



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:49 AM UTC

PDB ID : 3H6S / pdb_00003h6s
Title : Structure of cliticypin - cathepsin V complex
Authors : Renko, M.; Sabotic, J.; Brzin, J.; Turk, D.
Deposited on : 2009-04-23
Resolution : 2.22 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

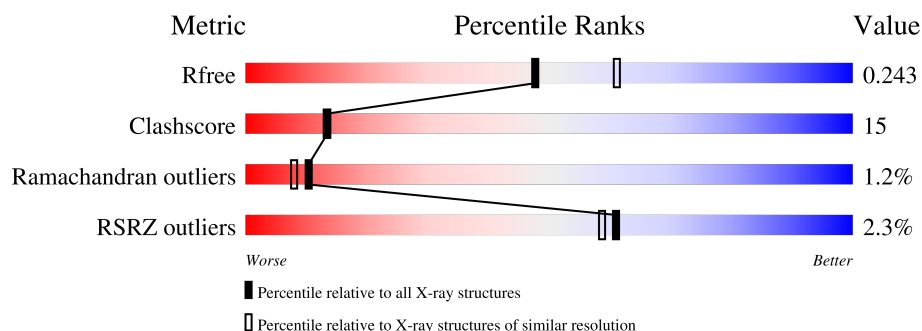
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	221	
1	B	221	
1	C	221	
1	D	221	
2	E	152	
2	F	152	

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Mol	Chain	Length	Quality of chain
2	G	152	
2	H	152	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	F	153	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12387 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 L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	7	0	0
			1683	1061	288	324	10			
1	B	220	Total	C	N	O	S	17	0	0
			1683	1061	288	324	10			
1	C	220	Total	C	N	O	S	8	0	0
			1683	1061	288	324	10			
1	D	220	Total	C	N	O	S	11	0	0
			1683	1061	288	324	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	GLN	ASN	engineered mutation	UNP O60911
A	179	ASP	ASN	engineered mutation	UNP O60911
B	108	GLN	ASN	engineered mutation	UNP O60911
B	179	ASP	ASN	engineered mutation	UNP O60911
C	108	GLN	ASN	engineered mutation	UNP O60911
C	179	ASP	ASN	engineered mutation	UNP O60911
D	108	GLN	ASN	engineered mutation	UNP O60911
D	179	ASP	ASN	engineered mutation	UNP O60911

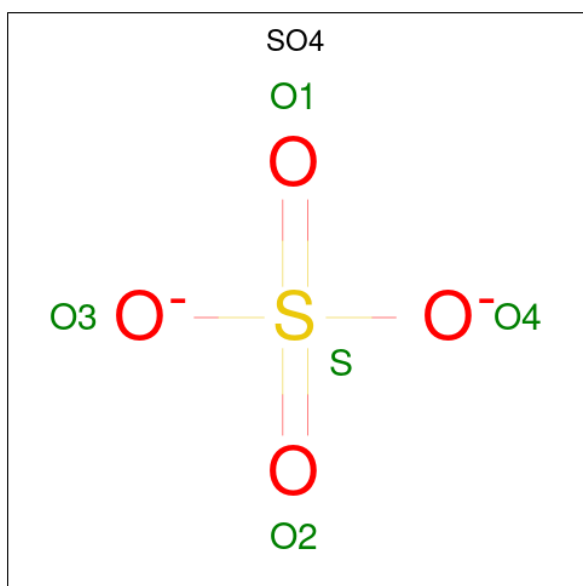
- Molecule 2 is a protein called Clitocypin analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	152	Total	C	N	O	S	47	0	0
			1192	752	204	233	3			
2	F	152	Total	C	N	O	S	38	0	0
			1192	752	204	233	3			
2	G	152	Total	C	N	O	S	64	0	0
			1192	752	204	233	3			
2	H	152	Total	C	N	O	S	51	0	0
			1192	752	204	233	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	82	SME	LEU	engineered mutation	UNP Q3Y9I6
E	89	SME	ILE	engineered mutation	UNP Q3Y9I6
F	82	SME	LEU	engineered mutation	UNP Q3Y9I6
F	89	SME	ILE	engineered mutation	UNP Q3Y9I6
G	82	SME	LEU	engineered mutation	UNP Q3Y9I6
G	89	SME	ILE	engineered mutation	UNP Q3Y9I6
H	82	SME	LEU	engineered mutation	UNP Q3Y9I6
H	89	SME	ILE	engineered mutation	UNP Q3Y9I6

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

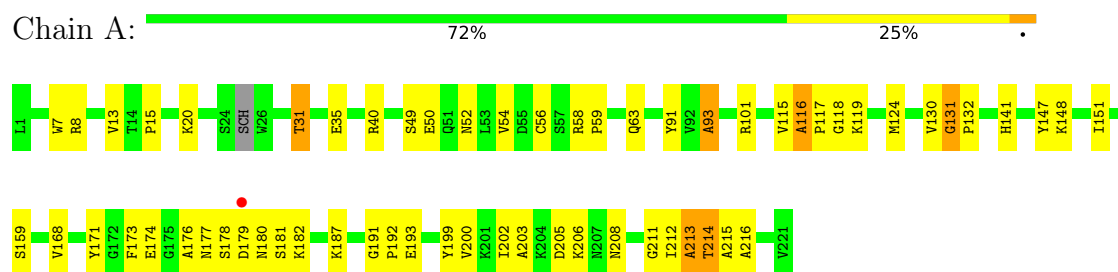
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total 169	O 169	0	0
4	B	124	Total 124	O 124	0	0
4	C	174	Total 174	O 174	0	0
4	D	97	Total 97	O 97	0	0
4	E	85	Total 85	O 85	0	0
4	F	81	Total 81	O 81	0	0
4	G	64	Total 64	O 64	0	0
4	H	63	Total 63	O 63	0	0

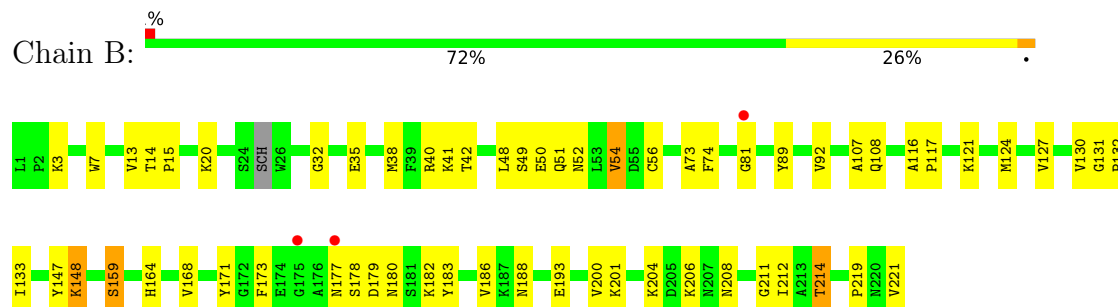
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

