



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:33 AM UTC

PDB ID : 3ENM / pdb_00003enm
Title : The structure of the MAP2K MEK6 reveals an autoinhibitory dimer
Authors : Min, X.; Akella, R.; He, H.; Humphreys, J.M.; Tsutakawa, S.; Lee, S.-J.;
Tainer, J.A.; Cobb, M.H.; Goldsmith, E.J.
Deposited on : 2008-09-25
Resolution : 2.35 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

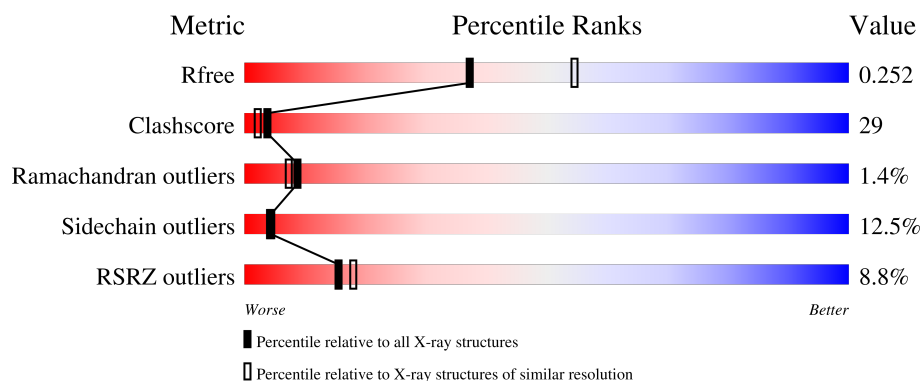
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	316	4% 57% 25% 7% 12%
1	B	316	15% 48% 29% 7% • 14%
1	C	316	8% 49% 28% 8% • 13%
1	D	316	3% 56% 27% 6% • 11%

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
2	SO4	B	4	-	-	X	-
3	GOL	A	1	-	-	X	-
4	EDO	B	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9174 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 Dual specificity mitogen-activated protein kinase kinase 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	Se	0	0	0
			2223	1429	368	411	4	11			
1	B	271	Total	C	N	O	S	Se	20	1	0
			2163	1388	360	400	4	11			
1	C	275	Total	C	N	O	S	Se	7	0	0
			2185	1403	363	404	4	11			
1	D	282	Total	C	N	O	S	Se	0	0	0
			2248	1443	372	417	4	12			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	-	expression tag	UNP P52564
A	19	SER	-	expression tag	UNP P52564
A	20	TYR	-	expression tag	UNP P52564
A	21	TYR	-	expression tag	UNP P52564
A	22	HIS	-	expression tag	UNP P52564
A	23	HIS	-	expression tag	UNP P52564
A	24	HIS	-	expression tag	UNP P52564
A	25	HIS	-	expression tag	UNP P52564
A	26	HIS	-	expression tag	UNP P52564
A	27	HIS	-	expression tag	UNP P52564
A	28	ASP	-	expression tag	UNP P52564
A	29	TYR	-	expression tag	UNP P52564
A	30	ASP	-	expression tag	UNP P52564
A	31	ILE	-	expression tag	UNP P52564
A	32	PRO	-	expression tag	UNP P52564
A	33	THR	-	expression tag	UNP P52564
A	34	THR	-	expression tag	UNP P52564
A	35	GLU	-	expression tag	UNP P52564
A	36	ASN	-	expression tag	UNP P52564
A	37	LEU	-	expression tag	UNP P52564
A	38	TYR	-	expression tag	UNP P52564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	-	expression tag	UNP P52564
A	40	GLN	-	expression tag	UNP P52564
A	41	GLY	-	expression tag	UNP P52564
A	42	ALA	-	expression tag	UNP P52564
A	43	MSE	-	expression tag	UNP P52564
A	44	GLU	-	expression tag	UNP P52564
A	207	ASP	SER	engineered mutation	UNP P52564
A	211	ASP	THR	engineered mutation	UNP P52564
A	333	ALA	-	expression tag	UNP P52564
B	18	MSE	-	expression tag	UNP P52564
B	19	SER	-	expression tag	UNP P52564
B	20	TYR	-	expression tag	UNP P52564
B	21	TYR	-	expression tag	UNP P52564
B	22	HIS	-	expression tag	UNP P52564
B	23	HIS	-	expression tag	UNP P52564
B	24	HIS	-	expression tag	UNP P52564
B	25	HIS	-	expression tag	UNP P52564
B	26	HIS	-	expression tag	UNP P52564
B	27	HIS	-	expression tag	UNP P52564
B	28	ASP	-	expression tag	UNP P52564
B	29	TYR	-	expression tag	UNP P52564
B	30	ASP	-	expression tag	UNP P52564
B	31	ILE	-	expression tag	UNP P52564
B	32	PRO	-	expression tag	UNP P52564
B	33	THR	-	expression tag	UNP P52564
B	34	THR	-	expression tag	UNP P52564
B	35	GLU	-	expression tag	UNP P52564
B	36	ASN	-	expression tag	UNP P52564
B	37	LEU	-	expression tag	UNP P52564
B	38	TYR	-	expression tag	UNP P52564
B	39	PHE	-	expression tag	UNP P52564
B	40	GLN	-	expression tag	UNP P52564
B	41	GLY	-	expression tag	UNP P52564
