61	THR	CA-C-O	-6.43	114.07	120.82
1	B	214	TYR	N-CA-C	6.42	117.91	108.14
2	D	39	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	131	ILE	CA-C-O	-6.41	114.75	121.93
2	C	52	HIS	N-CA-C	-6.41	104.22	111.14
1	B	217	VAL	N-CA-C	6.40	118.71	108.85
2	C	159	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	132	CYS	N-CA-C	6.32	118.29	109.31
1	B	145	HIS	CA-CB-CG	-6.29	107.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	PRO	N-CA-C	6.27	117.29	110.58
1	B	212	THR	CA-C-N	6.26	126.23	120.03
1	B	212	THR	C-N-CA	6.26	126.23	120.03
1	A	40	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	60	LEU	N-CA-CB	-6.21	100.84	109.91
2	D	95	VAL	CA-C-N	-6.20	112.38	120.44
2	D	95	VAL	C-N-CA	-6.20	112.38	120.44
1	B	107	PRO	CA-C-O	-6.18	114.38	121.36
2	D	117	HIS	N-CA-C	-6.16	104.65	111.36
2	C	60	GLU	N-CA-C	-6.16	104.49	111.14
2	C	24	ALA	N-CA-C	-6.12	105.57	113.16
1	B	35	VAL	CA-C-N	-6.12	112.28	120.54
1	B	35	VAL	C-N-CA	-6.12	112.28	120.54
1	B	127	LYS	CA-C-N	-6.11	112.88	121.99
1	B	127	LYS	C-N-CA	-6.11	112.88	121.99
2	C	42	ALA	N-CA-C	-6.11	101.16	110.14
1	B	136	TYR	N-CA-C	-6.11	99.85	109.50
1	B	75	TYR	CA-C-O	-6.10	112.49	119.32
1	B	55	SER	N-CA-C	6.10	123.79	110.80
1	A	133	GLU	CA-C-N	6.05	127.41	119.84
1	A	133	GLU	C-N-CA	6.05	127.41	119.84
1	A	93	LEU	N-CA-C	6.05	118.13	110.33
2	C	38	ALA	N-CA-C	-6.04	102.14	110.35
1	B	114	GLY	CA-C-N	6.00	129.15	120.38
1	B	114	GLY	C-N-CA	6.00	129.15	120.38
2	C	131	LEU	N-CA-C	-5.99	104.08	111.33
2	D	76	ASP	CA-CB-CG	5.99	118.59	112.60
2	C	119	ALA	N-CA-C	5.95	118.72	111.82
1	B	176	VAL	N-CA-C	5.95	117.58	108.71
1	A	123	GLY	N-CA-C	5.95	127.28	113.18
1	B	93	LEU	N-CA-C	5.90	123.37	110.80
1	B	213	PRO	N-CA-C	5.90	120.27	111.41
1	B	113	ASN	CA-CB-CG	5.88	118.48	112.60
2	D	101	ASN	OD1-CG-ND2	-5.88	116.72	122.60
2	D	117	HIS	CA-CB-CG	5.88	119.68	113.80
1	A	103	TYR	CA-C-N	-5.87	113.27	122.49
1	A	103	TYR	C-N-CA	-5.87	113.27	122.49
1	A	228	ASN	CB-CA-C	-5.85	103.27	111.80
1	A	208	VAL	CA-C-N	-5.83	114.54	122.77
1	A	208	VAL	C-N-CA	-5.83	114.54	122.77
2	D	136	ALA	N-CA-C	-5.83	101.66	110.28
1	A	117	PRO	CA-C-N	5.83	126.71	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PRO	C-N-CA	5.83	126.71	120.13
1	B	145	HIS	CA-C-O	-5.81	114.39	121.36
1	B	105	ILE	CB-CA-C	5.78	116.66	110.53
2	D	132	LEU	CA-C-N	-5.78	110.38	121.94
2	D	132	LEU	C-N-CA	-5.78	110.38	121.94
1	A	217	VAL	N-CA-C	5.75	117.71	108.85
1	A	97	HIS	CB-CA-C	5.75	120.60	111.23
1	B	82	PHE	N-CA-C	-5.74	104.93	111.07
1	A	222	ASN	CA-C-N	5.74	129.42	120.82
1	A	222	ASN	C-N-CA	5.74	129.42	120.82
1	A	61	THR	CA-C-N	-5.72	113.09	122.54
1	A	61	THR	C-N-CA	-5.72	113.09	122.54
1	B	122	GLU	CA-CB-CG	-5.72	102.66	114.10
1	B	32	PHE	CA-CB-CG	-5.71	108.09	113.80
2	C	64	VAL	N-CA-C	-5.71	104.94	110.42
1	B	52	VAL	CA-C-N	-5.70	110.35	121.06
1	B	52	VAL	C-N-CA	-5.70	110.35	121.06
1	A	179	ASP	N-CA-C	-5.69	106.29	113.18
1	B	56	ALA	N-CA-C	-5.69	105.22	111.82
1	B	149	ASN	CA-C-N	-5.69	112.39	122.74
1	B	149	ASN	C-N-CA	-5.69	112.39	122.74
1	A	203	ILE	N-CA-CB	-5.67	102.73	110.56
2	D	26	GLN	N-CA-CB	-5.66	100.93	110.49
2	D	121	THR	N-CA-C	5.65	117.89	111.11
2	D	89	GLU	N-CA-C	5.65	119.89	112.89
2	C	122	TRP	N-CA-CB	5.64	120.29	110.98
2	D	131	LEU	N-CA-C	-5.63	105.14	111.28
1	A	124	ASP	N-CA-C	5.63	118.71	107.62
1	A	40	ASP	CB-CA-C	-5.62	101.13	110.68
2	D	10	HIS	N-CA-C	5.61	119.74	113.01
2	C	70	ALA	CA-C-N	-5.61	110.83	121.54
2	C	70	ALA	C-N-CA	-5.61	110.83	121.54
1	B	6	ASP	CA-C-N	-5.61	112.20	120.38
1	B	6	ASP	C-N-CA	-5.61	112.20	120.38
1	A	133	GLU	CB-CA-C	5.60	117.43	109.08
1	B	253	THR	CA-C-O	-5.60	112.50	120.51
1	A	67	CYS	N-CA-C	-5.59	104.70	112.30
2	C	41	ASN	N-CA-CB	5.59	119.93	110.49
1	B	65	SER	N-CA-C	-5.57	105.79	112.59
1	A	129	SER	N-CA-C	-5.57	100.17	109.24
1	A	180	PHE	N-CA-C	-5.55	104.62	111.40
1	B	49	HIS	N-CA-C	-5.54	104.67	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLY	CA-C-N	-5.53	112.61	122.45
1	B	205	GLY	C-N-CA	-5.53	112.61	122.45
2	D	26	GLN	N-CA-C	5.53	122.57	110.80
1	A	137	SER	CA-C-N	-5.53	114.10	119.90
1	A	137	SER	C-N-CA	-5.53	114.10	119.90
1	B	35	VAL	CA-C-O	-5.52	114.92	121.05
2	D	94	ILE	CA-C-N	5.51	127.51	120.56
2	D	94	ILE	C-N-CA	5.51	127.51	120.56
1	A	228	ASN	CA-C-O	-5.51	115.15	121.54