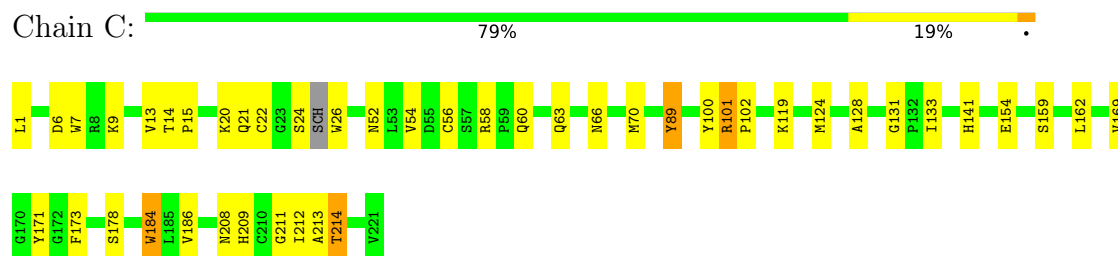
• Molecule 1: Cathepsin L2



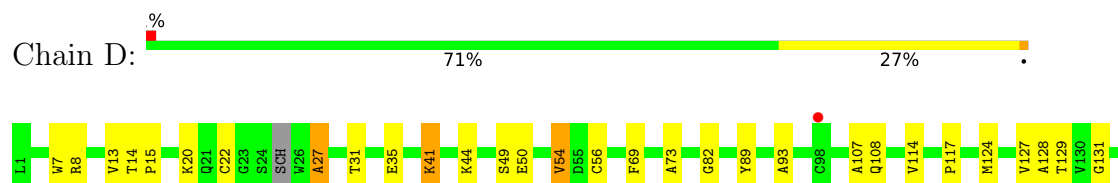
• Molecule 1: Cathepsin L2

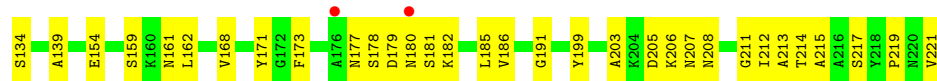


• Molecule 1: Cathepsin L2



• Molecule 1: Cathepsin L2

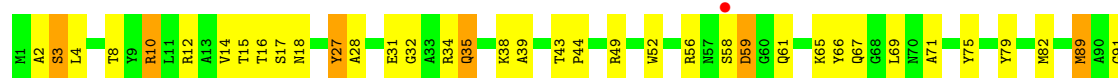




• Molecule 2: Clitocypin analog



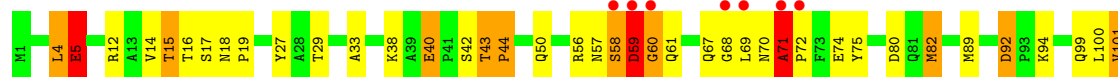
• Molecule 2: Clitocypin analog



• Molecule 2: Clitocypin analog



• Molecule 2: Clitocypin analog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.18Å 177.76Å 96.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.22 50.00 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.22) 99.1 (50.00-2.23)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.22Å)	Xtriage
Refinement program	REFMAC, MAIN	Depositor
R, R_{free}	0.182 , 0.239 (Not available) , 0.243	Depositor DCC
R_{free} test set	4098 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12387	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SME, SO4

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	1.47	7/1724 (0.4%)	1.36	18/2328 (0.8%)
1	B	1.34	5/1724 (0.3%)	1.39	16/2328 (0.7%)
1	C	1.51	8/1724 (0.5%)	1.37	15/2328 (0.6%)
1	D	1.41	13/1724 (0.8%)	1.36	14/2328 (0.6%)
2	E	1.49	11/1205 (0.9%)	1.55	18/1639 (1.1%)
2	F	1.38	4/1205 (0.3%)	1.54	19/1639 (1.2%)
2	G	1.40	8/1205 (0.7%)	1.59	23/1639 (1.4%)
2	H	1.38	3/1205 (0.2%)	1.63	23/1639 (1.4%)
All	All	1.43	59/11716 (0.5%)	1.46	146/15868 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	G	0	3
All	All	0	4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	ALA	CA-CB	11.38	1.65	1.53
1	C	54	VAL	CA-CB	8.69	1.65	1.54
1	D	139	ALA	CA-CB	8.32	1.67	1.53
2	F	43	THR	CA-C	7.83	1.60	1.52
2	H	109	ILE	CA-CB	-7.61	1.44	1.54
2	E	43	THR	CA-C	7.60	1.59	1.52
2	G	39	ALA	CA-CB	7.59	1.63	1.53
1	C	213	ALA	CA-CB	7.24	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	43	THR	CA-C	6.99	1.59	1.52
1	C	214	THR	CA-CB	6.87	1.64	1.53
1	D	27	ALA	CA-CB	6.87	1.64	1.53
1	B	212	ILE	CA-C	6.82	1.61	1.52
2	E	117	VAL	CA-CB	6.81	1.62	1.54
1	D	127	VAL	CA-CB	6.62	1.62	1.54
2	E	125	VAL	CA-CB	6.58	1.63	1.54
1	D	73	ALA	CA-CB	-6.56	1.43	1.53
2	E	16	THR	CA-C	6.51	1.61	1.52
1	D	89	TYR	CA-C	6.40	1.59	1.52
1	D	213	ALA	CA-CB	6.29	1.63	1.53
1	A	93	ALA	CA-CB	6.08	1.62	1.53
2	F	39	ALA	CA-CB	-6.05	1.45	1.53
1	D	44	LYS	CA-C	6.02	1.60	1.52
1	A	15	PRO	CA-C	5.88	1.59	1.52
2	G	78	SER	N-CA	-5.81	1.39	1.46
2	E	33	ALA	CA-CB	5.78	1.62	1.53
1	B	148	LYS	CA-C	5.77	1.58	1.52
1	C	89	TYR	CA-C	5.76	1.59	1.52
1	D	128	ALA	CA-CB	5.70	1.62	1.53
2	E	97	ILE	CA-C	5.67	1.59	1.52
1	A	130	VAL	CA-CB	-5.64	1.49	1.55
2	E	110	ILE	CA-CB	5.63	1.59	1.53
2	G	117	VAL	CA-CB	5.63	1.60	1.54
2	E	126	GLN	CA-C	5.62	1.59	1.52
2	E	51	ILE	CA-CB	5.58	1.60	1.54
1	D	168	VAL	CB-CG2	5.52	1.70	1.52
1	B	54	VAL	CA-CB	5.50	1.61	1.54
1	A	31	THR	CB-CG2	-5.48	1.34	1.52
1	C	100	TYR	CA-C	5.41	1.59	1.52
2	G	45	PRO	C-O	-5.39	1.16	1.24
2	G	112	ALA	CA-C	5.37	1.58	1.53
1	C	128	ALA	C-O	-5.34	1.17	1.24
2	H	15	THR	CB-CG2	-5.34	1.34	1.52
2	G	135	PHE	CA-C	5.27	1.57	1.52
2	G	44	PRO	C-O	-5.23	1.18	1.24
1	A	213	ALA	CA-CB	5.22	1.61	1.53
1	D	219	PRO	CA-C	5.19	1.59	1.52
2	F	44	PRO	C-O	-5.14	1.18	1.24
2	E	36	PRO	CA-C	5.13	1.58	1.52
1	D	215	ALA	CA-CB	5.13	1.57	1.53
1	B	73	ALA	CA-C	5.13	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	LEU	CA-C	-5.12	1.46	1.52
1	D	154	GLU	N-CA	-5.08	1.41	1.46
2	G	30	VAL	CA-CB	5.08	1.60	1.54
1	D	54	VAL	CA-CB	5.08	1.60	1.54
2	F	43	THR	N-CA	5.08	1.49	1.46
2	E	67	GLN	C-O	5.04	1.29	1.23
1	C	52	ASN	N-CA	5.04	1.52	1.46
1	B	32	GLY	CA-C	5.02	1.57	1.52
1	A	214	THR	CB-CG2	-5.01	1.36	1.52