B	42	ALA	-	expression tag	UNP P52564
B	43	MSE	-	expression tag	UNP P52564
B	44	GLU	-	expression tag	UNP P52564
B	207	ASP	SER	engineered mutation	UNP P52564
B	211	ASP	THR	engineered mutation	UNP P52564
B	333	ALA	-	expression tag	UNP P52564
C	18	MSE	-	expression tag	UNP P52564
C	19	SER	-	expression tag	UNP P52564
C	20	TYR	-	expression tag	UNP P52564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	TYR	-	expression tag	UNP P52564
C	22	HIS	-	expression tag	UNP P52564
C	23	HIS	-	expression tag	UNP P52564
C	24	HIS	-	expression tag	UNP P52564
C	25	HIS	-	expression tag	UNP P52564
C	26	HIS	-	expression tag	UNP P52564
C	27	HIS	-	expression tag	UNP P52564
C	28	ASP	-	expression tag	UNP P52564
C	29	TYR	-	expression tag	UNP P52564
C	30	ASP	-	expression tag	UNP P52564
C	31	ILE	-	expression tag	UNP P52564
C	32	PRO	-	expression tag	UNP P52564
C	33	THR	-	expression tag	UNP P52564
C	34	THR	-	expression tag	UNP P52564
C	35	GLU	-	expression tag	UNP P52564
C	36	ASN	-	expression tag	UNP P52564
C	37	LEU	-	expression tag	UNP P52564
C	38	TYR	-	expression tag	UNP P52564
C	39	PHE	-	expression tag	UNP P52564
C	40	GLN	-	expression tag	UNP P52564
C	41	GLY	-	expression tag	UNP P52564
C	42	ALA	-	expression tag	UNP P52564
C	43	MSE	-	expression tag	UNP P52564
C	44	GLU	-	expression tag	UNP P52564
C	207	ASP	SER	engineered mutation	UNP P52564
C	211	ASP	THR	engineered mutation	UNP P52564
C	333	ALA	-	expression tag	UNP P52564
D	18	MSE	-	expression tag	UNP P52564
D	19	SER	-	expression tag	UNP P52564
D	20	TYR	-	expression tag	UNP P52564
D	21	TYR	-	expression tag	UNP P52564
D	22	HIS	-	expression tag	UNP P52564
D	23	HIS	-	expression tag	UNP P52564
D	24	HIS	-	expression tag	UNP P52564
D	25	HIS	-	expression tag	UNP P52564
D	26	HIS	-	expression tag	UNP P52564
D	27	HIS	-	expression tag	UNP P52564
D	28	ASP	-	expression tag	UNP P52564
D	29	TYR	-	expression tag	UNP P52564
D	30	ASP	-	expression tag	UNP P52564
D	31	ILE	-	expression tag	UNP P52564
D	32	PRO	-	expression tag	UNP P52564

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	33	THR	-	expression tag	UNP P52564
D	34	THR	-	expression tag	UNP P52564
D	35	GLU	-	expression tag	UNP P52564
D	36	ASN	-	expression tag	UNP P52564
D	37	LEU	-	expression tag	UNP P52564
D	38	TYR	-	expression tag	UNP P52564
D	39	PHE	-	expression tag	UNP P52564
D	40	GLN	-	expression tag	UNP P52564
D	41	GLY	-	expression tag	UNP P52564
D	42	ALA	-	expression tag	UNP P52564
D	43	MSE	-	expression tag	UNP P52564
D	44	GLU	-	expression tag	UNP P52564
D	207	ASP	SER	engineered mutation	UNP P52564
D	211	ASP	THR	engineered mutation	UNP P52564
D	333	ALA	-	expression tag	UNP P52564

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



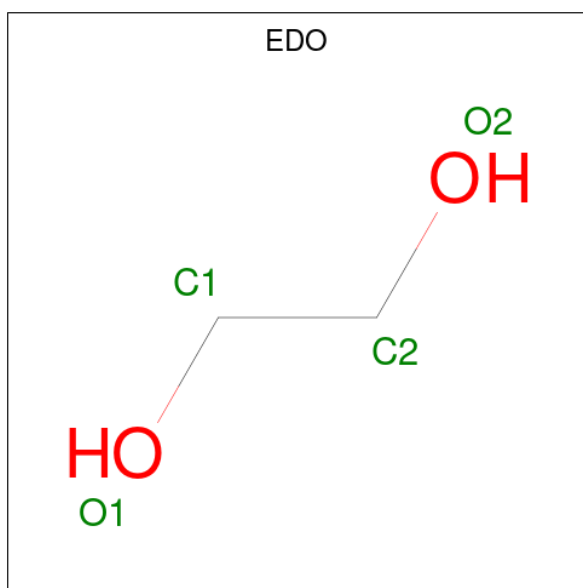
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

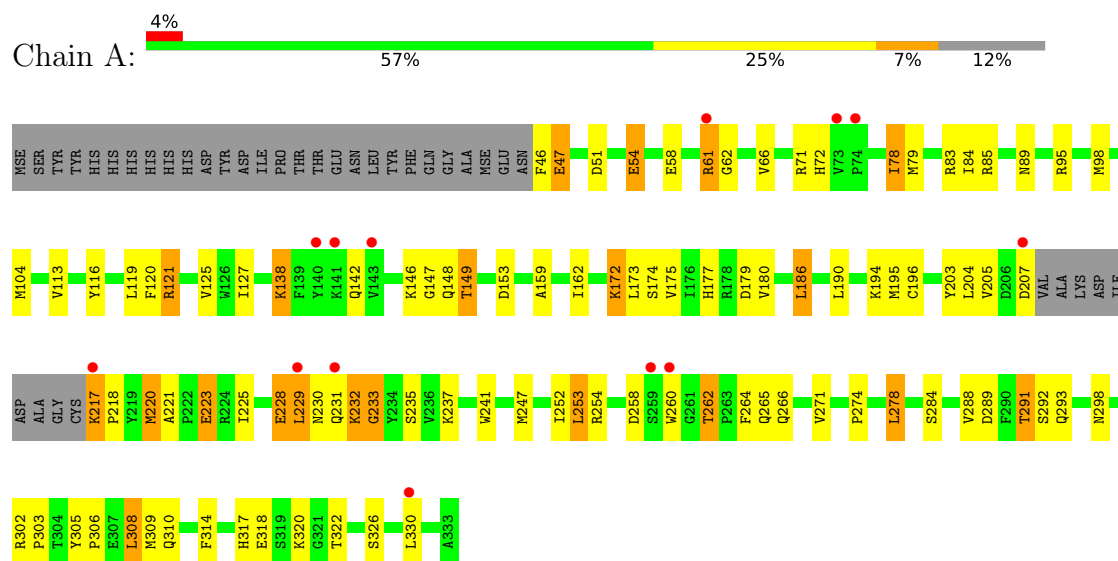
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total 93	O 93	0	0
5	B	74	Total 74	O 74	0	0
5	C	78	Total 78	O 78	0	0
5	D	80	Total 80	O 80	0	0

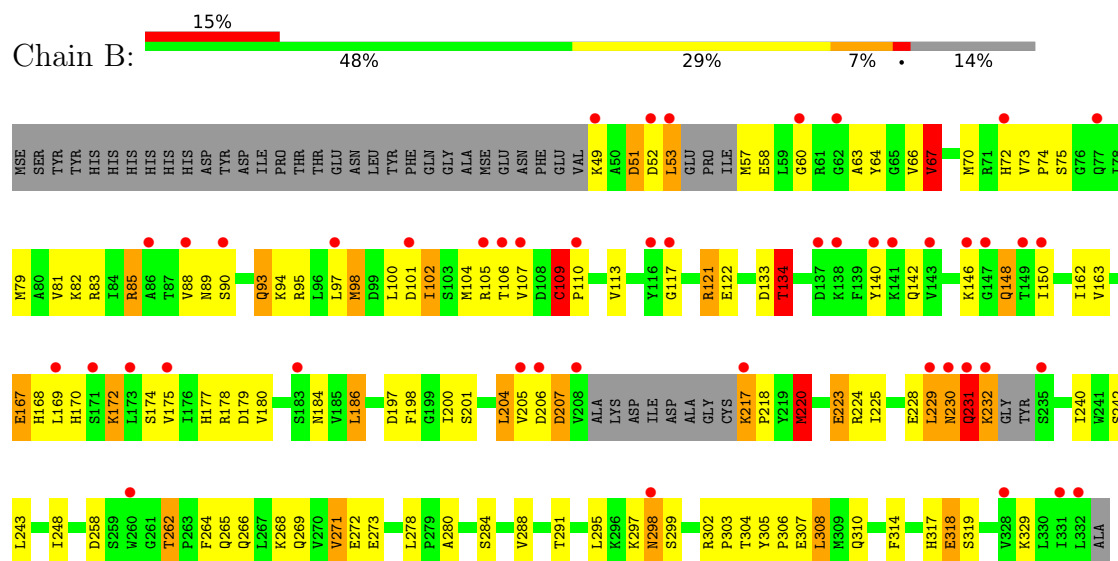
3 Residue-property plots

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: Dual specificity mitogen-activated protein kinase kinase 6



- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6



- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.66Å 122.66Å 195.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.35 19.97 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.97-2.35) 99.1 (19.97-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.212 , 0.269 0.207 , 0.252	Depositor DCC
R_{free} test set	3582 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9174	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: SO4, EDO, GOL

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	1.08	0/2260	1.20	5/3035 (0.2%)
1	B	1.04	1/2199 (0.0%)	1.27	12/2950 (0.4%)
1	C	1.03	0/2219	1.28	24/2980 (0.8%)
1	D	1.02	0/2285	1.27	14/3068 (0.5%)
All	All	1.05	1/8963 (0.0%)	1.25	55/12033 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	VAL	N-CA	-5.60	1.39	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	TRP	N-CA-C	-8.41	103.04	113.38
1	C	92	GLU	N-CA-C	-8.17	102.41	112.38
1	B	93	GLN	N-CA-C	-7.93	103.49	113.01
1	C	179	ASP	N-CA-C	7.88	119.90	110.44
1	D	149	THR	CA-C-N	-7.88	117.24	122.60
1	D	149	THR	C-N-CA	-7.88	117.24	122.60
1	C	77	GLN	N-CA-C	7.62	122.43	110.32
1	B	134	THR	CB-CA-C	-7.54	96.38	111.91
1	D	226	ASN	CA-C-N	7.49	127.47	119.76
1	D	226	ASN	C-N-CA	7.49	127.47	119.76
1	C	278	LEU	CA-C-N	-7.12	112.30	119.99
1	C	278	LEU	C-N-CA	-7.12	112.30	119.99
1	C	56	ILE	N-CA-C	7.05	124.00	109.34
1	B	109	CYS	N-CA-C	6.90	117.02	108.11
1	C	302	ARG	CA-C-N	6.86	126.82	120.03
1	C	302	ARG	C-N-CA	6.86	126.82	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	HIS	N-CA-C	6.83	118.61	111.03
1	B	67	VAL	N-CA-C	-6.77	98.47	108.97
1	B	280	ALA	N-CA-C	6.51	120.33	112.38
1	C	133	ASP	N-CA-C	6.49	118.15	111.14
1	D	177	HIS	N-CA-C	6.46	117.98	111.07
1	D	262	THR	N-CA-CB	-6.45	100.72	109.88
1	B	67	VAL	CA-C-N	-6.43	111.17	122.62
1	B	67	VAL	C-N-CA	-6.43	111.17	122.62
1	C	275	SER	CA-C-N	6.42	126.38	119.76
1	C	275	SER	C-N-CA	6.42	126.38	119.76
1	D	133	ASP	N-CA-C	6.41	118.07	111.14
1	C	134	THR	CB-CA-C	-6.16	97.28	111.95
1	D	280	ALA	N-CA-C	6.14	118.95	111.82
1	A	190	LEU	N-CA-C	-6.13	105.78	113.20
1	B	133	ASP	N-CA-C	6.04	117.53	111.07
1	D	102	ILE	CB-CA-C	-5.79	104.33	112.14
1	C	148	GLN	N-CA-C	5.57	117.97	109.95
1	D	179	ASP	N-CA-C	5.56	118.88	107.37
1	B	107	VAL	CB-CA-C	-5.50	105.97	111.80
1	D	117	GLY	N-CA-C	5.48	118.17	110.38
1	A	78	ILE	CB-CA-C	-5.48	104.02	111.15
1	B	220	MSE	CG-SE-CE	-5.35	87.15	98.92
1	D	70	MSE	N-CA-C	5.33	118.13	109.06
1	C	280	ALA	N-CA-C	5.23	117.89	111.82
1	C	257	TYR	CA-C-N	-5.16	115.44	122.87
1	C	257	TYR	C-N-CA	-5.16	115.44	122.87
1	D	218	PRO	N-CA-C	5.13	118.92	110.55
1	A	221	ALA	CA-C-N	5.12	125.16	119.32
1	A	221	ALA	C-N-CA	5.12	125.16	119.32
1	C	288	VAL	CB-CA-C	-5.11	105.16	112.22
1	D	252	ILE	N-CA-C	-5.10	107.78	112.83
1	C	273	GLU	CA-C-N	-5.08	115.00	120.03
1	C	273	GLU	C-N-CA	-5.08	115.00	120.03
1	B	85	ARG	CB-CA-C	-5.05	101.56	109.70
1	C	257	TYR	N-CA-C	-5.05	102.58	110.42
1	B	150	ILE	CA-C-O	5.03	121.93	119.12
1	A	230	ASN	N-CA-C	5.01	116.33	107.61
1	C	221	ALA	CA-C-N	5.00	125.02	119.32
1	C	221	ALA	C-N-CA	5.00	125.02	119.32

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	2223	0	2248	125	0
1	B	2163	0	2194	132	0
1	C	2185	0	2215	160	0
1	D	2248	0	2269	111	0
2	A	5	0	0	1	0
2	B	5	0	0	5	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	6	0	8	7	0
4	B	4	0	6	7	0
5	A	93	0	0	9	0
5	B	74	0	0	12	0
5	C	78	0	0	9	0
5	D	80	0	0	4	0