1	B	140	TYR	CA-C-N	-5.50	111.18	120.58
1	B	140	TYR	C-N-CA	-5.50	111.18	120.58
1	B	224	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	181	LEU	N-CA-C	-5.49	103.11	110.24
1	B	122	GLU	CB-CA-C	5.48	121.32	110.42
2	C	150	ASP	N-CA-C	-5.47	104.34	111.02
1	B	83	TRP	CA-C-N	-5.47	111.58	120.71
1	B	83	TRP	C-N-CA	-5.47	111.58	120.71
1	B	40	ASP	CA-CB-CG	5.38	117.98	112.60
2	D	164	LEU	CA-C-O	-5.38	115.17	120.82
1	B	31	ALA	CA-C-N	-5.36	112.16	120.31
1	B	31	ALA	C-N-CA	-5.36	112.16	120.31
1	A	180	PHE	CA-C-N	-5.36	112.94	120.82
1	A	180	PHE	C-N-CA	-5.36	112.94	120.82
2	C	115	PRO	N-CA-C	-5.36	106.22	113.40
1	A	150	SER	CA-C-N	-5.34	112.67	121.80
1	A	150	SER	C-N-CA	-5.34	112.67	121.80
1	A	19	GLU	N-CA-C	5.33	117.82	110.35
1	A	210	ASN	N-CA-C	-5.33	106.36	112.86
2	D	11	GLY	N-CA-C	-5.32	106.06	112.49
2	C	41	ASN	CB-CA-C	-5.30	99.87	110.42
1	A	111	HIS	N-CA-CB	-5.28	103.97	111.84
2	D	124	HIS	CA-CB-CG	-5.27	108.53	113.80
2	D	96	GLU	CA-C-O	-5.25	115.31	120.82
1	B	141	LYS	N-CA-C	-5.23	105.26	111.69
1	B	237	GLN	CA-C-N	-5.23	115.08	122.34
1	B	237	GLN	C-N-CA	-5.23	115.08	122.34
2	D	114	THR	N-CA-CB	5.20	115.36	109.49
2	C	122	TRP	N-CA-C	-5.19	105.62	112.94
1	B	106	PRO	N-CA-CB	-5.19	100.52	103.22
1	B	72	ASN	CB-CA-C	-5.17	102.61	111.46
2	C	56	TRP	N-CA-C	-5.17	99.95	108.48
2	C	164	LEU	CA-C-N	-5.16	113.73	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	164	LEU	C-N-CA	-5.16	113.73	120.44
1	A	24	GLY	N-CA-C	5.15	125.39	113.18
1	B	223	THR	CA-C-N	-5.14	114.05	122.79
1	B	223	THR	C-N-CA	-5.14	114.05	122.79
1	B	200	ALA	N-CA-C	5.13	118.09	110.14
1	B	82	PHE	CA-CB-CG	-5.13	108.67	113.80
2	C	139	ASN	CA-CB-CG	-5.12	107.48	112.60
1	A	230	PHE	N-CA-C	5.11	118.08	109.95
2	D	51	LEU	CA-C-N	-5.11	112.00	120.68
2	D	51	LEU	C-N-CA	-5.11	112.00	120.68
2	C	117	HIS	CA-C-N	-5.09	113.35	120.53
2	C	117	HIS	C-N-CA	-5.09	113.35	120.53
1	A	42	ILE	CB-CA-C	-5.08	105.28	112.14
1	B	31	ALA	CA-C-O	-5.08	115.47	120.70
2	C	76	ASP	N-CA-C	5.06	116.98	109.69
1	B	231	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	147	GLY	CA-C-N	-5.05	111.95	120.58
1	A	147	GLY	C-N-CA	-5.05	111.95	120.58
1	B	172	GLY	N-CA-C	5.05	118.48	110.96
2	D	101	ASN	N-CA-C	-5.04	105.83	112.94
1	B	139	THR	CA-C-N	-5.04	112.32	121.14
1	B	139	THR	C-N-CA	-5.04	112.32	121.14
1	B	248	ALA	CA-C-N	-5.03	113.44	121.03
1	B	248	ALA	C-N-CA	-5.03	113.44	121.03
2	D	158	GLU	CA-C-O	-5.02	115.10	120.42
1	B	236	GLY	N-CA-C	-5.02	108.21	113.58
1	A	156	SER	CA-C-N	5.01	127.45	120.63
1	A	156	SER	C-N-CA	5.01	127.45	120.63

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	1971	0	1823	169	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1963	0	1812	163	1
2	C	1211	0	1164	139	2
2	D	1211	0	1164	82	2
3	A	47	0	0	3	0
3	B	51	0	0	3	0
3	C	22	0	0	3	0
3	D	23	0	0	1	0
All	All	6499	0	5963	518	3

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 43.

All (518) 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:108:CYS:SG	1:B:109:GLU:N	2.41	0.94
2:C:168:ALA:O	2:C:171:ASN:HB2	1.72	0.89
1:A:29:SCH:HA	1:A:199:HIS:CE1	2.09	0.88
2:C:110:GLN:HE21	2:C:110:GLN:HA	1.39	0.86
1:A:177:TYR:CD2	1:A:190:HIS:CE1	2.65	0.84
2:C:110:GLN:HA	2:C:110:GLN:NE2	1.93	0.81
1:A:85:ARG:HD3	2:C:56:TRP:CH2	2.17	0.80
1:A:242:ILE:HG23	1:A:243:GLU:HG3	1.65	0.79
1:A:65:SER:H	2:C:88:ASN:ND2	1.81	0.79
1:A:29:SCH:HB2	1:A:200:ALA:H	1.46	0.78
1:B:29:SCH:SG	1:B:30:TRP:CE3	2.75	0.78
1:A:66:MET:HE2	2:C:56:TRP:CD1	2.20	0.77
2:D:93:GLU:CD	2:D:93:GLU:H	1.94	0.75
1:A:0:LYS:H	1:A:0:LYS:HD3	1.51	0.75
1:A:85:ARG:HD2	2:C:56:TRP:CZ2	2.20	0.75
1:B:75:TYR:CZ	2:D:48:ARG:HG3	2.21	0.75
1:A:177:TYR:CG	1:A:190:HIS:CE1	2.75	0.75
2:C:66:LEU:HD13	2:C:101:ASN:ND2	2.03	0.74
2:D:50:PRO:HB2	2:D:65:LEU:HD21	1.69	0.73
1:A:23:GLN:NE2	1:A:26:CYS:O	2.21	0.73
1:A:66:MET:HE1	2:C:56:TRP:HB2	1.69	0.73
2:D:33:LEU:O	2:D:38:ALA:HB2	1.88	0.73
1:A:66:MET:CE	2:C:56:TRP:HB2	2.20	0.72
2:C:72:VAL:HG12	3:C:205:HOH:O	1.90	0.72
1:A:21:ARG:NH1	1:A:35:VAL:HG23	2.06	0.70
1:B:29:SCH:SG	1:B:30:TRP:HE3	2.14	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:HB2	2:C:78:TRP:CD1	2.27	0.69
1:A:24:GLY:HA2	1:A:108:CYS:SG	2.33	0.69
1:A:17:ILE:HG12	1:A:40:ASP:HB3	1.75	0.69
2:D:59:LEU:O	2:D:62:VAL:N	2.26	0.69