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	59	ASP	N-CA-C	-16.18	76.33	110.80
2	G	18	ASN	CA-C-N	9.64	129.40	119.56
2	G	18	ASN	C-N-CA	9.64	129.40	119.56
2	H	58	SER	N-CA-C	9.54	124.28	108.73
2	G	44	PRO	N-CA-C	9.03	121.72	110.70
2	E	101	VAL	CA-C-N	9.00	129.08	119.90
2	E	101	VAL	C-N-CA	9.00	129.08	119.90
1	B	89	TYR	CA-C-N	8.95	129.00	119.78
1	B	89	TYR	C-N-CA	8.95	129.00	119.78
2	E	115	GLN	N-CA-C	8.81	121.84	111.71
1	C	214	THR	N-CA-C	8.80	122.03	111.82
2	H	112	ALA	N-CA-C	-8.79	98.57	109.65
2	H	115	GLN	N-CA-C	8.45	120.57	111.36
1	D	13	VAL	N-CA-C	8.43	120.24	107.77
2	H	101	VAL	N-CA-CB	8.36	119.17	110.23
1	A	191	GLY	CA-C-N	8.35	128.08	119.56
1	A	191	GLY	C-N-CA	8.35	128.08	119.56
2	G	59	ASP	N-CA-C	-7.94	97.40	109.79
2	E	44	PRO	N-CA-C	7.94	120.38	110.70
2	F	112	ALA	N-CA-C	-7.84	100.21	109.93
1	A	31	THR	OG1-CB-CG2	7.62	124.54	109.30
2	G	112	ALA	N-CA-C	-7.50	100.31	109.83
1	C	56	CYS	N-CA-C	7.42	123.36	113.72
2	F	44	PRO	N-CA-C	7.36	119.67	110.70
1	B	52	ASN	N-CA-C	-7.35	103.20	111.07
2	H	71	ALA	N-CA-C	7.31	125.97	109.81
1	C	20	LYS	CB-CA-C	-7.26	108.21	116.63
1	D	191	GLY	CA-C-N	7.23	126.86	119.56
1	D	191	GLY	C-N-CA	7.23	126.86	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	CYS	N-CA-C	7.21	122.25	113.38
2	E	112	ALA	N-CA-C	-7.07	101.16	109.93
2	H	57	ASN	CA-C-N	-7.05	113.40	122.77
2	H	57	ASN	C-N-CA	-7.05	113.40	122.77
2	F	67	GLN	N-CA-C	7.03	122.03	113.17
2	H	67	GLN	N-CA-C	7.03	120.88	110.48
2	E	73	PHE	N-CA-CB	-6.99	98.68	110.49
2	G	59	ASP	CB-CA-C	-6.98	97.56	113.33
1	D	49	SER	N-CA-C	6.94	119.58	108.41
2	E	141	GLY	N-CA-C	-6.90	101.35	112.31
2	H	40	GLU	CA-C-N	-6.86	113.59	120.31
2	H	40	GLU	C-N-CA	-6.86	113.59	120.31
2	H	44	PRO	N-CA-C	6.82	119.02	110.70
1	B	159	SER	N-CA-C	-6.79	104.19	113.30
2	G	10	ARG	N-CA-C	-6.78	98.34	109.40
2	F	3	SER	N-CA-C	6.76	120.04	109.96
1	C	89	TYR	CA-C-N	6.75	126.73	119.78
1	C	89	TYR	C-N-CA	6.75	126.73	119.78
1	B	56	CYS	N-CA-C	6.73	123.48	114.12
2	G	55	THR	N-CA-C	6.71	125.09	110.80
1	D	129	THR	N-CA-C	6.71	121.75	113.50
1	A	20	LYS	CB-CA-C	-6.63	108.94	116.63
1	B	13	VAL	N-CA-C	6.58	117.60	108.12
2	E	10	ARG	N-CA-C	-6.58	98.48	109.07
1	D	212	ILE	CB-CA-C	-6.51	102.54	112.05
1	C	13	VAL	N-CA-C	6.51	117.22	108.11
2	G	39	ALA	N-CA-C	-6.50	97.93	108.52
1	B	214	THR	N-CA-C	6.46	120.37	112.23
2	F	10	ARG	N-CA-C	-6.45	99.20	109.59
1	B	186	VAL	N-CA-C	6.43	117.74	108.48
2	E	14	VAL	N-CA-CB	-6.43	100.63	111.23
1	A	101	ARG	CA-C-N	6.30	126.50	119.32
1	A	101	ARG	C-N-CA	6.30	126.50	119.32
1	D	89	TYR	CA-C-N	6.27	126.21	119.76
1	D	89	TYR	C-N-CA	6.27	126.21	119.76
2	F	111	ARG	N-CA-C	6.25	120.02	109.76
2	E	71	ALA	N-CA-C	-6.17	100.43	109.50
2	G	3	SER	N-CA-C	6.14	118.39	108.32
1	C	52	ASN	N-CA-C	-6.12	104.61	111.28
2	G	109	ILE	N-CA-C	-6.11	99.63	108.36
2	G	49	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	D	186	VAL	N-CA-C	6.06	116.60	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	120	ASP	CB-CA-C	-6.04	99.79	109.75
2	E	14	VAL	CG1-CB-CG2	5.98	123.95	110.80
2	F	69	LEU	N-CA-C	5.97	118.75	111.82
1	B	81	GLY	N-CA-C	-5.96	99.05	113.18
1	A	13	VAL	N-CA-C	5.95	116.44	108.11
2	H	92	ASP	CA-C-N	5.94	127.27	119.84
2	H	92	ASP	C-N-CA	5.94	127.27	119.84
1	A	118	GLY	CA-C-N	-5.88	114.68	122.85
1	A	118	GLY	C-N-CA	-5.88	114.68	122.85
1	A	176	ALA	N-CA-C	5.88	120.60	112.90
2	G	143	ASP	N-CA-CB	5.87	120.41	110.49
2	H	80	ASP	N-CA-C	-5.87	98.30	110.80
2	G	14	VAL	CB-CA-C	5.86	120.89	111.29
2	H	4	LEU	N-CA-C	-5.85	98.34	110.80
2	G	14	VAL	N-CA-CB	-5.80	101.67	111.23
2	E	67	GLN	N-CA-C	-5.75	99.29	109.06
1	A	214	THR	N-CA-C	5.73	120.00	112.89
1	C	54	VAL	N-CA-CB	5.68	119.10	110.58
1	C	54	VAL	N-CA-C	5.64	116.42	110.72
2	G	145	PRO	N-CA-C	-5.64	102.27	111.68
1	A	56	CYS	N-CA-C	5.62	121.03	113.72
1	C	184	TRP	N-CA-C	-5.62	100.03	109.07
2	G	61	GLN	N-CA-C	5.58	119.20	110.32
2	F	2	ALA	N-CA-C	-5.55	102.18	110.23
2	F	49	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	D	127	VAL	N-CA-CB	5.53	118.88	110.58
1	D	212	ILE	CG1-CB-CG2	-5.47	94.30	110.70
1	B	130	VAL	CB-CA-C	-5.46	105.56	110.91
2	F	136	PRO	CB-CA-C	-5.46	105.61	111.56
2	H	5	GLU	N-CA-C	-5.45	99.20	110.80
2	E	58	SER	N-CA-C	5.41	118.98	112.38
2	F	27	TYR	N-CA-C	5.41	118.04	109.50
1	B	212	ILE	N-CA-C	5.38	116.75	110.62
1	B	164	HIS	CA-C-N	-5.34	117.12	122.20
1	B	164	HIS	C-N-CA	-5.34	117.12	122.20
2	G	60	GLY	N-CA-C	-5.34	106.42	115.34
1	C	169	VAL	CB-CA-C	-5.33	105.08	111.85
2	E	63	THR	N-CA-C	-5.33	101.43	109.85
2	F	109	ILE	N-CA-C	-5.32	100.92	108.58
1	D	207	ASN	N-CA-C	5.32	119.05	111.92
2	F	49	ARG	NE-CZ-NH1	-5.30	116.19	121.50
2	G	26	GLU	N-CA-C	5.30	117.88	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ALA	CA-C-N	5.30	125.60	119.93
1	A	116	ALA	C-N-CA	5.30	125.60	119.93
1	C	119	LYS	N-CA-C	5.25	117.52	107.75
2	E	6	ASP	N-CA-C	-5.24	102.53	110.28
2	F	4	LEU	N-CA-C	-5.23	101.74	110.17
1	A	31	THR	N-CA-CB	-5.22	102.44	110.12
1	B	20	LYS	CB-CA-C	-5.22	109.03	116.34
1	A	131	GLY	CA-C-N	5.19	125.20	119.90
1	A	131	GLY	C-N-CA	5.19	125.20	119.90
2	E	120	ASP	CB-CA-C	-5.18	101.80	110.19
2	F	35	GLN	CA-C-N	5.17	125.09	119.76
2	F	35	GLN	C-N-CA	5.17	125.09	119.76
2	G	6	ASP	N-CA-C	-5.16	103.53	110.24
2	G	104	THR	N-CA-C	-5.16	100.89	108.99
1	D	41	LYS	N-CA-C	5.15	116.58	111.07
2	H	15	THR	N-CA-CB	-5.13	103.10	111.66
2	H	130	LEU	N-CA-C	-5.12	101.62	109.76
2	F	92	ASP	N-CA-C	-5.10	101.88	109.42
2	H	137	VAL	N-CA-C	5.10	115.25	108.11
2	H	111	ARG	CB-CA-C	-5.09	100.22	109.38
2	F	28	ALA	N-CA-C	-5.08	102.33	109.96
1	C	186	VAL	N-CA-C	5.07	115.41	108.12
1	A	49	SER	N-CA-C	5.06	116.56	108.41
2	E	108	TYR	N-CA-C	5.05	117.67	109.24
2	H	58	SER	CA-C-N	5.04	131.16	121.54
2	H	58	SER	C-N-CA	5.04	131.16	121.54
2	E	73	PHE	N-CA-C	5.04	121.53	110.80
2	F	143	ASP	N-CA-CB	5.03	118.99	110.49
1	B	206	LYS	N-CA-C	-5.03	104.41	110.44
1	B	49	SER	N-CA-C	5.01	116.48	108.41
1	C	101	ARG	CA-C-N	5.01	125.03	119.32
1	C	101	ARG	C-N-CA	5.01	125.03	119.32
2	G	47	PHE	N-CA-C	5.00	117.39	111.33