All	All	9174	0	8940	508	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (508) 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:C:56:ILE:CG2	1:C:57:MSE:N	1.70	1.41
1:A:119:LEU:HD21	1:C:208:VAL:CG1	1.46	1.41
1:A:119:LEU:CD2	1:C:208:VAL:HG11	1.55	1.33
1:C:177:HIS:CD2	1:C:179:ASP:H	1.50	1.30
1:D:43:MSE:O	1:D:44:GLU:HG3	1.43	1.18
1:C:56:ILE:HG22	1:C:57:MSE:N	1.21	1.16
1:A:159:ALA:HA	1:A:247:MSE:CE	1.77	1.15
1:C:177:HIS:HD2	1:C:179:ASP:N	1.45	1.13
1:D:162:ILE:HD12	1:D:247:MSE:HE1	1.31	1.13
1:B:217:LYS:HB3	1:B:218:PRO:CD	1.80	1.11
1:A:220:MSE:HE3	1:A:225:ILE:HD11	1.30	1.10
1:D:231:GLN:CD	1:D:232:LYS:H	1.58	1.10
1:A:274:PRO:HA	3:A:1:GOL:C3	1.82	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:O	1:B:97:LEU:HG	1.51	1.09
1:C:56:ILE:HG23	1:C:57:MSE:N	1.68	1.08
1:C:89:ASN:OD1	1:C:91:GLN:HG3	1.53	1.08
1:C:217:LYS:HD2	5:C:467:HOH:O	1.52	1.08
1:A:159:ALA:HA	1:A:247:MSE:HE3	1.11	1.08
1:D:95:ARG:NH2	1:D:98:MSE:HE2	1.67	1.08
1:A:253:LEU:N	1:A:253:LEU:HD22	1.62	1.06
1:D:231:GLN:HG2	1:D:232:LYS:N	1.68	1.06
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.32	1.06
1:B:262:THR:HG22	1:B:265:GLN:H	1.18	1.05
1:A:274:PRO:HB3	3:A:1:GOL:H32	1.37	1.05
1:C:55:PRO:HD3	1:C:71:ARG:O	1.55	1.05
1:D:231:GLN:CG	1:D:232:LYS:H	1.68	1.04
1:D:231:GLN:CG	1:D:232:LYS:N	2.19	1.04
1:A:274:PRO:HA	3:A:1:GOL:H31	1.36	1.04
1:B:49:LYS:HB3	1:B:117:GLY:HA3	1.38	1.04
1:B:83:ARG:H	4:B:1:EDO:H22	1.23	1.04
1:C:230:ASN:O	1:C:231:GLN:HG3	1.57	1.03
1:A:229:LEU:HD22	1:A:229:LEU:O	1.59	1.01
1:B:248:ILE:HD11	1:B:291:THR:HG21	1.38	1.01
1:B:319:SER:HB3	5:B:386:HOH:O	1.61	1.00
1:A:121:ARG:HG3	1:C:208:VAL:HG13	1.42	1.00
1:C:152:GLU:OE2	1:C:284:SER:HB2	1.61	1.00
1:C:259:SER:HB3	1:C:266:GLN:HG2	1.45	0.99
1:C:55:PRO:HG3	1:C:71:ARG:HB3	1.44	0.99
1:A:229:LEU:HD22	1:A:229:LEU:C	1.88	0.99
1:A:274:PRO:CB	3:A:1:GOL:H32	1.93	0.98
1:A:159:ALA:CA	1:A:247:MSE:HE3	1.94	0.98
1:C:91:GLN:HE21	1:C:92:GLU:N	1.61	0.97
1:A:262:THR:HG22	1:A:265:GLN:H	1.29	0.97
1:C:55:PRO:CG	1:C:71:ARG:HB3	1.95	0.97
1:A:218:PRO:HB3	1:A:220:MSE:HE1	1.45	0.96
1:C:55:PRO:O	1:C:56:ILE:HG13	1.65	0.96
1:A:326:SER:O	1:A:330:LEU:HD23	1.66	0.96
1:B:248:ILE:HD11	1:B:291:THR:CG2	1.97	0.95
1:B:100:LEU:HG	1:B:104:MSE:HE2	1.45	0.94
1:A:177:HIS:HD2	1:A:179:ASP:H	1.01	0.93
1:C:48:VAL:HG12	1:C:49:LYS:HG2	1.49	0.92
1:A:274:PRO:CA	3:A:1:GOL:H32	2.01	0.89
1:B:52:ASP:OD2	1:B:72:HIS:HE1	1.55	0.88
1:A:218:PRO:CB	1:A:220:MSE:HE1	2.04	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:MSE:HE2	1:D:58:GLU:O	1.72	0.88
1:C:291:THR:HG22	5:C:441:HOH:O	1.73	0.87
1:D:262:THR:HG22	1:D:265:GLN:H	1.39	0.87
1:B:231:GLN:HG2	1:B:232:LYS:N	1.88	0.87
1:D:217:LYS:HG2	1:D:266:GLN:OE1	1.75	0.87
1:B:205:VAL:HB	4:B:1:EDO:H12	1.54	0.86
1:D:182:PRO:HD3	1:D:246:THR:HB	1.57	0.86
1:C:48:VAL:HG13	1:C:49:LYS:HD3	1.54	0.86
1:D:43:MSE:O	1:D:44:GLU:CG	2.23	0.86
1:C:55:PRO:O	1:C:56:ILE:CG1	2.24	0.85
1:C:91:GLN:HE21	1:C:92:GLU:CA	1.88	0.85
1:C:67:VAL:O	1:C:68:GLU:HB2	1.74	0.85
1:C:50:ALA:O	1:C:51:ASP:CB	2.24	0.84
1:B:52:ASP:O	1:B:53:LEU:HB2	1.75	0.84
1:C:291:THR:CG2	5:C:441:HOH:O	2.22	0.84
1:D:243:LEU:HD11	1:D:247:MSE:HE3	1.59	0.84
1:A:274:PRO:HA	3:A:1:GOL:H32	1.59	0.83
1:B:94:LYS:HG2	1:B:98:MSE:HE3	1.58	0.83
1:C:104:MSE:HG2	1:C:115:PHE:O	1.78	0.83
1:D:95:ARG:NH2	1:D:98:MSE:CE	2.41	0.83
1:A:252:ILE:C	1:A:253:LEU:HD22	2.03	0.83