2:D:110:GLN:NE2	2:D:110:GLN:HA	2.08	0.68
1:B:116:ARG:HG3	1:B:117:PRO:HD2	1.76	0.68
2:C:165:GLN:HE21	2:C:169:LYS:H	1.39	0.68
1:B:30:TRP:CG	1:B:31:ALA:N	2.63	0.67
1:A:37:ALA:HB3	1:A:80:TRP:CH2	2.30	0.67
1:A:94:TYR:CD2	1:A:106:PRO:HA	2.30	0.67
2:D:120:ALA:HB1	2:D:152:ALA:HB2	1.78	0.66
1:A:38:ILE:HG23	1:A:83:TRP:CZ2	2.30	0.66
2:D:57:GLY:HA3	3:D:209:HOH:O	1.96	0.66
2:D:109:SER:O	2:D:111:ARG:N	2.29	0.66
1:A:85:ARG:CD	2:C:56:TRP:CH2	2.78	0.66
2:C:72:VAL:HG22	2:C:72:VAL:O	1.95	0.66
1:B:30:TRP:CE3	1:B:74:GLY:N	2.64	0.65
1:B:38:ILE:HG12	1:B:80:TRP:CZ3	2.31	0.65
1:A:130:LYS:O	1:A:140:TYR:CG	2.50	0.65
1:B:89:VAL:HG13	1:B:144:LYS:HZ3	1.62	0.65
2:D:56:TRP:CE3	2:D:57:GLY:N	2.65	0.65
1:B:30:TRP:CZ2	1:B:70:GLY:O	2.49	0.65
1:A:30:TRP:CE3	1:A:79:ALA:HB2	2.31	0.64
1:A:146:TYR:HB2	1:A:252:ARG:HE	1.63	0.64
2:C:106:ASN:N	2:C:106:ASN:HD22	1.96	0.64
1:B:85:ARG:HB3	2:D:56:TRP:CZ2	2.33	0.64
1:A:17:ILE:HA	1:A:40:ASP:OD1	1.98	0.64
1:B:26:CYS:SG	1:B:60:LEU:HD21	2.38	0.64
1:B:35:VAL:HG21	1:B:56:ALA:HB2	1.80	0.64
1:B:99:GLY:O	1:B:133:GLU:HG2	1.97	0.64
1:A:65:SER:H	2:C:88:ASN:HD22	1.43	0.64
1:A:2:PRO:HG2	1:A:5:PHE:HB2	1.79	0.63
2:C:40:VAL:O	2:C:40:VAL:CG1	2.46	0.63
2:C:128:VAL:O	2:C:132:LEU:HD13	1.98	0.63
1:A:23:GLN:NE2	1:A:28:SER:H	1.97	0.63
1:A:65:SER:HB2	2:C:85:LEU:HD23	1.79	0.63
1:A:66:MET:HE2	2:C:56:TRP:HD1	1.63	0.63
1:B:85:ARG:HG3	2:D:56:TRP:CE2	2.33	0.63
1:A:26:CYS:HB2	1:A:105:ILE:HD13	1.81	0.62
1:B:41:ARG:NH2	1:B:248:ALA:HB1	2.15	0.62
2:C:149:PHE:HE1	2:C:161:ALA:O	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:CYS:SG	1:B:105:ILE:CD1	2.88	0.62
1:B:173:ALA:O	1:B:174:PHE:HB3	1.99	0.62
1:B:25:SER:O	1:B:122:GLU:O	2.16	0.62
2:C:54:ALA:C	2:C:56:TRP:H	2.08	0.62
2:C:30:VAL:HG21	2:C:61:ILE:CD1	2.28	0.62
1:B:30:TRP:CZ3	1:B:74:GLY:N	2.68	0.61
1:B:6:ASP:HB3	1:B:9:GLU:CB	2.30	0.61
2:D:141:ASN:N	2:D:141:ASN:HD22	1.98	0.61
1:A:38:ILE:HG21	1:A:83:TRP:CE2	2.35	0.61
1:A:43:CYS:HA	1:A:50:VAL:O	2.00	0.61
1:A:30:TRP:CG	1:A:31:ALA:H	2.18	0.61
1:B:234:LEU:HB3	1:B:239:HIS:CB	2.31	0.61
1:A:177:TYR:CE2	1:A:195:MET:HB2	2.36	0.60
1:A:85:ARG:HD2	2:C:56:TRP:CE2	2.35	0.60
1:A:214:TYR:CE1	1:A:232:LYS:HG2	2.36	0.60
1:A:38:ILE:O	1:A:42:ILE:HG13	2.01	0.60
2:C:29:GLU:HG3	2:C:33:LEU:HD23	1.83	0.60
1:B:136:TYR:CE1	1:B:138:PRO:HG2	2.36	0.60
2:C:106:ASN:N	2:C:106:ASN:ND2	2.50	0.60
1:B:234:LEU:HB3	1:B:239:HIS:HB3	1.83	0.60
1:B:239:HIS:O	1:B:240:CYS:HB2	2.00	0.60
1:A:30:TRP:CG	1:A:31:ALA:N	2.69	0.59
1:A:85:ARG:CD	2:C:56:TRP:CZ2	2.85	0.59
1:A:94:TYR:CD2	1:A:107:PRO:HD3	2.37	0.59
1:B:65:SER:O	2:D:85:LEU:HD22	2.02	0.59
1:B:30:TRP:CZ3	1:B:73:GLY:CA	2.85	0.59
2:C:45:THR:O	2:C:46:TYR:HB2	2.02	0.59
1:B:89:VAL:HG13	1:B:144:LYS:NZ	2.17	0.59
2:D:54:ALA:HB1	2:D:62:VAL:HG23	1.85	0.59
2:D:33:LEU:O	2:D:38:ALA:CB	2.51	0.59
1:B:157:GLU:O	1:B:161:MET:SD	2.61	0.59
1:A:183:TYR:CE2	1:A:231:PHE:CB	2.86	0.58
1:B:82:PHE:CE1	1:B:86:LYS:HD2	2.38	0.58
1:A:87:GLY:O	1:A:144:LYS:HE3	2.03	0.58
2:C:142:ASP:HB3	2:C:146:LYS:O	2.03	0.58
1:B:66:MET:O	2:D:48:ARG:NH2	2.36	0.58
1:A:29:SCH:HA	1:A:199:HIS:ND1	2.18	0.58
1:B:85:ARG:CB	2:D:56:TRP:CZ2	2.88	0.57
2:D:109:SER:C	2:D:111:ARG:H	2.11	0.57
2:C:34:ILE:HD11	2:C:64:VAL:HG11	1.86	0.57
1:B:29:SCH:HE3	1:B:73:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TYR:CE2	1:A:138:PRO:HG2	2.40	0.57
1:A:109:GLU:O	1:A:119:CYS:SG	2.63	0.57
1:B:78:GLU:HA	1:B:81:ASN:HB2	1.87	0.57
1:B:38:ILE:HG23	1:B:83:TRP:CZ2	2.39	0.57
1:B:80:TRP:CD1	1:B:247:VAL:HG21	2.40	0.57
2:D:147:THR:HB	2:D:148:PRO:HD2	1.86	0.57
1:A:8:ARG:HG2	1:A:17:ILE:HG22	1.87	0.57
1:A:29:SCH:HE2	1:A:198:GLY:O	2.04	0.57
1:A:103:TYR:CE2	1:A:105:ILE:HB	2.40	0.57
1:A:0:LYS:H	1:A:0:LYS:CD	2.17	0.56
1:A:75:TYR:CE1	2:C:48:ARG:NH1	2.74	0.56
1:B:65:SER:OG	2:D:88:ASN:ND2	2.38	0.56
2:D:93:GLU:CD	2:D:93:GLU:N	2.63	0.56
1:B:29:SCH:SG	1:B:30:TRP:CZ3	2.98	0.56
2:C:143:ARG:C	2:C:145:GLY:N	2.63	0.56
2:C:21:ALA:O	2:C:25:GLY:N	2.37	0.56
1:B:73:GLY:O	2:D:78:TRP:NE1	2.38	0.56
1:B:77:ALA:HB2	3:B:328:HOH:O	2.06	0.56
1:A:75:TYR:HE1	2:C:48:ARG:NH1	2.03	0.56
1:B:47:ASN:C	1:B:49:HIS:H	2.14	0.56
2:C:34:ILE:CD1	2:C:64:VAL:CG1	2.83	0.56
2:C:40:VAL:O	2:C:41:ASN:CG	2.48	0.56
1:A:29:SCH:C	1:A:200:ALA:HB3	2.36	0.56
1:A:63:CYS:SG	1:A:82:PHE:CD1	2.99	0.56