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	89	TYR	Sidechain
2	G	142	GLY	Mainchain
2	G	79	TYR	Sidechain
2	G	86	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1683	0	1612	40	1
1	B	1683	0	1612	41	1
1	C	1683	0	1612	27	0
1	D	1683	0	1612	35	1
2	E	1192	0	1141	42	2
2	F	1192	0	1141	49	0
2	G	1192	0	1140	57	1
2	H	1192	0	1140	46	2
3	A	5	0	0	0	0
3	B	10	0	0	2	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	1	0
4	A	169	0	0	6	0
4	B	124	0	0	4	0
4	C	174	0	0	4	2
4	D	97	0	0	1	0
4	E	85	0	0	4	0
4	F	81	0	0	6	0
4	G	64	0	0	5	0
4	H	63	0	0	3	0
All	All	12387	0	11010	323	5

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 15.

All (323) 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:D:208:ASN:HD21	1:D:214:THR:HG22	0.97	1.14
1:A:177:ASN:HB3	1:A:180:ASN:HB2	1.31	1.09
1:B:177:ASN:HB3	1:B:180:ASN:HB2	1.34	1.07
2:G:16:THR:HG22	2:G:143:ASP:HA	1.43	1.00
1:D:208:ASN:ND2	1:D:214:THR:HG22	1.77	0.98
1:A:208:ASN:HD21	1:A:214:THR:HG22	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASN:HD21	1:C:214:THR:HG22	1.32	0.94
2:E:104:THR:HG21	2:E:107:VAL:HB	1.50	0.92
2:E:16:THR:HG22	2:E:143:ASP:HA	1.52	0.92
2:E:16:THR:HG23	4:E:837:HOH:O	1.70	0.92
2:F:16:THR:HG22	2:F:143:ASP:HA	1.49	0.92
1:B:3:LYS:HD2	1:B:178:SER:HB2	1.53	0.88
2:F:15:THR:HG22	2:F:18:ASN:H	1.39	0.87
2:G:59:ASP:HB2	2:G:61:GLN:H	1.41	0.85
1:B:38:MET:HE2	1:B:107:ALA:HA	1.57	0.85
2:G:92:ASP:HB2	4:G:831:HOH:O	1.76	0.84
2:E:81:GLN:HA	2:E:81:GLN:OE1	1.77	0.83
2:H:15:THR:HG22	2:H:18:ASN:H	1.42	0.83
1:B:208:ASN:HD21	1:B:214:THR:HG22	1.44	0.82
2:F:34:ARG:HD3	4:F:853:HOH:O	1.81	0.81
2:G:15:THR:HG22	2:G:18:ASN:H	1.45	0.81
1:C:58:ARG:HH12	1:C:63:GLN:HE22	1.28	0.81
1:D:31:THR:HG21	1:D:50:GLU:OE2	1.81	0.81
1:D:208:ASN:HD21	1:D:214:THR:CG2	1.90	0.81
1:A:179:ASP:HA	1:A:182:LYS:HD3	1.60	0.80
1:C:159:SER:O	1:C:214:THR:HG21	1.81	0.80
2:H:104:THR:CG2	2:H:107:VAL:H	1.96	0.79
1:A:31:THR:HG21	1:A:50:GLU:OE2	1.82	0.79
2:E:15:THR:HG22	2:E:18:ASN:H	1.47	0.79
2:F:59:ASP:HB3	4:F:264:HOH:O	1.82	0.78
2:H:4:LEU:O	2:H:5:GLU:HB2	1.84	0.77
2:G:104:THR:HG21	2:G:107:VAL:HB	1.65	0.77
1:C:21:GLN:HB3	4:C:835:HOH:O	1.85	0.76
1:B:51:GLN:NE2	1:B:92:VAL:H	1.84	0.76
2:F:101:VAL:O	2:F:104:THR:HB	1.86	0.76
1:A:159:SER:O	1:A:214:THR:HG21	1.87	0.75
2:E:82:SME:HE1	2:E:114:ILE:HD13	1.68	0.75
2:E:101:VAL:O	2:E:104:THR:HB	1.86	0.75
1:D:8:ARG:NH1	1:D:185:LEU:HD21	2.01	0.75
1:A:208:ASN:ND2	1:A:214:THR:HG22	2.02	0.75
2:H:71:ALA:HB3	2:H:72:PRO:HD3	1.69	0.74
2:H:16:THR:HG21	2:H:142:GLY:HA2	1.68	0.74
2:G:16:THR:CG2	2:G:143:ASP:HA	2.15	0.74
1:A:203:ALA:HB1	1:A:206:LYS:HD2	1.71	0.73
2:G:10:ARG:CZ	2:G:51:ILE:HD11	2.21	0.70
2:G:101:VAL:O	2:G:104:THR:HB	1.91	0.70
1:B:159:SER:O	1:B:214:THR:HG21	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:ASP:O	2:H:61:GLN:N	2.25	0.69
1:C:58:ARG:HH12	1:C:63:GLN:NE2	1.91	0.68
2:G:104:THR:CG2	2:G:107:VAL:H	2.06	0.68
2:H:29:THR:HG21	2:H:40:GLU:HB2	1.76	0.68
1:C:208:ASN:ND2	1:C:214:THR:HG22	2.07	0.68
2:F:104:THR:CG2	2:F:107:VAL:H	2.07	0.68
2:H:114:ILE:O	2:H:114:ILE:HG23	1.94	0.67
2:F:16:THR:CG2	2:F:143:ASP:HA	2.22	0.67
2:H:104:THR:HG23	2:H:107:VAL:H	1.59	0.67
1:D:159:SER:O	1:D:214:THR:HG21	1.96	0.66
1:B:3:LYS:HD2	1:B:178:SER:CB	2.25	0.66
2:H:14:VAL:HG13	2:H:15:THR:H	1.60	0.66
2:F:104:THR:HG21	2:F:107:VAL:HB	1.77	0.66
1:C:124:MET:HE3	1:C:171:TYR:CE1	2.31	0.65
2:G:56:ARG:HD3	2:H:58:SER:OG	1.95	0.65
2:G:99:GLN:OE1	2:G:111:ARG:NH1	2.29	0.65
2:H:16:THR:HG21	2:H:142:GLY:CA	2.25	0.65
2:F:15:THR:HG22	2:F:18:ASN:N	2.09	0.65
2:G:3:SER:CB	2:G:56:ARG:HH12	2.10	0.65
2:G:15:THR:HG22	2:G:18:ASN:N	2.10	0.65