1:B:52:ASP:OD2	1:B:72:HIS:CE1	2.32	0.83
1:C:206:ASP:O	1:C:207:ASP:CB	2.27	0.83
1:D:95:ARG:HH21	1:D:98:MSE:HE2	1.41	0.82
1:A:253:LEU:N	1:A:253:LEU:CD2	2.42	0.82
1:B:134:THR:HG23	5:B:361:HOH:O	1.80	0.82
1:A:274:PRO:CA	3:A:1:GOL:C3	2.57	0.81
1:B:217:LYS:HD3	1:B:266:GLN:OE1	1.79	0.81
1:A:232:LYS:NZ	1:A:232:LYS:HB3	1.95	0.81
1:A:142:GLN:NE2	1:A:146:LYS:HE3	1.97	0.80
1:A:162:ILE:HD12	1:A:247:MSE:HE1	1.63	0.80
1:B:83:ARG:H	4:B:1:EDO:C2	1.94	0.80
1:A:220:MSE:HE3	1:A:225:ILE:CD1	2.11	0.80
1:A:225:ILE:O	1:B:262:THR:HG21	1.81	0.80
1:C:152:GLU:OE2	1:C:284:SER:CB	2.30	0.80
1:C:177:HIS:CD2	1:C:179:ASP:N	2.29	0.80
1:D:113:VAL:HG11	1:D:186:LEU:HD22	1.64	0.80
1:B:200:ILE:HG13	1:B:204:LEU:HD22	1.63	0.79
1:A:153:ASP:OD1	1:A:320:LYS:HE2	1.83	0.79
1:C:177:HIS:O	1:C:178:ARG:HG2	1.83	0.78
1:D:131:LEU:CD1	1:D:131:LEU:C	2.55	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:THR:HG21	1:B:225:ILE:O	1.83	0.78
1:A:162:ILE:HD12	1:A:247:MSE:CE	2.14	0.78
1:C:217:LYS:HB2	1:C:217:LYS:NZ	1.99	0.77
1:A:113:VAL:HG21	1:A:186:LEU:HD22	1.66	0.77
1:D:231:GLN:OE1	1:D:232:LYS:N	2.16	0.77
1:A:220:MSE:CE	1:A:225:ILE:HD11	2.13	0.77
1:C:217:LYS:HB2	1:C:217:LYS:HZ2	1.50	0.76
1:D:303:PRO:HG2	1:D:308:LEU:HD13	1.68	0.76
1:D:243:LEU:CD1	1:D:247:MSE:HE3	2.15	0.76
1:C:50:ALA:O	1:C:51:ASP:HB3	1.83	0.75
1:B:93:GLN:HB3	2:B:4:SO4:S	2.26	0.75
1:B:248:ILE:CD1	1:B:291:THR:HG21	2.15	0.75
1:D:43:MSE:HG3	1:D:46:PHE:CD2	2.21	0.75
1:D:243:LEU:CD1	1:D:247:MSE:CE	2.64	0.75
1:C:206:ASP:O	1:C:207:ASP:HB2	1.85	0.75
1:B:298:ASN:OD1	1:B:298:ASN:C	2.28	0.75
1:C:259:SER:CB	1:C:266:GLN:HG2	2.17	0.75
1:C:294:CYS:O	1:C:302:ARG:HD3	1.87	0.74
1:A:232:LYS:HB3	1:A:232:LYS:HZ2	1.49	0.74
1:C:56:ILE:HG22	1:C:57:MSE:CA	2.17	0.74
1:A:177:HIS:CD2	1:A:179:ASP:H	1.94	0.73
1:C:200:ILE:HG13	1:C:204:LEU:HD22	1.68	0.73
1:A:83:ARG:HH22	1:C:124:ASP:CG	1.95	0.73
1:A:159:ALA:CA	1:A:247:MSE:CE	2.62	0.73
1:D:262:THR:H	1:D:265:GLN:HE21	1.37	0.73
1:B:109:CYS:SG	1:B:110:PRO:HD2	2.29	0.73
1:A:119:LEU:HD21	1:C:208:VAL:HG11	0.76	0.73
1:A:119:LEU:HD21	1:C:208:VAL:HG12	1.63	0.73
1:A:320:LYS:HE3	5:A:383:HOH:O	1.87	0.72
1:A:252:ILE:C	1:A:253:LEU:CD2	2.62	0.72
1:D:162:ILE:CD1	1:D:247:MSE:HE1	2.17	0.72
1:A:84:ILE:HD11	1:A:127:ILE:HD11	1.72	0.72
1:C:55:PRO:CD	1:C:71:ARG:O	2.37	0.71
1:A:217:LYS:HE3	1:A:266:GLN:NE2	2.05	0.71
1:C:230:ASN:HA	5:C:419:HOH:O	1.89	0.71
1:D:131:LEU:HD13	1:D:132:MSE:N	2.06	0.71
1:C:50:ALA:HB1	1:C:53:LEU:HG	1.73	0.71
1:A:177:HIS:HD2	1:A:179:ASP:N	1.84	0.71
1:C:50:ALA:HB2	1:C:53:LEU:HD12	1.71	0.71
1:D:43:MSE:HB3	1:D:46:PHE:HB3	1.71	0.71
1:B:72:HIS:HD2	1:B:75:SER:OG	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:N	4:B:1:EDO:H22	2.01	0.70
1:B:284:SER:O	1:B:288:VAL:HG23	1.91	0.70
1:C:298:ASN:C	1:C:298:ASN:HD22	2.00	0.70
1:C:55:PRO:HG2	1:C:71:ARG:HB3	1.72	0.70
1:B:52:ASP:OD2	1:B:74:PRO:HG2	1.91	0.70
1:D:79:MSE:HE2	1:D:116:TYR:CD2	2.26	0.70
1:B:205:VAL:HB	4:B:1:EDO:C1	2.21	0.70
1:C:284:SER:O	1:C:288:VAL:HG23	1.91	0.70
1:A:89:ASN:HB2	2:A:2:SO4:O3	1.92	0.69
1:A:54:GLU:OE1	1:A:71:ARG:NH1	2.25	0.69
1:C:55:PRO:HG3	1:C:71:ARG:CB	2.21	0.69
1:B:72:HIS:HD2	1:B:75:SER:CB	2.05	0.69
1:C:77:GLN:NE2	1:C:116:TYR:OH	2.25	0.69
1:A:217:LYS:HG3	1:A:218:PRO:HD3	1.75	0.69
1:D:121:ARG:HH11	1:D:121:ARG:HG3	1.57	0.68
1:B:304:THR:HG23	1:B:307:GLU:OE1	1.92	0.68
1:C:113:VAL:HG21	1:C:186:LEU:HD22	1.74	0.68