2:D:117:HIS:HE1	2:D:140:ALA:HB3	1.71	0.56
2:C:168:ALA:O	2:C:171:ASN:N	2.34	0.55
1:B:6:ASP:HB3	1:B:9:GLU:H	1.70	0.55
2:D:109:SER:O	2:D:112:GLY:N	2.37	0.55
1:B:30:TRP:HZ2	1:B:70:GLY:O	1.88	0.55
1:A:171:GLU:HG2	1:A:172:GLY:N	2.20	0.55
1:B:69:ASP:HB3	1:B:72:ASN:HB2	1.87	0.55
1:A:177:TYR:CD2	1:A:190:HIS:HE1	2.22	0.55
1:A:183:TYR:CE2	1:A:231:PHE:HB2	2.42	0.55
1:B:195:MET:O	1:B:195:MET:HG2	2.06	0.55
2:D:59:LEU:O	2:D:60:GLU:C	2.47	0.55
1:B:176:VAL:HG21	1:B:199:HIS:ND1	2.22	0.55
1:B:204:LEU:HD23	1:B:204:LEU:H	1.72	0.55
2:C:149:PHE:CE1	2:C:161:ALA:O	2.60	0.55
1:B:30:TRP:CD1	1:B:31:ALA:N	2.76	0.55
1:B:41:ARG:NH2	1:B:170:VAL:HG12	2.22	0.55
1:B:89:VAL:HG12	1:B:143:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:O	1:B:42:ILE:HG13	2.07	0.54
1:B:234:LEU:HD22	1:B:239:HIS:HB2	1.89	0.54
1:A:38:ILE:CG2	1:A:83:TRP:CE2	2.91	0.54
1:A:47:ASN:O	1:A:48:ALA:HB3	2.08	0.54
1:A:70:GLY:HA3	1:A:125:THR:HG23	1.89	0.54
1:B:30:TRP:CZ3	1:B:73:GLY:HA2	2.42	0.54
1:A:20:ILE:HD11	1:A:230:PHE:CE2	2.42	0.54
1:A:29:SCH:CB	1:A:199:HIS:ND1	2.70	0.54
1:A:227:ASP:C	1:A:228:ASN:HD22	2.16	0.54
1:B:214:TYR:CD1	1:B:214:TYR:C	2.85	0.54
2:C:16:LYS:HZ1	2:C:44:ASP:HB3	1.73	0.54
2:C:40:VAL:O	2:C:41:ASN:CB	2.55	0.54
2:C:143:ARG:HD3	2:C:143:ARG:O	2.08	0.54
1:B:38:ILE:CG1	1:B:80:TRP:CZ3	2.90	0.54
1:A:29:SCH:CB	1:A:199:HIS:HD1	2.20	0.53
1:B:47:ASN:HD21	1:B:49:HIS:CE1	2.27	0.53
1:B:234:LEU:CD2	1:B:237:GLN:HB2	2.38	0.53
2:D:18:LEU:HD22	2:D:50:PRO:HB3	1.90	0.53
1:B:180:PHE:O	1:B:182:LEU:N	2.40	0.53
1:B:202:ARG:HG2	1:B:218:ALA:HB3	1.89	0.53
2:C:127:ILE:O	2:C:131:LEU:HD13	2.08	0.53
1:B:48:ALA:O	1:B:49:HIS:C	2.52	0.53
2:D:73:ASN:OD1	2:D:103:ALA:HA	2.08	0.53
2:D:44:ASP:O	2:D:46:TYR:N	2.42	0.53
1:A:239:HIS:CD2	1:A:240:CYS:HG	2.26	0.53
1:B:44:ILE:O	1:B:47:ASN:N	2.34	0.53
2:C:34:ILE:HG13	2:C:35:ALA:N	2.23	0.53
1:B:181:LEU:HD11	1:B:196:MET:SD	2.48	0.53
2:D:116:LEU:O	2:D:116:LEU:HD23	2.09	0.53
1:A:29:SCH:HB2	1:A:200:ALA:N	2.20	0.53
2:C:66:LEU:HD13	2:C:101:ASN:HD22	1.71	0.53
2:C:30:VAL:HG21	2:C:61:ILE:HG12	1.91	0.53
2:C:51:LEU:HB2	3:C:209:HOH:O	2.09	0.53
2:C:143:ARG:C	2:C:145:GLY:H	2.17	0.53
2:C:143:ARG:O	2:C:145:GLY:N	2.42	0.52
1:A:17:ILE:HG12	1:A:40:ASP:OD1	2.09	0.52
1:A:30:TRP:HE3	1:A:79:ALA:HB2	1.74	0.52
2:C:54:ALA:C	2:C:56:TRP:N	2.67	0.52
2:C:70:ALA:HB1	3:C:209:HOH:O	2.08	0.52
1:B:24:GLY:O	1:B:119:CYS:SG	2.68	0.52
2:C:34:ILE:O	2:C:37:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:ASP:O	2:C:77:LYS:C	2.53	0.52
1:A:58:ASP:HA	1:A:101:ARG:NH1	2.25	0.52
1:A:253:THR:O	1:A:254:ASP:CB	2.57	0.52
2:C:40:VAL:O	2:C:40:VAL:HG13	2.10	0.52
1:A:221:TRP:O	1:A:222:ASN:HB3	2.10	0.51
1:A:107:PRO:HB2	1:A:116:ARG:CD	2.40	0.51
1:B:44:ILE:HG22	1:B:45:HIS:N	2.25	0.51
2:C:153:ILE:O	2:C:154:ASP:C	2.53	0.51
1:B:6:ASP:HB3	1:B:9:GLU:HB2	1.92	0.51
1:A:17:ILE:CG1	1:A:40:ASP:HB3	2.39	0.51
1:B:35:VAL:O	1:B:39:SER:OG	2.29	0.51
2:C:105:VAL:O	2:C:115:PRO:HD2	2.11	0.51
2:C:153:ILE:O	2:C:155:ASN:O	2.28	0.51
2:C:167:ALA:O	2:C:168:ALA:C	2.52	0.51
1:A:120:THR:HG22	1:A:120:THR:O	2.11	0.51
2:C:153:ILE:HG22	2:C:154:ASP:N	2.26	0.51
1:A:23:GLN:NE2	1:A:28:SER:N	2.57	0.51
1:B:68:GLY:HA3	1:B:74:GLY:HA2	1.91	0.51
1:B:71:CYS:O	1:B:122:GLU:HB3	2.11	0.51
1:B:38:ILE:HG23	1:B:83:TRP:CH2	2.45	0.51
1:B:164:ILE:HG12	1:B:170:VAL:HG13	1.93	0.51
1:A:109:GLU:N	1:A:119:CYS:SG	2.84	0.50
2:C:18:LEU:HD12	2:C:38:ALA:HB3	1.92	0.50
2:D:123:GLY:O	2:D:124:HIS:CD2	2.63	0.50
1:A:65:SER:HB2	2:C:85:LEU:CD2	2.42	0.50
1:B:222:ASN:CG	1:B:223:THR:N	2.69	0.50
2:C:14:LEU:CD1	2:C:33:LEU:CD1	2.90	0.50
2:C:61:ILE:O	2:C:65:LEU:HD13	2.11	0.50
1:B:41:ARG:HH21	1:B:170:VAL:HG12	1.75	0.50
1:A:80:TRP:CZ3	1:A:248:ALA:HA	2.47	0.50
2:C:110:GLN:HE21	2:C:110:GLN:CA	2.19	0.50
2:C:116:LEU:HD22	2:C:148:PRO:CB	2.42	0.50
1:A:148:TYR:N	1:A:250:ILE:O	2.42	0.50
2:C:41:ASN:OD1	2:C:70:ALA:HA	2.11	0.50
1:B:57:GLU:OE2	1:B:61:THR:HG21	2.12	0.50
2:D:44:ASP:O	2:D:45:THR:C	2.54	0.49
2:D:39:ASP:O	2:D:40:VAL:HG12	2.11	0.49
2:D:141:ASN:N	2:D:141:ASN:ND2	2.60	0.49
1:B:233:ILE:HG12	1:B:234:LEU:N	2.27	0.49
1:B:253:THR:O	1:B:254:ASP:O	2.31	0.49
2:D:126:GLU:O	2:D:130:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD11	1:A:230:PHE:CZ	2.47	0.49
1:B:5:PHE:HE1	1:B:10:GLN:OE1	1.95	0.49