2:F:65:LYS:HG3	4:F:420:HOH:O	1.96	0.65
1:B:41:LYS:HG2	1:B:42:THR:HG23	1.78	0.65
2:G:4:LEU:HD12	2:G:4:LEU:N	2.12	0.64
2:H:42:SER:HA	2:H:50:GLN:HE22	1.62	0.64
1:B:177:ASN:HB3	1:B:180:ASN:CB	2.22	0.64
2:E:82:SME:HE1	2:E:114:ILE:CD1	2.29	0.64
1:B:124:MET:HE3	1:B:171:TYR:CE1	2.34	0.63
2:H:104:THR:HG21	2:H:107:VAL:HB	1.81	0.63
2:E:104:THR:CG2	2:E:107:VAL:H	2.12	0.63
2:H:152:GLU:OE1	2:H:152:GLU:HA	1.99	0.63
1:A:40:ARG:HD2	4:A:387:HOH:O	1.98	0.63
2:E:8:THR:HG22	2:E:152:GLU:HB2	1.81	0.62
2:G:57:ASN:O	2:G:59:ASP:O	2.19	0.61
1:D:114:VAL:HG11	2:F:114:ILE:HG12	1.83	0.61
2:E:8:THR:HG23	2:E:51:ILE:HG23	1.83	0.60
2:F:31:GLU:HG3	2:F:38:LYS:HG3	1.84	0.60
2:F:3:SER:HA	2:F:56:ARG:HH12	1.66	0.60
1:B:51:GLN:HE21	1:B:92:VAL:H	1.48	0.60
2:E:73:PHE:C	2:E:73:PHE:HD1	2.09	0.60
1:A:7:TRP:CE2	1:A:131:GLY:HA2	2.38	0.59
2:E:99:GLN:OE1	2:E:111:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:PHE:C	2:E:73:PHE:CD1	2.80	0.59
1:C:211:GLY:O	1:C:214:THR:HG23	2.03	0.59
1:C:131:GLY:O	1:C:133:ILE:HD12	2.03	0.58
2:H:102:PRO:O	2:H:103:SER:HB2	2.03	0.58
1:A:180:ASN:O	1:A:181:SER:HB2	2.03	0.58
2:F:56:ARG:CB	2:F:56:ARG:HH21	2.17	0.58
2:G:54:VAL:O	2:G:63:THR:O	2.21	0.58
2:G:111:ARG:HG3	2:G:111:ARG:HH11	1.69	0.58
2:E:104:THR:HG21	2:E:107:VAL:CB	2.31	0.58
2:H:29:THR:HB	2:H:50:GLN:HG2	1.85	0.58
2:H:15:THR:CG2	2:H:18:ASN:H	2.13	0.58
2:E:49:ARG:NH2	2:E:49:ARG:HG3	2.19	0.58
1:B:127:VAL:HG12	1:B:133:ILE:CG1	2.34	0.57
2:H:27:TYR:O	2:H:29:THR:HG22	2.05	0.57
1:D:31:THR:O	1:D:35:GLU:HG3	2.04	0.57
1:C:1:LEU:N	4:C:629:HOH:O	2.38	0.57
2:G:9:TYR:CE2	2:G:151:ARG:HG2	2.40	0.57
1:A:63:GLN:HG2	2:E:18:ASN:ND2	2.20	0.56
1:A:63:GLN:HE21	2:E:18:ASN:HD22	1.52	0.56
1:C:60:GLN:H	1:C:60:GLN:NE2	2.04	0.56
2:E:16:THR:CG2	2:E:143:ASP:HA	2.31	0.56
1:B:173:PHE:CD1	1:B:178:SER:HA	2.41	0.56
2:H:92:ASP:O	2:H:94:LYS:HE3	2.04	0.56
2:F:114:ILE:HG13	2:F:117:VAL:HG21	1.88	0.56
2:G:57:ASN:HB2	2:G:59:ASP:OD2	2.06	0.56
2:H:100:LEU:HD13	2:H:101:VAL:O	2.06	0.55
1:D:117:PRO:HD2	2:F:79:TYR:CE2	2.42	0.55
2:F:114:ILE:O	2:F:117:VAL:HB	2.07	0.55
1:C:184:TRP:NE1	1:C:212:ILE:HD11	2.22	0.55
2:G:30:VAL:O	2:G:49:ARG:HD2	2.06	0.55
1:D:41:LYS:HE3	1:D:221:VAL:O	2.06	0.55
2:E:30:VAL:HG12	2:E:49:ARG:HB3	1.87	0.55
2:G:3:SER:OG	2:G:56:ARG:NH1	2.40	0.55
1:D:7:TRP:CE2	1:D:131:GLY:HA2	2.42	0.55
2:G:79:TYR:CD2	2:G:79:TYR:O	2.60	0.55
2:E:73:PHE:O	2:E:74:GLU:HB3	2.07	0.54
2:E:57:ASN:ND2	2:E:95:GLU:OE2	2.40	0.54
2:G:31:GLU:HG3	2:G:38:LYS:HG3	1.88	0.54
2:F:111:ARG:NH1	2:F:111:ARG:HG2	2.22	0.54
2:H:14:VAL:HG13	2:H:15:THR:N	2.23	0.54
2:H:71:ALA:CB	2:H:72:PRO:HD3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:GLN:OE1	2:H:111:ARG:NH1	2.42	0.53
1:B:108:GLN:O	1:B:221:VAL:HG12	2.09	0.53
1:D:8:ARG:HD3	1:D:199:TYR:CZ	2.44	0.53
2:H:101:VAL:O	2:H:104:THR:HB	2.08	0.53
2:H:12:ARG:HD3	2:H:14:VAL:HG23	1.90	0.53
1:D:177:ASN:HB3	1:D:180:ASN:ND2	2.24	0.53
2:H:16:THR:HG22	2:H:143:ASP:OD1	2.09	0.53
2:G:81:GLN:HA	2:G:81:GLN:OE1	2.08	0.52
1:A:63:GLN:NE2	2:E:18:ASN:HD22	2.07	0.52
1:D:177:ASN:HB3	1:D:180:ASN:HD22	1.73	0.52
2:F:104:THR:HG23	2:F:107:VAL:H	1.74	0.52
1:D:27:ALA:O	1:D:31:THR:HB	2.10	0.52
2:F:32:GLY:HA3	2:F:35:GLN:OE1	2.10	0.52
1:B:7:TRP:CE2	1:B:131:GLY:HA2	2.45	0.52
2:F:75:TYR:HA	2:F:91:GLY:O	2.10	0.52
1:A:31:THR:O	1:A:35:GLU:HG3	2.10	0.52
2:G:137:VAL:HG13	4:G:784:HOH:O	2.09	0.52
1:A:91:TYR:CE1	1:A:93:ALA:HB2	2.46	0.51
2:E:15:THR:HG22	2:E:18:ASN:N	2.22	0.51
1:C:7:TRP:CE2	1:C:131:GLY:HA2	2.46	0.51
1:D:50:GLU:O	1:D:54:VAL:HG13	2.10	0.51
1:D:82:GLY:HA2	1:D:107:ALA:O	2.10	0.51
2:F:52:TRP:CZ3	2:F:66:TYR:HB2	2.46	0.51