1:B:94:LYS:O	1:B:97:LEU:HB2	1.94	0.68
1:C:50:ALA:CB	1:C:53:LEU:HD12	2.24	0.68
1:A:142:GLN:NE2	1:A:146:LYS:CE	2.56	0.67
1:A:172:LYS:C	1:A:173:LEU:HD23	2.19	0.67
1:A:217:LYS:HE3	1:A:266:GLN:HE22	1.60	0.67
1:C:53:LEU:HD22	1:D:190:LEU:HD11	1.77	0.67
1:D:243:LEU:HD12	1:D:247:MSE:HE2	1.77	0.67
1:D:57:MSE:CE	1:D:58:GLU:O	2.43	0.67
1:A:121:ARG:HG3	1:C:208:VAL:CG1	2.21	0.67
1:B:73:VAL:N	1:B:74:PRO:CD	2.58	0.66
1:C:56:ILE:CG2	1:C:57:MSE:O	2.43	0.66
1:C:224:ARG:NH2	1:C:231:GLN:O	2.28	0.66
1:C:48:VAL:CG1	1:C:49:LYS:HG2	2.24	0.66
1:C:89:ASN:HB2	2:C:3:SO4:O1	1.96	0.66
1:D:131:LEU:C	1:D:131:LEU:HD13	2.21	0.66
1:B:93:GLN:O	1:B:97:LEU:CG	2.38	0.65
1:A:284:SER:O	1:A:288:VAL:HG23	1.96	0.65
1:C:267:LEU:O	1:C:271:VAL:HG12	1.96	0.65
1:B:262:THR:HG22	1:B:265:GLN:N	2.03	0.65
1:D:101:ASP:OD1	1:D:105:ARG:NH2	2.20	0.65
1:A:47:GLU:OE2	1:A:120:PHE:HD1	1.81	0.64
1:A:207:ASP:HB3	1:C:66:VAL:HG22	1.80	0.64
1:C:50:ALA:HB1	1:C:53:LEU:CG	2.27	0.64
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HD22	1:D:190:LEU:CD1	2.28	0.63
1:D:223:GLU:CD	1:D:223:GLU:H	2.06	0.63
1:A:278:LEU:HB2	1:A:291:THR:HG21	1.80	0.63
1:A:95:ARG:HD3	5:A:398:HOH:O	1.98	0.63
1:A:232:LYS:O	1:A:233:GLY:O	2.17	0.63
1:D:95:ARG:HH22	1:D:98:MSE:HE2	1.59	0.63
1:D:217:LYS:HB3	1:D:218:PRO:CD	2.29	0.62
1:C:59:LEU:HG	1:C:60:GLY:H	1.63	0.62
1:C:173:LEU:O	1:C:175:VAL:HG23	1.98	0.62
1:D:224:ARG:HD2	1:D:234:TYR:CE1	2.33	0.62
1:A:153:ASP:OD1	1:A:320:LYS:CE	2.48	0.62
1:B:197:ASP:OD2	1:B:198:PHE:HD2	1.83	0.62
1:A:138:LYS:HE3	5:A:397:HOH:O	2.00	0.62
1:B:314:PHE:CE2	1:B:318:GLU:HG3	2.35	0.62
1:A:262:THR:HG22	1:A:265:GLN:N	2.08	0.62
1:A:148:GLN:HG3	1:A:149:THR:H	1.65	0.61
1:B:73:VAL:N	1:B:74:PRO:HD2	2.15	0.61
1:C:48:VAL:O	1:C:49:LYS:O	2.19	0.61
1:D:242:SER:O	1:D:246:THR:HG23	1.99	0.61
1:A:83:ARG:NH2	1:C:124:ASP:OD1	2.34	0.61
1:C:89:ASN:CG	1:C:91:GLN:HG3	2.26	0.61
1:C:159:ALA:O	1:C:163:VAL:HG23	2.01	0.61
1:A:262:THR:CG2	1:A:264:PHE:HB3	2.31	0.61
1:D:243:LEU:CD1	1:D:247:MSE:HE2	2.30	0.61
1:B:148:GLN:HG3	5:B:351:HOH:O	2.00	0.60
1:B:303:PRO:CG	1:B:308:LEU:HD13	2.31	0.60
1:D:43:MSE:C	1:D:44:GLU:HG3	2.25	0.60
1:D:72:HIS:HD2	1:D:75:SER:H	1.49	0.60
1:C:100:LEU:HG	1:C:104:MSE:HE2	1.83	0.60
1:C:170:HIS:O	1:C:174:SER:HA	2.01	0.60
1:A:83:ARG:NH2	1:C:124:ASP:CG	2.60	0.59
1:B:93:GLN:HB3	2:B:4:SO4:O4	2.02	0.59
1:B:148:GLN:CG	5:B:351:HOH:O	2.50	0.59
1:A:159:ALA:HA	1:A:247:MSE:HE1	1.79	0.59
1:B:72:HIS:HD2	1:B:75:SER:HB3	1.68	0.59
1:C:91:GLN:NE2	1:C:92:GLU:N	2.42	0.59
1:A:172:LYS:O	1:A:173:LEU:HD23	2.02	0.58
1:A:142:GLN:HE21	1:A:146:LYS:HE3	1.67	0.58
1:D:303:PRO:CG	1:D:308:LEU:HD13	2.32	0.58
1:A:85:ARG:HA	1:A:205:VAL:HG22	1.84	0.58
1:D:43:MSE:HB2	1:D:46:PHE:HD2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:CYS:SG	1:B:110:PRO:CD	2.92	0.58
1:C:72:HIS:ND1	1:C:75:SER:HB3	2.19	0.58
1:C:230:ASN:O	1:C:231:GLN:CG	2.44	0.58
1:D:72:HIS:CD2	1:D:74:PRO:HD2	2.39	0.58
1:A:262:THR:HG23	1:A:264:PHE:H	1.69	0.58
1:B:167:GLU:HG3	5:B:364:HOH:O	2.04	0.58
1:D:101:ASP:CG	1:D:105:ARG:HH21	2.10	0.58
1:A:262:THR:HB	1:A:265:GLN:NE2	2.19	0.57
1:B:121:ARG:NH1	5:B:340:HOH:O	2.37	0.57
1:B:168:HIS:CE1	1:B:172:LYS:HD3	2.40	0.57
1:C:177:HIS:CD2	1:C:179:ASP:CA	2.87	0.57
1:D:54:GLU:OE1	1:D:71:ARG:HD2	2.04	0.57
1:B:109:CYS:SG	1:B:110:PRO:N	2.76	0.57
1:D:217:LYS:CG	1:D:266:GLN:OE1	2.49	0.57