2:C:83:LEU:CD1	2:C:95:VAL:HG23	2.42	0.49
2:D:39:ASP:O	2:D:41:ASN:N	2.46	0.49
1:A:0:LYS:O	1:A:1:LEU:HD23	2.13	0.49
1:A:209:GLU:HB2	1:A:214:TYR:CE2	2.48	0.49
1:A:221:TRP:O	1:A:222:ASN:CB	2.61	0.49
1:B:41:ARG:HH12	1:B:167:ASN:HB2	1.77	0.49
1:A:38:ILE:CG2	1:A:83:TRP:CZ2	2.96	0.49
1:A:66:MET:HE3	1:A:78:GLU:OE1	2.12	0.49
1:B:31:ALA:O	1:B:35:VAL:HG22	2.13	0.49
2:C:30:VAL:HG11	2:C:61:ILE:HG23	1.95	0.49
1:A:223:THR:O	1:A:228:ASN:HA	2.13	0.49
2:D:26:GLN:HB3	2:D:29:GLU:HB3	1.94	0.49
1:A:21:ARG:NH1	1:A:35:VAL:CG2	2.75	0.48
1:A:37:ALA:HB3	1:A:80:TRP:HH2	1.78	0.48
1:A:234:LEU:HB3	1:A:239:HIS:HB2	1.95	0.48
1:B:78:GLU:HA	1:B:81:ASN:CB	2.43	0.48
1:B:94:TYR:O	1:B:95:GLU:C	2.56	0.48
2:C:34:ILE:HD12	2:C:64:VAL:HG12	1.95	0.48
1:A:24:GLY:O	1:A:25:SER:CB	2.59	0.48
1:B:80:TRP:CD1	1:B:247:VAL:CG2	2.96	0.48
2:D:76:ASP:OD2	2:D:80:TYR:HB2	2.14	0.48
1:B:40:ASP:O	1:B:43:CYS:HB3	2.13	0.48
1:A:209:GLU:HB2	1:A:214:TYR:HE2	1.78	0.48
1:A:225:TRP:CD2	1:A:226:GLY:N	2.81	0.48
1:A:239:HIS:CD2	1:A:240:CYS:SG	3.06	0.48
1:B:237:GLN:O	1:B:238:ASP:HB3	2.12	0.48
1:B:38:ILE:CG2	1:B:83:TRP:CZ2	2.96	0.48
2:C:168:ALA:O	2:C:171:ASN:CB	2.53	0.48
1:B:222:ASN:CG	1:B:223:THR:H	2.22	0.48
2:D:116:LEU:HD12	2:D:136:ALA:HB1	1.96	0.48
1:B:30:TRP:HZ3	1:B:73:GLY:HA2	1.79	0.48
1:B:60:LEU:HD11	1:B:70:GLY:O	2.13	0.48
2:C:29:GLU:O	2:C:33:LEU:HD23	2.14	0.48
2:C:168:ALA:O	2:C:169:LYS:C	2.55	0.48
2:D:60:GLU:O	2:D:63:ASP:HB2	2.13	0.48
1:B:224:ASP:O	1:B:225:TRP:C	2.55	0.48
1:B:38:ILE:HG21	1:B:83:TRP:CE2	2.49	0.48
2:C:150:ASP:O	2:C:154:ASP:N	2.47	0.48
1:A:41:ARG:HH21	1:A:170:VAL:HG12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:TRP:CE3	1:A:226:GLY:N	2.82	0.48
1:B:75:TYR:CE1	2:D:46:TYR:HB2	2.48	0.47
2:C:14:LEU:HD11	2:C:33:LEU:CD1	2.44	0.47
2:C:34:ILE:CD1	2:C:64:VAL:HG12	2.44	0.47
2:D:121:THR:HG23	2:D:155:ASN:ND2	2.29	0.47
1:B:164:ILE:HA	1:B:168:GLY:O	2.14	0.47
2:C:44:ASP:C	2:C:45:THR:O	2.56	0.47
1:A:176:VAL:O	1:A:195:MET:HA	2.14	0.47
1:B:112:VAL:HG11	1:B:225:TRP:HA	1.96	0.47
2:C:45:THR:O	2:C:46:TYR:CB	2.62	0.47
1:A:90:SER:HB2	1:A:100:CYS:H	1.79	0.47
1:A:100:CYS:HB2	1:A:143:ASP:OD2	2.14	0.47
1:A:180:PHE:O	1:A:181:LEU:C	2.56	0.47
1:B:5:PHE:CE1	1:B:10:GLN:OE1	2.68	0.47
2:C:83:LEU:HD12	2:C:95:VAL:HG23	1.97	0.47
1:A:214:TYR:CD1	1:A:232:LYS:HG2	2.50	0.47
2:C:75:SER:HA	2:C:80:TYR:O	2.15	0.47
1:A:84:THR:HG21	1:A:149:ASN:C	2.40	0.47
1:A:45:HIS:CG	1:A:251:PRO:HG2	2.50	0.46
1:A:57:GLU:O	1:A:61:THR:HG23	2.14	0.46
1:A:140:TYR:OH	1:A:144:LYS:NZ	2.48	0.46
1:B:92:GLY:O	1:B:93:LEU:O	2.33	0.46
2:C:14:LEU:CD1	2:C:33:LEU:HD12	2.46	0.46
1:A:78:GLU:O	1:A:82:PHE:N	2.46	0.46
1:A:133:GLU:HA	1:A:134:PRO:HD2	1.77	0.46
1:B:29:SCH:HB3	1:B:200:ALA:H	1.80	0.46
1:A:9:GLU:O	1:A:12:PRO:HD3	2.16	0.46
2:D:123:GLY:HA2	2:D:160:ILE:HD12	1.98	0.46
1:A:43:CYS:O	1:A:48:ALA:N	2.46	0.46
1:A:174:PHE:HA	3:A:316:HOH:O	2.15	0.46
2:C:30:VAL:HG21	2:C:61:ILE:CG1	2.45	0.46
2:C:54:ALA:O	2:C:56:TRP:N	2.48	0.46
1:A:69:ASP:O	1:A:70:GLY:C	2.55	0.46
1:A:234:LEU:HB3	1:A:239:HIS:CB	2.46	0.46
1:B:30:TRP:CH2	1:B:70:GLY:O	2.69	0.46
2:C:30:VAL:HG21	2:C:61:ILE:HD13	1.97	0.46
2:D:110:GLN:NE2	2:D:110:GLN:CA	2.78	0.46
1:A:35:VAL:HG13	1:A:59:LEU:HD23	1.98	0.46
1:A:38:ILE:HD13	1:A:83:TRP:CD2	2.51	0.46
1:A:209:GLU:C	1:A:211:GLY:N	2.73	0.46
1:B:178:SER:C	1:B:180:PHE:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:VAL:HG21	2:C:134:ASN:O	2.16	0.46
1:A:64:GLY:HA3	2:C:88:ASN:HD21	1.81	0.46
1:B:180:PHE:C	1:B:182:LEU:N	2.74	0.46
1:A:39:SER:O	1:A:40:ASP:C	2.54	0.45
1:B:214:TYR:HA	1:B:235:ARG:H	1.81	0.45
3:B:306:HOH:O	2:D:53:ALA:HB1	2.15	0.45
2:C:127:ILE:N	2:C:127:ILE:HD12	2.31	0.45
1:B:55:SER:OG	1:B:57:GLU:HB3	2.17	0.45
1:A:29:SCH:SG	1:A:199:HIS:ND1	2.79	0.45
1:B:20:ILE:HG22	1:B:21:ARG:N	2.31	0.45
2:C:30:VAL:O	2:C:34:ILE:HG12	2.17	0.45
1:A:57:GLU:O	1:A:58:ASP:C	2.59	0.45
1:A:76:PRO:O	1:A:77:ALA:C	2.60	0.45
1:B:6:ASP:O	1:B:7:ALA:C	2.57	0.45
1:B:26:CYS:HB2	1:B:105:ILE:HD13	1.99	0.45
2:C:116:LEU:HD12	2:C:136:ALA:HB1	1.99	0.45
1:B:160:ILE:O	1:B:163:GLU:HB3	2.16	0.45
1:B:20:ILE:CG2	1:B:21:ARG:N	2.80	0.45
1:B:43:CYS:SG	1:B:48:ALA:HA	2.57	0.45
2:C:70:ALA:O	2:C:71:ASP:C	2.57	0.45
1:B:75:TYR:OH	2:D:48:ARG:HB2	2.16	0.45
1:B:75:TYR:CE2	2:D:48:ARG:HG3	2.51	0.45