2:G:10:ARG:C	2:G:11:LEU:HD12	2.35	0.51
2:E:8:THR:HG23	2:E:51:ILE:CG2	2.40	0.51
2:F:92:ASP:N	3:F:153:SO4:O3	2.38	0.51
2:G:10:ARG:NE	2:G:51:ILE:HD11	2.26	0.51
1:B:74:PHE:CZ	1:B:219:PRO:HD3	2.45	0.51
2:F:15:THR:HG23	2:F:143:ASP:OD1	2.11	0.51
1:A:124:MET:HE3	1:A:171:TYR:CE1	2.45	0.50
1:C:141:HIS:HD2	4:C:281:HOH:O	1.94	0.50
1:D:179:ASP:HA	1:D:182:LYS:HD2	1.92	0.50
2:F:114:ILE:HG13	2:F:117:VAL:CG2	2.41	0.50
2:H:15:THR:HG23	2:H:17:SER:H	1.77	0.50
1:D:182:LYS:HE2	1:D:205:ASP:OD1	2.12	0.50
1:C:22:CYS:SG	1:C:24:SER:HB3	2.52	0.50
2:H:71:ALA:O	2:H:74:GLU:HG2	2.10	0.50
2:G:3:SER:HB3	2:G:56:ARG:HH12	1.76	0.50
2:G:9:TYR:CZ	2:G:151:ARG:HG2	2.47	0.50
1:B:127:VAL:HG12	1:B:133:ILE:HG13	1.94	0.49
1:B:50:GLU:O	1:B:54:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:95:GLU:HG3	4:E:715:HOH:O	2.11	0.49
1:A:148:LYS:CD	4:A:627:HOH:O	2.61	0.49
1:B:179:ASP:HA	1:B:182:LYS:HD2	1.93	0.49
1:C:58:ARG:NH1	1:C:63:GLN:NE2	2.57	0.49
1:B:41:LYS:HG2	1:B:42:THR:CG2	2.43	0.49
1:A:63:GLN:CG	2:E:18:ASN:ND2	2.76	0.48
1:C:173:PHE:CG	1:C:178:SER:HA	2.48	0.48
2:G:4:LEU:HD11	2:G:108:TYR:CE2	2.48	0.48
2:F:101:VAL:HG13	2:F:107:VAL:HG12	1.95	0.48
2:F:14:VAL:HG13	2:F:15:THR:N	2.29	0.48
2:G:73:PHE:O	2:G:74:GLU:HB3	2.13	0.48
2:E:34:ARG:O	2:E:89:SME:HE2	2.14	0.48
2:H:16:THR:CG2	2:H:144:ARG:H	2.27	0.48
2:F:61:GLN:NE2	2:F:95:GLU:OE2	2.44	0.48
1:A:147:TYR:CZ	1:A:200:VAL:HG23	2.49	0.47
2:H:14:VAL:CG1	2:H:15:THR:N	2.77	0.47
2:F:3:SER:HA	2:F:56:ARG:NH1	2.29	0.47
2:H:16:THR:HG23	4:H:175:HOH:O	2.14	0.47
1:B:127:VAL:HG12	1:B:133:ILE:HG12	1.95	0.47
2:F:12:ARG:HB2	2:F:27:TYR:CE1	2.48	0.47
2:G:10:ARG:NH1	2:G:51:ILE:HD11	2.29	0.47
1:A:177:ASN:HB3	1:A:180:ASN:CB	2.23	0.47
1:B:211:GLY:O	1:B:214:THR:HG23	2.13	0.47
1:A:151:ILE:HD11	1:A:174:GLU:HG3	1.97	0.47
1:C:6:ASP:OD2	1:C:9:LYS:HE3	2.14	0.47
2:F:111:ARG:HG2	2:F:111:ARG:HH11	1.77	0.47
2:H:104:THR:HG21	2:H:107:VAL:H	1.78	0.47
1:B:188:ASN:HB3	4:B:585:HOH:O	2.15	0.47
1:B:204:LYS:HE2	4:B:421:HOH:O	2.13	0.47
1:B:177:ASN:CB	1:B:180:ASN:HD22	2.27	0.47
2:G:15:THR:HG23	2:G:17:SER:H	1.79	0.47
1:B:14:THR:HB	1:B:15:PRO:CD	2.45	0.47
2:H:33:ALA:HB2	2:H:75:TYR:CD2	2.50	0.47
1:C:184:TRP:NE1	1:C:212:ILE:CD1	2.78	0.47
2:F:16:THR:CG2	2:F:144:ARG:H	2.28	0.47
1:A:212:ILE:HD12	1:A:213:ALA:N	2.30	0.46
2:E:49:ARG:HG3	2:E:49:ARG:HH21	1.81	0.46
2:E:101:VAL:HA	2:E:102:PRO:HD3	1.73	0.46
2:H:14:VAL:HG13	2:H:19:PRO:HA	1.97	0.46
1:A:119:LYS:HE3	4:A:700:HOH:O	2.16	0.46
2:H:94:LYS:HA	2:H:94:LYS:HD3	1.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:PRO:HB3	4:G:166:HOH:O	2.15	0.46
1:A:116:ALA:HA	1:A:117:PRO:HD3	1.82	0.46
1:B:183:TYR:CD1	1:B:201:LYS:HD3	2.51	0.46
2:H:102:PRO:HA	4:H:177:HOH:O	2.15	0.46
2:F:71:ALA:HB3	2:F:75:TYR:HE1	1.81	0.45
2:H:38:LYS:HE3	2:H:38:LYS:HB3	1.67	0.45
1:B:148:LYS:HD2	1:B:148:LYS:HA	1.63	0.45
1:B:177:ASN:HB2	1:B:180:ASN:HD22	1.81	0.45
1:D:14:THR:HB	1:D:15:PRO:CD	2.46	0.45
1:B:173:PHE:CE1	1:B:178:SER:HA	2.51	0.45
2:G:111:ARG:NH1	2:G:111:ARG:HG3	2.31	0.45
1:D:211:GLY:O	1:D:214:THR:HG23	2.17	0.45
2:F:8:THR:HA	2:F:52:TRP:O	2.16	0.45
2:G:4:LEU:HD12	2:G:4:LEU:H	1.78	0.45
2:H:69:LEU:HD23	2:H:69:LEU:HA	1.75	0.45
2:F:117:VAL:HG12	2:F:119:VAL:HG22	1.98	0.45
2:G:30:VAL:HG12	2:G:49:ARG:HB3	1.98	0.45
1:A:58:ARG:N	1:A:59:PRO:CD	2.80	0.45
2:E:73:PHE:HD1	2:E:73:PHE:O	1.99	0.45
1:A:173:PHE:CD2	1:A:178:SER:HA	2.52	0.45
2:E:15:THR:HG23	2:E:17:SER:H	1.82	0.45
2:G:73:PHE:CE1	2:G:75:TYR:HB3	2.52	0.45
2:G:122:GLU:OE1	2:G:144:ARG:HD2	2.17	0.44
1:D:69:PHE:CE2	2:F:116:ARG:O	2.70	0.44
2:F:111:ARG:HH11	2:F:111:ARG:CG	2.30	0.44
2:E:114:ILE:O	2:E:114:ILE:HG23	2.17	0.44