1:B:89:ASN:OD1	1:B:89:ASN:C	2.48	0.57
1:B:113:VAL:HG21	1:B:186:LEU:HD22	1.86	0.57
1:A:119:LEU:CD2	1:C:208:VAL:CG1	2.39	0.57
1:A:177:HIS:HE1	1:A:196:CYS:O	1.87	0.56
1:D:231:GLN:O	1:D:232:LYS:HB2	2.05	0.56
1:A:217:LYS:CG	1:A:218:PRO:HD3	2.36	0.56
1:D:46:PHE:CE1	1:D:100:LEU:HD23	2.40	0.56
1:B:134:THR:CG2	5:B:361:HOH:O	2.43	0.56
1:C:55:PRO:CG	1:C:71:ARG:CB	2.78	0.56
1:C:93:GLN:O	1:C:97:LEU:HG	2.06	0.56
1:D:131:LEU:C	1:D:131:LEU:HD12	2.29	0.56
1:C:220:MSE:H	1:C:220:MSE:SE	2.38	0.56
1:D:95:ARG:HH22	1:D:98:MSE:CE	2.12	0.56
1:B:184:ASN:HD21	1:B:201:SER:H	1.54	0.56
1:B:94:LYS:CE	1:B:98:MSE:HE1	2.35	0.56
1:D:231:GLN:HG2	1:D:232:LYS:CA	2.36	0.56
1:C:291:THR:HG21	5:C:441:HOH:O	1.99	0.56
1:B:223:GLU:CD	1:B:223:GLU:H	2.14	0.55
1:A:121:ARG:CG	1:C:208:VAL:HG13	2.27	0.55
1:B:169:LEU:HB3	1:B:175:VAL:HB	1.88	0.55
1:C:230:ASN:ND2	5:C:463:HOH:O	2.33	0.55
1:B:220:MSE:O	1:B:220:MSE:HG2	2.03	0.55
1:B:229:LEU:HD11	1:D:316:LEU:HB2	1.87	0.55
1:A:303:PRO:HG2	1:A:308:LEU:HD13	1.88	0.55
1:B:94:LYS:HG2	1:B:98:MSE:CE	2.34	0.55
1:C:91:GLN:NE2	1:C:92:GLU:HG3	2.22	0.55
1:B:81:VAL:HG23	1:B:81:VAL:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PRO:CG	1:A:308:LEU:HD13	2.37	0.54
1:C:91:GLN:HE21	1:C:92:GLU:HA	1.69	0.54
1:B:72:HIS:CD2	1:B:75:SER:OG	2.57	0.54
1:B:94:LYS:HE2	1:B:98:MSE:HE1	1.88	0.54
1:C:177:HIS:CD2	1:C:177:HIS:C	2.85	0.54
1:C:55:PRO:HG2	1:C:56:ILE:H	1.72	0.54
1:A:61:ARG:HH12	1:A:66:VAL:N	2.06	0.54
1:B:94:LYS:CE	1:B:98:MSE:CE	2.85	0.54
1:C:240:ILE:HD13	1:C:303:PRO:O	2.07	0.54
1:A:217:LYS:CB	1:A:218:PRO:HD3	2.38	0.54
1:B:248:ILE:HG12	1:B:278:LEU:HD13	1.90	0.54
1:C:119:LEU:HD23	1:C:128:CYS:SG	2.48	0.54
1:C:259:SER:HB3	1:C:266:GLN:CG	2.29	0.54
1:D:298:ASN:HB3	1:D:301:GLU:OE1	2.08	0.53
1:A:289:ASP:O	1:A:293:GLN:HG2	2.08	0.53
1:B:90:SER:O	2:B:4:SO4:O4	2.26	0.53
1:C:91:GLN:HG3	1:C:92:GLU:H	1.73	0.53
1:C:55:PRO:HG2	1:C:71:ARG:H	1.73	0.53
1:A:194:LYS:NZ	5:A:371:HOH:O	2.40	0.53
1:B:101:ASP:O	1:B:105:ARG:HG2	2.08	0.53
1:D:137:ASP:O	1:D:141:LYS:HG2	2.09	0.53
1:D:105:ARG:HG2	1:D:106:THR:HG23	1.91	0.53
1:C:48:VAL:HG13	1:C:49:LYS:CD	2.33	0.53
1:C:184:ASN:HD21	1:C:201:SER:H	1.57	0.52
1:B:72:HIS:CD2	1:B:75:SER:HB3	2.43	0.52
1:D:143:VAL:HG13	1:D:148:GLN:HB3	1.91	0.52
1:D:148:GLN:HG3	1:D:149:THR:H	1.73	0.52
1:B:82:LYS:HA	4:B:1:EDO:H22	1.92	0.52
1:C:84:ILE:HD13	1:C:204:LEU:CD1	2.39	0.52
1:D:298:ASN:OD1	1:D:298:ASN:C	2.53	0.52
1:C:55:PRO:CG	1:C:71:ARG:H	2.21	0.52
1:D:271:VAL:HG22	1:D:272:GLU:HG3	1.92	0.52
1:A:254:ARG:HD2	5:A:392:HOH:O	2.09	0.52
1:B:317:HIS:HD2	5:B:347:HOH:O	1.93	0.52
1:A:113:VAL:HG21	1:A:186:LEU:CD2	2.37	0.52
1:B:262:THR:CG2	1:B:264:PHE:HB3	2.40	0.52
1:A:326:SER:O	1:A:330:LEU:CD2	2.50	0.51
1:C:149:THR:CG2	1:C:150:ILE:N	2.72	0.51
1:D:109:CYS:SG	1:D:111:PHE:HB2	2.50	0.51
1:B:63:ALA:O	1:B:64:TYR:HB2	2.10	0.51
1:A:309:MSE:HE3	1:A:314:PHE:CZ	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH2	1:C:124:ASP:OD2	2.29	0.51
1:B:168:HIS:ND1	1:B:172:LYS:HD3	2.25	0.51
1:C:77:GLN:NE2	1:C:116:TYR:CZ	2.79	0.51
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.91	0.51
1:A:305:TYR:O	1:A:309:MSE:HG3	2.11	0.51
1:D:73:VAL:N	1:D:74:PRO:CD	2.73	0.51
1:D:221:ALA:HB1	1:D:223:GLU:OE2	2.10	0.51
1:A:228:GLU:O	1:A:229:LEU:C	2.53	0.51
1:B:102:ILE:HD13	1:B:102:ILE:N	2.26	0.51
1:C:248:ILE:HD11	1:C:291:THR:CG2	2.41	0.51
1:A:223:GLU:CD	1:A:223:GLU:H	2.17	0.51