1:B:190:HIS:H	1:B:239:HIS:CE1	2.34	0.45
1:B:239:HIS:O	1:B:240:CYS:CB	2.64	0.45
2:C:147:THR:HB	2:C:148:PRO:HD2	1.98	0.45
1:B:162:ALA:O	1:B:166:LYS:N	2.45	0.45
2:D:61:ILE:O	2:D:65:LEU:HD13	2.16	0.45
2:D:110:GLN:HA	2:D:110:GLN:HE21	1.82	0.45
1:A:63:CYS:HB3	1:A:67:CYS:HB2	1.78	0.45
1:A:171:GLU:HG3	1:A:201:ILE:O	2.17	0.45
1:A:181:LEU:O	1:A:182:LEU:CB	2.64	0.45
2:C:66:LEU:HB3	2:C:101:ASN:HD22	1.81	0.45
2:D:34:ILE:HA	2:D:38:ALA:HB3	1.98	0.45
1:B:37:ALA:O	1:B:38:ILE:C	2.58	0.44
1:A:30:TRP:CZ3	1:A:79:ALA:HB2	2.52	0.44
1:B:177:TYR:O	1:B:180:PHE:HB3	2.17	0.44
2:C:125:LEU:O	2:C:126:GLU:C	2.60	0.44
2:D:55:ALA:O	2:D:56:TRP:C	2.59	0.44
2:D:140:ALA:C	2:D:141:ASN:HD22	2.24	0.44
1:A:6:ASP:HB3	1:A:9:GLU:HB2	1.99	0.44
1:A:57:GLU:HB2	1:A:103:TYR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PRO:HB2	1:A:116:ARG:HD2	1.97	0.44
2:D:59:LEU:HD13	2:D:94:ILE:CG1	2.47	0.44
1:A:35:VAL:HG21	1:A:56:ALA:CA	2.48	0.44
1:B:142:GLN:O	1:B:142:GLN:HG2	2.17	0.44
2:C:116:LEU:N	2:C:131:LEU:HD23	2.33	0.44
1:A:134:PRO:HB2	2:D:35:ALA:HB1	1.98	0.44
1:A:136:TYR:HE2	1:A:138:PRO:HG2	1.83	0.44
1:A:181:LEU:O	1:A:182:LEU:HG	2.18	0.44
1:A:225:TRP:CE3	1:A:226:GLY:HA3	2.52	0.44
2:C:50:PRO:O	2:C:53:ALA:N	2.51	0.44
1:B:17:ILE:HG12	1:B:40:ASP:OD2	2.18	0.44
2:C:128:VAL:HG12	2:C:132:LEU:HD13	1.99	0.44
2:C:131:LEU:O	2:C:136:ALA:HB2	2.18	0.44
2:D:18:LEU:HD12	2:D:38:ALA:HB1	1.99	0.44
2:D:33:LEU:HD23	2:D:33:LEU:N	2.31	0.44
1:A:147:GLY:HA2	1:A:251:PRO:HA	2.00	0.44
1:B:186:GLY:O	1:B:232:LYS:HB2	2.18	0.44
1:B:226:GLY:C	1:B:228:ASN:H	2.26	0.44
2:C:39:ASP:OD2	2:C:41:ASN:O	2.36	0.44
2:C:92:LEU:HG	2:C:96:GLU:OE2	2.17	0.44
1:B:232:LYS:HD2	1:B:232:LYS:N	2.33	0.43
2:C:57:GLY:C	2:C:58:HIS:CG	2.96	0.43
1:B:75:TYR:HE1	2:D:46:TYR:HB2	1.83	0.43
1:B:214:TYR:CA	1:B:235:ARG:HB3	2.47	0.43
2:C:39:ASP:O	2:C:40:VAL:O	2.35	0.43
2:C:84:HIS:O	2:C:85:LEU:C	2.61	0.43
2:D:56:TRP:HE3	2:D:57:GLY:N	2.11	0.43
1:A:14:CYS:HA	1:A:15:PRO:HD2	1.88	0.43
1:A:139:THR:O	1:A:143:ASP:N	2.48	0.43
1:B:35:VAL:HG13	1:B:59:LEU:HD23	1.99	0.43
1:B:58:ASP:OD2	1:B:144:LYS:NZ	2.47	0.43
2:C:105:VAL:HB	2:C:106:ASN:ND2	2.32	0.43
2:C:116:LEU:HD11	2:C:132:LEU:HD11	2.00	0.43
2:D:142:ASP:HB2	2:D:145:GLY:H	1.83	0.43
1:A:85:ARG:C	1:A:86:LYS:HG3	2.44	0.43
1:A:103:TYR:OH	1:A:105:ILE:HD12	2.17	0.43
1:B:80:TRP:NE1	1:B:247:VAL:HG23	2.32	0.43
1:B:238:ASP:HB2	1:B:243:GLU:OE1	2.18	0.43
2:C:34:ILE:HG13	2:C:35:ALA:H	1.83	0.43
2:C:132:LEU:C	2:C:134:ASN:N	2.76	0.43
2:D:64:VAL:O	2:D:65:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:ALA:CB	2:C:160:ILE:HG21	2.48	0.43
1:A:181:LEU:C	1:A:182:LEU:HG	2.44	0.43
2:C:64:VAL:O	2:C:65:LEU:C	2.62	0.43
2:C:105:VAL:O	2:C:105:VAL:HG12	2.18	0.43
2:D:142:ASP:HB3	2:D:144:GLN:H	1.83	0.43
1:A:29:SCH:CA	1:A:199:HIS:ND1	2.82	0.43
2:C:158:GLU:O	2:C:159:ASP:C	2.61	0.43
2:D:105:VAL:HB	2:D:106:ASN:ND2	2.33	0.43
1:A:26:CYS:HB2	1:A:105:ILE:CD1	2.49	0.43
1:B:40:ASP:O	1:B:43:CYS:N	2.52	0.43
1:B:41:ARG:NH1	1:B:167:ASN:CB	2.81	0.43
1:B:48:ALA:C	1:B:50:VAL:N	2.73	0.43
1:B:56:ALA:O	1:B:57:GLU:C	2.61	0.43
1:B:164:ILE:CG1	1:B:170:VAL:HG13	2.49	0.43
1:A:21:ARG:HH11	1:A:35:VAL:HG23	1.83	0.43
2:D:52:HIS:HE1	2:D:81:THR:CA	2.32	0.43
2:D:55:ALA:C	2:D:56:TRP:O	2.57	0.43
1:A:61:THR:O	1:A:128:CYS:HB2	2.18	0.42
2:D:16:LYS:O	2:D:20:ASP:N	2.48	0.42
2:D:40:VAL:CG1	2:D:41:ASN:H	2.32	0.42
2:D:115:PRO:O	2:D:118:VAL:HG13	2.19	0.42
1:A:96:SER:O	1:A:97:HIS:HB2	2.19	0.42
1:A:107:PRO:HB2	1:A:116:ARG:HD3	2.01	0.42
1:B:26:CYS:SG	1:B:105:ILE:HD12	2.57	0.42
1:B:47:ASN:C	1:B:49:HIS:N	2.75	0.42
2:D:120:ALA:HA	2:D:160:ILE:HG21	2.01	0.42
1:B:6:ASP:CB	1:B:9:GLU:HB2	2.50	0.42
1:B:41:ARG:NH2	1:B:248:ALA:CB	2.81	0.42
1:B:157:GLU:HG2	1:B:161:MET:SD	2.59	0.42
2:C:162:GLU:O	2:C:163:VAL:C	2.63	0.42
2:D:111:ARG:HH11	2:D:111:ARG:CG	2.32	0.42
1:B:148:TYR:CD2	1:B:149:ASN:HB3	2.55	0.42
2:D:164:LEU:O	2:D:165:GLN:C	2.62	0.42
1:A:23:GLN:HE21	1:A:28:SER:H	1.64	0.42
1:B:148:TYR:HD2	1:B:149:ASN:HB3	1.84	0.42
1:A:94:TYR:CE2	1:A:106:PRO:HA	2.54	0.42
1:B:208:VAL:HG12	1:B:209:GLU:N	2.34	0.42
2:C:66:LEU:CB	2:C:101:ASN:HD22	2.32	0.42
2:C:110:GLN:NE2	2:C:110:GLN:CA	2.75	0.42
2:C:118:VAL:HG23	2:C:119:ALA:N	2.35	0.42
2:D:109:SER:C	2:D:111:ARG:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HG21	1:A:229:GLY:HA3	2.02	0.42