2:G:10:ARG:HG2	2:G:51:ILE:HD13	1.99	0.44
2:G:18:ASN:N	2:G:19:PRO:CD	2.80	0.44
1:D:134:SER:HB2	1:D:217:SER:O	2.18	0.44
1:B:147:TYR:CZ	1:B:200:VAL:HG23	2.52	0.44
1:B:183:TYR:CE1	1:B:201:LYS:HD3	2.52	0.44
2:H:16:THR:HG22	2:H:143:ASP:HA	2.00	0.44
1:C:14:THR:HB	1:C:15:PRO:HD2	2.00	0.44
2:F:125:VAL:HG11	4:F:411:HOH:O	2.18	0.44
2:G:15:THR:CG2	2:G:18:ASN:H	2.24	0.44
2:H:15:THR:HG22	2:H:18:ASN:N	2.21	0.44
1:A:205:ASP:C	4:A:339:HOH:O	2.61	0.43
1:D:69:PHE:HE2	2:F:116:ARG:O	2.01	0.43
2:E:33:ALA:HB2	2:E:75:TYR:CE2	2.53	0.43
1:A:52:ASN:C	1:A:52:ASN:HD22	2.27	0.43
1:A:63:GLN:CG	2:E:18:ASN:HD22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:THR:CG2	4:D:259:HOH:O	2.66	0.43
2:G:111:ARG:NH1	2:G:111:ARG:CG	2.80	0.43
1:C:66:ASN:C	2:G:25:GLY:HA2	2.44	0.43
1:D:20:LYS:HE2	1:D:20:LYS:HA	2.00	0.43
2:F:56:ARG:HH21	2:F:56:ARG:HB2	1.84	0.43
1:A:8:ARG:HD3	1:A:199:TYR:CZ	2.54	0.43
1:A:211:GLY:O	1:A:214:THR:HG23	2.19	0.43
2:E:10:ARG:HD3	4:E:405:HOH:O	2.18	0.43
2:G:14:VAL:HG13	2:G:15:THR:H	1.82	0.43
1:B:177:ASN:CB	1:B:180:ASN:HB2	2.25	0.43
1:D:173:PHE:CD1	1:D:178:SER:HA	2.53	0.43
2:E:82:SME:CE	2:E:114:ILE:HD13	2.41	0.43
1:A:31:THR:HG23	4:A:476:HOH:O	2.18	0.43
2:G:8:THR:HA	2:G:52:TRP:O	2.19	0.43
2:G:15:THR:HG23	2:G:16:THR:N	2.33	0.43
2:E:14:VAL:HG13	2:E:15:THR:N	2.34	0.42
2:E:80:ASP:HB3	2:E:81:GLN:H	1.69	0.42
1:A:192:PRO:HD2	1:A:193:GLU:OE2	2.19	0.42
1:A:202:ILE:O	1:A:203:ALA:C	2.61	0.42
2:G:116:ARG:HG3	4:G:780:HOH:O	2.19	0.42
1:D:117:PRO:HB3	2:F:114:ILE:CD1	2.49	0.42
2:H:4:LEU:HD23	2:H:4:LEU:HA	1.91	0.42
2:G:10:ARG:HD3	4:G:189:HOH:O	2.19	0.42
1:A:132:PRO:HA	1:A:168:VAL:O	2.18	0.42
2:G:5:GLU:O	2:G:6:ASP:C	2.62	0.42
1:B:116:ALA:HA	1:B:117:PRO:HD2	1.84	0.42
1:B:201:LYS:NZ	3:B:222:SO4:O3	2.52	0.42
1:D:124:MET:HE3	1:D:171:TYR:CE1	2.55	0.42
2:E:38:LYS:NZ	4:E:524:HOH:O	2.42	0.42
2:F:10:ARG:NH2	4:F:744:HOH:O	2.50	0.42
1:A:50:GLU:O	1:A:54:VAL:HG13	2.19	0.42
2:F:10:ARG:HD3	4:F:744:HOH:O	2.19	0.42
1:A:187:LYS:HB2	1:A:199:TYR:CE2	2.54	0.42
1:B:193:GLU:HG3	4:B:639:HOH:O	2.19	0.42
1:D:22:CYS:HB2	1:D:93:ALA:O	2.20	0.42
2:H:128:ASN:ND2	4:H:787:HOH:O	2.52	0.42
1:B:35:GLU:HG3	1:B:48:LEU:HD12	2.02	0.42
1:C:26:TRP:O	1:C:70:MET:HG3	2.20	0.42
2:E:4:LEU:HG	2:E:108:TYR:CZ	2.55	0.41
2:F:34:ARG:O	2:F:89:SME:HE1	2.20	0.41
2:H:56:ARG:HG2	2:H:60:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLN:NE2	2:G:40:GLU:OE2	2.52	0.41
1:B:14:THR:HB	1:B:15:PRO:HD2	2.02	0.41
2:G:12:ARG:HB2	2:G:27:TYR:CE1	2.55	0.41
1:C:101:ARG:HA	1:C:102:PRO:HD2	1.76	0.41
2:F:114:ILE:CG1	2:F:117:VAL:HG21	2.49	0.41
2:F:56:ARG:HB2	2:F:56:ARG:NH2	2.36	0.41
2:F:58:SER:O	2:F:59:ASP:HB2	2.21	0.41
2:H:82:SME:HE3	2:H:82:SME:HB3	2.02	0.41
2:E:14:VAL:HG13	2:E:15:THR:H	1.85	0.41
1:D:173:PHE:HA	1:D:181:SER:O	2.21	0.41
1:D:203:ALA:HB1	1:D:206:LYS:HD3	2.03	0.41
2:G:4:LEU:HD11	2:G:108:TYR:CZ	2.55	0.41
2:G:51:ILE:HD13	2:G:51:ILE:HA	1.84	0.41
1:B:132:PRO:HA	1:B:168:VAL:O	2.20	0.41
1:C:14:THR:HB	1:C:15:PRO:CD	2.50	0.41
1:C:154:GLU:O	1:C:209:HIS:HE1	2.03	0.41
1:C:63:GLN:CG	2:G:18:ASN:ND2	2.83	0.40
1:D:161:ASN:C	1:D:162:LEU:HD23	2.46	0.40
1:A:115:VAL:HB	1:A:216:ALA:HB3	2.02	0.40
1:A:141:HIS:HD2	4:A:453:HOH:O	2.03	0.40
1:D:162:LEU:HD23	1:D:162:LEU:N	2.36	0.40
2:F:15:THR:HG23	2:F:17:SER:H	1.87	0.40
1:B:121:LYS:HB2	3:B:223:SO4:O3	2.21	0.40
4:C:668:HOH:O	2:G:21:PRO:HA	2.21	0.40
2:G:31:GLU:HG3	2:G:38:LYS:CG	2.51	0.40
1:B:40:ARG:HG3	4:B:436:HOH:O	2.22	0.40
2:H:43:THR:HB	2:H:44:PRO:CD	2.52	0.40
1:A:212:ILE:H	1:A:212:ILE:HG13	1.76	0.40
1:D:173:PHE:CG	1:D:178:SER:HA	2.57	0.40
2:F:102:PRO:O	2:F:103:SER:HB2	2.21	0.40