1:A:157:GLU:O	1:A:160:ILE:N	2.53	0.42
1:A:234:LEU:HD11	3:A:327:HOH:O	2.18	0.42
1:B:30:TRP:CZ3	1:B:73:GLY:C	2.97	0.42
1:A:32:PHE:HB3	1:A:36:GLU:OE2	2.19	0.42
1:A:61:THR:HG22	1:A:126:PRO:HG2	2.01	0.42
1:A:227:ASP:OD1	1:A:228:ASN:ND2	2.53	0.42
1:B:32:PHE:HA	1:B:35:VAL:HG22	2.02	0.42
1:B:179:ASP:HB3	1:B:192:THR:O	2.19	0.42
2:C:29:GLU:HG3	2:C:29:GLU:O	2.20	0.42
2:C:49:THR:HB	2:C:50:PRO:CD	2.50	0.42
2:C:146:LYS:HA	2:C:150:ASP:OD2	2.20	0.42
2:C:34:ILE:CD1	2:C:64:VAL:HG11	2.48	0.42
2:C:149:PHE:CE1	2:C:165:GLN:HB2	2.55	0.42
1:A:227:ASP:HB3	1:A:230:PHE:O	2.20	0.42
2:C:80:TYR:HD2	2:C:84:HIS:CD2	2.38	0.41
1:A:34:ALA:C	1:A:36:GLU:N	2.74	0.41
1:A:100:CYS:O	1:A:132:CYS:HB3	2.20	0.41
2:C:73:ASN:HD21	2:C:103:ALA:HA	1.84	0.41
2:C:159:ASP:O	2:C:162:GLU:N	2.49	0.41
1:A:35:VAL:HG13	1:A:59:LEU:CD2	2.51	0.41
1:A:69:ASP:HB3	1:A:72:ASN:HB2	2.01	0.41
1:B:65:SER:O	2:D:85:LEU:CD2	2.66	0.41
2:C:70:ALA:O	2:C:72:VAL:N	2.52	0.41
2:C:74:ALA:O	2:C:81:THR:HA	2.21	0.41
2:C:90:GLY:O	2:C:91:HIS:HB2	2.20	0.41
2:D:44:ASP:O	2:D:44:ASP:CG	2.62	0.41
1:A:65:SER:N	2:C:88:ASN:ND2	2.61	0.41
1:A:171:GLU:HG2	1:A:172:GLY:H	1.84	0.41
1:A:242:ILE:HG13	1:A:242:ILE:O	2.20	0.41
1:B:41:ARG:NH1	1:B:167:ASN:HB2	2.35	0.41
1:B:85:ARG:CB	2:D:56:TRP:HZ2	2.31	0.41
2:C:142:ASP:O	2:C:143:ARG:C	2.60	0.41
2:C:93:GLU:H	2:C:93:GLU:CD	2.29	0.41
2:D:93:GLU:O	2:D:94:ILE:C	2.60	0.41
2:D:142:ASP:CB	2:D:144:GLN:H	2.33	0.41
1:A:130:LYS:HD2	3:A:333:HOH:O	2.19	0.41
1:B:174:PHE:HE2	1:B:201:ILE:HG12	1.86	0.41
1:B:250:ILE:HG22	1:B:251:PRO:N	2.35	0.41
2:C:39:ASP:O	2:C:40:VAL:HG12	2.20	0.41
2:C:165:GLN:NE2	2:C:169:LYS:H	2.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:GLN:O	2:D:27:ASP:C	2.63	0.41
1:A:177:TYR:O	1:A:180:PHE:HB3	2.21	0.41
1:B:177:TYR:HA	1:B:194:GLU:O	2.21	0.41
1:B:189:GLN:O	1:B:191:VAL:HG23	2.21	0.41
2:D:40:VAL:HG13	2:D:41:ASN:N	2.36	0.41
1:B:161:MET:O	1:B:162:ALA:C	2.63	0.41
1:B:173:ALA:O	1:B:174:PHE:CB	2.69	0.41
2:C:83:LEU:HD22	2:C:103:ALA:HB1	2.02	0.41
1:A:109:GLU:OE2	1:A:116:ARG:HB2	2.21	0.41
1:A:110:HIS:O	1:A:112:VAL:HG13	2.20	0.41
1:A:171:GLU:CG	1:A:201:ILE:O	2.68	0.41
1:B:28:SER:O	1:B:29:SCH:C	2.69	0.41
1:B:178:SER:OG	1:B:194:GLU:N	2.54	0.41
1:B:242:ILE:O	1:B:242:ILE:HG13	2.20	0.41
2:C:10:HIS:O	2:C:14:LEU:HB2	2.21	0.41
2:C:18:LEU:HD23	2:C:18:LEU:O	2.21	0.41
2:C:106:ASN:O	2:C:107:ALA:C	2.64	0.41
2:D:66:LEU:CD1	2:D:97:VAL:HG12	2.51	0.41
1:B:47:ASN:O	1:B:47:ASN:ND2	2.54	0.41
1:A:55:SER:HB2	1:A:91:GLY:HA3	2.02	0.40
1:B:85:ARG:HB3	2:D:56:TRP:HZ2	1.79	0.40
1:B:178:SER:C	1:B:180:PHE:N	2.80	0.40
2:C:34:ILE:HG21	2:C:34:ILE:HD13	1.82	0.40
1:A:64:GLY:HA2	2:C:122:TRP:CZ2	2.56	0.40
1:A:79:ALA:O	1:A:82:PHE:HB3	2.22	0.40
1:B:38:ILE:CG2	1:B:83:TRP:CE2	3.04	0.40
2:C:116:LEU:C	2:C:116:LEU:HD23	2.46	0.40
1:B:10:GLN:HB3	1:B:11:TRP:CE3	2.56	0.40
2:D:128:VAL:O	2:D:129:ASP:C	2.61	0.40
1:A:68:GLY:HA3	1:A:74:GLY:HA2	2.03	0.40
1:A:80:TRP:O	1:A:83:TRP:HB3	2.22	0.40
1:B:21:ARG:HB2	1:B:36:GLU:OE1	2.21	0.40
1:B:44:ILE:HG21	1:B:167:ASN:O	2.21	0.40
1:B:209:GLU:O	1:B:210:ASN:HB2	2.21	0.40
2:C:95:VAL:O	2:C:96:GLU:C	2.61	0.40
1:B:25:SER:HB2	3:B:312:HOH:O	2.21	0.40
1:B:42:ILE:O	1:B:43:CYS:C	2.64	0.40
1:B:106:PRO:HA	1:B:107:PRO:HD3	2.00	0.40
2:C:14:LEU:O	2:C:15:GLY:C	2.65	0.40
2:C:14:LEU:HD12	2:C:33:LEU:CD1	2.51	0.40
2:D:66:LEU:HD21	2:D:72:VAL:HG23	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:TYR:CD2	2:D:31:ARG:NH1[4_558]	1.52	0.68
1:B:111:HIS:CD2	1:B:141:LYS:NZ[1_554]	2.15	0.05
2:C:68:TYR:CG	2:D:31:ARG:NH1[4_558]	2.15	0.05

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	253/256 (99%)	210 (83%)	39 (15%)	4 (2%)	7	14
1	B	252/256 (98%)	195 (77%)	48 (19%)	9 (4%)	2	4
2	C	161/171 (94%)	117 (73%)	34 (21%)	10 (6%)	1	1
2	D	161/171 (94%)	136 (84%)	14 (9%)	11 (7%)	1	1
All	All	827/854 (97%)	658 (80%)	135 (16%)	34 (4%)	2	3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	B	93	LEU
1	B	253	THR
2	C	41	ASN
2	C	154	ASP
2	D	26	GLN
2	D	45	THR
2	D	57	GLY
2	D	110	GLN
1	B	117	PRO
1	B	181	LEU
2	D	41	ASN
1	B	174	PHE

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Mol	Chain	Res	Type
2	C	155	ASN
2	C	169	LYS
2	D	31	ARG
2	D	37	GLY
1	A	25	SER
2	C	40	VAL