All (5) 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:E:116:ARG:NH2	4:C:288:HOH:O[1_455]	1.18	1.02
1:B:108:GLN:OE1	1:D:108:GLN:NE2[2_655]	1.85	0.35
1:A:117:PRO:CG	2:H:114:ILE:CD1[4_455]	2.02	0.18
2:E:116:ARG:CZ	4:C:288:HOH:O[1_455]	2.11	0.09
2:G:69:LEU:CD1	2:H:68:GLY:CA[4_455]	2.14	0.06

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	216/221 (98%)	209 (97%)	7 (3%)	0	100	100
1	B	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
1	C	216/221 (98%)	211 (98%)	5 (2%)	0	100	100
1	D	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
2	E	148/152 (97%)	133 (90%)	11 (7%)	4 (3%)	4	2
2	F	148/152 (97%)	139 (94%)	7 (5%)	2 (1%)	9	7
2	G	148/152 (97%)	127 (86%)	16 (11%)	5 (3%)	3	1
2	H	148/152 (97%)	127 (86%)	14 (10%)	7 (5%)	2	0
All	All	1456/1492 (98%)	1358 (93%)	80 (6%)	18 (1%)	10	8

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	69	LEU
2	F	59	ASP
2	G	69	LEU
2	H	5	GLU
2	H	59	ASP
2	H	60	GLY
2	H	71	ALA
2	E	143	ASP
2	F	143	ASP
2	G	68	GLY
2	G	71	ALA
2	G	142	GLY
2	H	70	ASN
2	H	142	GLY
2	E	74	GLU
2	H	138	ASP
2	E	73	PHE

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Mol	Chain	Res	Type
2	G	55	THR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
2	SME	H	89	2	6,7,9	1.90	2 (33%)	2,7,11	0.42	0
2	SME	F	82	2	6,7,9	1.76	1 (16%)	2,7,11	0.85	0
2	SME	F	89	2	6,7,9	1.66	1 (16%)	2,7,11	1.01	0
2	SME	E	89	2	6,7,9	1.81	2 (33%)	2,7,11	0.16	0
2	SME	H	82	2	6,7,9	2.00	2 (33%)	2,7,11	0.39	0
2	SME	E	82	2	6,7,9	2.24	2 (33%)	2,7,11	1.78	1 (50%)
2	SME	G	82	2	6,7,9	1.76	2 (33%)	2,7,11	0.29	0
2	SME	G	89	2	6,7,9	1.79	2 (33%)	2,7,11	0.47	0

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
2	SME	H	89	2	-	0/5/6/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SME	F	82	2	-	0/5/6/9	-
2	SME	F	89	2	-	0/5/6/9	-
2	SME	E	89	2	-	0/5/6/9	-
2	SME	H	82	2	-	4/5/6/9	-
2	SME	E	82	2	-	3/5/6/9	-
2	SME	G	82	2	-	1/5/6/9	-
2	SME	G	89	2	-	0/5/6/9	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	82	SME	CB-CA	-3.98	1.47	1.53
2	F	82	SME	CG-S	3.66	1.99	1.81
2	H	82	SME	CG-S	3.30	1.98	1.81
2	F	89	SME	CG-S	3.28	1.97	1.81
2	E	89	SME	CG-S	3.22	1.97	1.81
2	H	89	SME	CG-S	3.17	1.97	1.81
2	G	89	SME	CG-S	3.11	1.97	1.81
2	H	89	SME	CE-S	3.08	1.97	1.78
2	G	82	SME	CG-S	2.86	1.95	1.81
2	E	89	SME	CE-S	2.79	1.95	1.78
2	E	82	SME	CG-S	2.76	1.95	1.81
2	G	89	SME	CE-S	2.61	1.94	1.78
2	H	82	SME	CE-S	2.60	1.94	1.78
2	G	82	SME	CE-S	2.18	1.92	1.78

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	82	SME	CB-CG-S	-2.52	97.21	113.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	82	SME	C-CA-CB-CG
2	G	82	SME	O-C-CA-CB
2	H	82	SME	N-CA-CB-CG
2	H	82	SME	C-CA-CB-CG
2	H	82	SME	CB-CG-S-CE
2	H	82	SME	CA-CB-CG-S

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Mol	Chain	Res	Type	Atoms
2	E	82	SME	CA-CB-CG-S
2	E	82	SME	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	89	SME	1	0
2	E	89	SME	1	0
2	H	82	SME	1	0
2	E	82	SME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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
3	SO4	F	153	-	4,4,4	2.65	3 (75%)	6,6,6	3.22	4 (66%)
3	SO4	D	222	-	4,4,4	0.94	0	6,6,6	0.58	0
3	SO4	B	223	-	4,4,4	0.67	0	6,6,6	0.47	0
3	SO4	C	222	-	4,4,4	0.78	0	6,6,6	0.98	0
3	SO4	B	222	-	4,4,4	1.50	1 (25%)	6,6,6	0.44	0
3	SO4	A	222	-	4,4,4	0.92	0	6,6,6	0.61	0

All (4) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	153	SO4	O1-S	3.58	1.66	1.44
3	F	153	SO4	O4-S	3.13	1.73	1.48
3	B	222	SO4	O2-S	2.73	1.61	1.44
3	F	153	SO4	O2-S	2.29	1.58	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	153	SO4	O4-S-O1	-4.70	84.99	109.56
3	F	153	SO4	O4-S-O2	4.33	132.17	109.56
3	F	153	SO4	O3-S-O1	-3.53	91.09	109.56
3	F	153	SO4	O4-S-O3	2.34	121.44	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	153	SO4	1	0
3	B	223	SO4	1	0
3	B	222	SO4	1	0

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	220/221 (99%)	-0.58	1 (0%) 87 86	15, 25, 40, 80	3 (1%)
1	B	220/221 (99%)	-0.27	3 (1%) 73 72	16, 30, 49, 81	8 (3%)
1	C	220/221 (99%)	-0.58	0 100 100	10, 24, 38, 53	2 (0%)
1	D	220/221 (99%)	-0.15	3 (1%) 73 72	18, 32, 56, 91	4 (1%)
2	E	143/152 (94%)	-0.13	6 (4%) 40 37	15, 27, 57, 81	1 (0%)
2	F	144/152 (94%)	-0.28	3 (2%) 63 61	14, 27, 54, 66	1 (0%)
2	G	140/152 (92%)	-0.01	8 (5%) 29 26	19, 32, 60, 67	0
2	H	143/152 (94%)	0.14	10 (6%) 22 19	19, 35, 62, 77	2 (1%)
All	All	1450/1492 (97%)	-0.27	34 (2%) 61 59	10, 28, 55, 91	21 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	71	ALA	4.2
2	H	137	VAL	4.1
2	F	137	VAL	3.6
2	H	136	PRO	3.6
2	H	69	LEU	3.6
2	G	80	ASP	3.2
2	G	81	GLN	3.1
2	H	72	PRO	3.1
2	F	142	GLY	3.1
2	H	59	ASP	3.1
2	E	73	PHE	3.1
2	E	80	ASP	3.0
2	G	137	VAL	3.0
2	E	72	PRO	2.7
2	G	3	SER	2.6
1	A	179	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	71	ALA	2.5
2	G	59	ASP	2.5
2	E	137	VAL	2.4
1	B	81	GLY	2.4
1	D	176	ALA	2.3
2	E	136	PRO	2.3
1	D	98	CYS	2.3
1	D	180	ASN	2.3
1	B	175	GLY	2.3
1	B	177	ASN	2.2
2	G	136	PRO	2.2
2	E	142	GLY	2.2
2	H	58	SER	2.2
2	H	152	GLU	2.1
2	H	68	GLY	2.1
2	H	60	GLY	2.1
2	F	58	SER	2.0
2	G	74	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SME	G	82	8/10	0.83	0.20	40,46,51,57	0
2	SME	F	82	8/10	0.85	0.18	26,30,34,41	0
2	SME	F	89	8/10	0.87	0.16	23,30,36,44	0
2	SME	E	89	8/10	0.87	0.17	23,26,39,41	0
2	SME	E	82	8/10	0.88	0.18	29,36,41,49	0
2	SME	G	89	8/10	0.88	0.18	22,30,34,42	0
2	SME	H	82	8/10	0.88	0.19	31,37,38,45	0
2	SME	H	89	8/10	0.89	0.18	30,37,46,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	F	153	5/5	0.88	0.13	56,57,61,65	0
3	SO4	B	222	5/5	0.93	0.07	63,64,68,69	0
3	SO4	B	223	5/5	0.95	0.09	43,43,48,53	0
3	SO4	C	222	5/5	0.97	0.07	40,41,46,47	0
3	SO4	A	222	5/5	0.97	0.11	44,46,51,51	0
3	SO4	D	222	5/5	0.98	0.06	39,42,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.