2	C	153	ILE
2	D	77	LYS
1	A	121	GLY
2	C	126	GLU
2	C	27	ASP
2	D	46	TYR
1	B	137	SER
2	C	11	GLY
2	C	72	VAL
2	D	30	VAL
2	D	40	VAL
1	A	92	GLY
1	B	89	VAL
1	B	44	ILE
1	B	102	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	210/210 (100%)	188 (90%)	22 (10%)	6	13
1	B	209/210 (100%)	187 (90%)	22 (10%)	6	13
2	C	122/129 (95%)	106 (87%)	16 (13%)	4	7
2	D	122/129 (95%)	101 (83%)	21 (17%)	2	3
All	All	663/678 (98%)	582 (88%)	81 (12%)	5	8

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	LEU
1	A	0	LYS
1	A	4	SER
1	A	28	SER
1	A	40	ASP
1	A	61	THR
1	A	65	SER
1	A	69	ASP
1	A	72	ASN
1	A	115	SER
1	A	125	THR
1	A	128	CYS
1	A	142	GLN
1	A	144	LYS
1	A	152	SER
1	A	155	ASN
1	A	194	GLU
1	A	196	MET
1	A	201	ILE
1	A	228	ASN
1	A	244	SER
1	A	245	GLU
1	B	16	THR
1	B	25	SER
1	B	39	SER
1	B	40	ASP
1	B	51	SER
1	B	66	MET
1	B	75	TYR
1	B	108	CYS
1	B	115	SER
1	B	119	CYS
1	B	133	GLU
1	B	152	SER
1	B	154	SER
1	B	155	ASN
1	B	178	SER
1	B	181	LEU
1	B	195	MET
1	B	202	ARG
1	B	210	ASN
1	B	232	LYS
1	B	237	GLN

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Mol	Chain	Res	Type
1	B	253	THR
2	C	12	SER
2	C	31	ARG
2	C	40	VAL
2	C	43	SER
2	C	45	THR
2	C	75	SER
2	C	99	LEU
2	C	106	ASN
2	C	110	GLN
2	C	113	GLN
2	C	118	VAL
2	C	126	GLU
2	C	129	ASP
2	C	142	ASP
2	C	159	ASP
2	C	166	LYS
2	D	12	SER
2	D	17	LYS
2	D	19	LEU
2	D	20	ASP
2	D	23	SER
2	D	26	GLN
2	D	33	LEU
2	D	36	ASN
2	D	48	ARG
2	D	56	TRP
2	D	95	VAL
2	D	99	LEU
2	D	105	VAL
2	D	106	ASN
2	D	110	GLN
2	D	111	ARG
2	D	118	VAL
2	D	126	GLU
2	D	141	ASN
2	D	159	ASP
2	D	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	113	ASN
1	A	190	HIS
1	A	228	ASN
1	A	237	GLN
1	B	47	ASN
1	B	72	ASN
1	B	142	GLN
1	B	145	HIS
1	B	167	ASN
1	B	189	GLN
1	B	190	HIS
1	B	210	ASN
1	B	237	GLN
2	C	36	ASN
2	C	73	ASN
2	C	88	ASN
2	C	101	ASN
2	C	106	ASN
2	C	110	GLN
2	C	157	ASN
2	C	165	GLN
2	D	36	ASN
2	D	88	ASN
2	D	110	GLN
2	D	124	HIS
2	D	141	ASN
2	D	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SCH	A	29	1	6,7,8	0.55	0	4,7,9	0.67	0
1	SCH	B	29	1	6,7,8	0.46	0	4,7,9	1.53	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCH	A	29	1	-	1/2/6/8	-
1	SCH	B	29	1	-	1/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	SCH	CB-SG-SD	2.75	110.98	103.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	29	SCH	CA-CB-SG-SD
1	B	29	SCH	CA-CB-SG-SD

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	29	SCH	10	0
1	B	29	SCH	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/256 (99%)	0.21	11 (4%) 40 38	13, 49, 92, 99	2 (0%)
1	B	254/256 (99%)	1.03	40 (15%) 5 4	20, 77, 98, 99	5 (1%)
2	C	163/171 (95%)	0.67	15 (9%) 14 14	28, 71, 99, 99	0
2	D	161/171 (94%)	0.34	7 (4%) 40 38	21, 55, 87, 99	3 (1%)
All	All	832/854 (97%)	0.57	73 (8%) 15 15	13, 61, 98, 99	10 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ILE	5.2
1	B	164	ILE	4.4
1	B	217	VAL	4.2
1	B	181	LEU	4.0
1	B	205	GLY	3.9
1	A	192	THR	3.8
1	B	192	THR	3.7
1	B	231	PHE	3.5
2	C	145	GLY	3.4
1	B	191	VAL	3.4
1	B	173	ALA	3.3
1	B	246	VAL	3.3
1	B	203	ILE	3.2
1	B	177	TYR	3.2
2	D	40	VAL	3.1
1	B	174	PHE	3.1
1	B	199	HIS	3.0
1	B	153	VAL	3.0
1	B	215	TRP	3.0
1	B	254	ASP	3.0
1	A	123	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	121	GLY	2.9
1	A	196	MET	2.8
1	B	206	TRP	2.8
2	D	38	ALA	2.8
1	B	180	PHE	2.8
1	B	213	PRO	2.8
2	C	168	ALA	2.8
2	D	144	GLN	2.7
1	B	20	ILE	2.7
1	B	182	LEU	2.7
2	C	77	LYS	2.7
2	C	18	LEU	2.6
2	C	110	GLN	2.6
2	D	170	LEU	2.6
2	D	65	LEU	2.5
1	B	253	THR	2.5
1	B	50	VAL	2.4
1	B	176	VAL	2.4
2	C	22	ALA	2.4
1	A	198	GLY	2.4
1	B	3	ALA	2.4
2	C	32	ILE	2.4
2	D	139	ASN	2.4
2	C	148	PRO	2.4
1	B	242	ILE	2.3
2	C	144	GLN	2.3
2	C	140	ALA	2.3
1	B	15	PRO	2.3
1	B	188	TYR	2.3
1	B	187	VAL	2.3
1	A	181	LEU	2.3
1	A	49	HIS	2.2
1	B	112	VAL	2.2
2	C	34	ILE	2.2
1	B	165	TYR	2.2
1	B	33	GLY	2.2
1	B	16	THR	2.2
1	B	240	CYS	2.2
1	A	1	LEU	2.2
2	C	112	GLY	2.2
1	B	148	TYR	2.1
2	C	58	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	2.1
1	B	30	TRP	2.1
2	D	19	LEU	2.1
1	B	234	LEU	2.1
2	C	19	LEU	2.1
1	A	20	ILE	2.1
1	A	75	TYR	2.1
1	A	13	GLN	2.0
2	C	31	ARG	2.0
1	A	124	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SCH	A	29	8/9	0.76	0.20	54,65,70,84	0
1	SCH	B	29	8/9	0.82	0.14	56,66,70,71	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.