1:C:91:GLN:NE2	1:C:92:GLU:CA	2.66	0.51
1:D:44:GLU:C	1:D:46:PHE:H	2.18	0.51
1:D:231:GLN:HG2	1:D:232:LYS:O	2.12	0.50
1:B:303:PRO:HG2	1:B:308:LEU:HD13	1.93	0.50
1:C:170:HIS:CD2	1:C:236:VAL:HG11	2.47	0.50
1:D:83:ARG:O	1:D:205:VAL:HG23	2.12	0.50
1:A:153:ASP:OD2	1:A:153:ASP:N	2.45	0.50
1:C:55:PRO:CD	1:C:71:ARG:H	2.24	0.50
1:C:67:VAL:O	1:C:68:GLU:CB	2.51	0.50
1:D:57:MSE:HB2	5:D:401:HOH:O	2.10	0.50
1:D:286:GLU:CD	1:D:286:GLU:H	2.20	0.50
1:A:159:ALA:CB	1:A:247:MSE:HE3	2.42	0.50
1:D:217:LYS:HG3	1:D:218:PRO:HD3	1.93	0.50
1:B:51:ASP:OD1	1:B:51:ASP:O	2.30	0.50
1:A:180:VAL:HG22	1:A:195:MSE:HE1	1.94	0.50
1:B:314:PHE:O	1:B:318:GLU:HB2	2.12	0.50
1:C:263:PRO:HD2	5:C:456:HOH:O	2.11	0.50
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.94	0.50
1:A:305:TYR:HB2	1:A:306:PRO:HD3	1.94	0.49
5:A:364:HOH:O	1:C:129:MSE:SE	2.79	0.49
1:B:93:GLN:HB3	2:B:4:SO4:O3	2.11	0.49
1:C:217:LYS:NZ	1:C:217:LYS:CB	2.74	0.49
1:D:131:LEU:CD1	1:D:132:MSE:N	2.75	0.49
1:D:253:LEU:O	1:D:254:ARG:HB3	2.12	0.49
1:B:248:ILE:CD1	1:B:291:THR:CG2	2.80	0.49
1:D:154:ILE:HD13	1:D:327:PHE:CG	2.47	0.49
1:B:262:THR:H	1:B:265:GLN:HE21	1.59	0.49
1:C:48:VAL:CG1	1:C:49:LYS:HD3	2.34	0.49
1:B:162:ILE:HG21	1:B:243:LEU:HD13	1.94	0.49
1:B:94:LYS:HE3	1:B:98:MSE:CE	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLN:HG3	5:D:439:HOH:O	2.11	0.49
1:A:62:GLY:HA2	1:C:132:MSE:O	2.13	0.49
1:C:55:PRO:O	1:C:56:ILE:CD1	2.60	0.49
1:B:70:MSE:HG2	1:B:81:VAL:HG11	1.95	0.49
1:B:262:THR:HG23	5:B:356:HOH:O	2.11	0.49
1:C:184:ASN:ND2	1:C:201:SER:H	2.11	0.49
1:D:43:MSE:HB2	1:D:46:PHE:CD2	2.46	0.49
1:D:157:LYS:HE3	1:D:317:HIS:O	2.12	0.49
1:A:262:THR:HG23	5:A:347:HOH:O	2.14	0.48
1:D:217:LYS:CG	1:D:218:PRO:HD3	2.43	0.48
1:D:217:LYS:CB	1:D:218:PRO:HD3	2.43	0.48
1:D:262:THR:CG2	1:D:264:PHE:HB3	2.43	0.48
1:A:237:LYS:HD2	1:A:302:ARG:HB2	1.95	0.48
1:C:134:THR:HG21	1:C:138:LYS:HB2	1.95	0.48
1:C:304:THR:HB	1:C:306:PRO:HD2	1.95	0.48
1:B:94:LYS:CG	1:B:98:MSE:CE	2.91	0.48
1:B:94:LYS:CG	1:B:98:MSE:HE3	2.36	0.48
1:D:56:ILE:HD12	1:D:56:ILE:N	2.27	0.48
1:D:43:MSE:CB	1:D:46:PHE:CD2	2.96	0.48
1:D:72:HIS:CD2	1:D:75:SER:OG	2.67	0.48
1:B:220:MSE:SE	1:B:220:MSE:H	2.47	0.48
1:B:248:ILE:CG1	1:B:291:THR:HG21	2.43	0.48
1:C:217:LYS:HB3	1:C:218:PRO:CD	2.44	0.48
1:D:121:ARG:NH1	1:D:121:ARG:CG	2.76	0.48
1:A:104:MSE:HE3	1:A:116:TYR:O	2.14	0.48
1:A:262:THR:HG21	1:A:264:PHE:HB3	1.96	0.48
1:C:50:ALA:O	1:C:51:ASP:HB2	2.07	0.48
1:B:72:HIS:CD2	1:B:75:SER:CB	2.91	0.48
1:B:228:GLU:O	1:B:229:LEU:C	2.56	0.48
1:A:138:LYS:HD3	1:A:138:LYS:N	2.28	0.47
1:B:66:VAL:HG12	1:B:67:VAL:O	2.13	0.47
1:C:279:PRO:HD2	1:C:283:PHE:CE2	2.50	0.47
1:B:83:ARG:O	4:B:1:EDO:H11	2.14	0.47
1:A:232:LYS:NZ	1:A:232:LYS:CB	2.68	0.47
1:C:89:ASN:OD1	1:C:91:GLN:CG	2.44	0.47
1:B:81:VAL:O	1:B:81:VAL:CG2	2.60	0.47
1:B:258[A]:ASP:CG	1:B:269:GLN:HE22	2.22	0.47
1:C:73:VAL:N	1:C:74:PRO:CD	2.77	0.47
1:D:89:ASN:OD1	1:D:89:ASN:C	2.58	0.47
1:D:286:GLU:HA	5:D:455:HOH:O	2.14	0.47
1:A:162:ILE:HD12	1:A:247:MSE:HE2	1.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:THR:HA	1:D:195:MSE:O	2.14	0.47
1:B:90:SER:HA	2:B:4:SO4:S	2.55	0.47
1:B:168:HIS:O	1:B:172:LYS:HB2	2.14	0.47
1:D:121:ARG:HG3	1:D:121:ARG:NH1	2.27	0.47
1:B:271:VAL:HG22	1:B:272:GLU:HG3	1.95	0.46
1:C:61:ARG:HH11	1:C:61:ARG:HB2	1.80	0.46
1:C:104:MSE:CG	1:C:115:PHE:O	2.56	0.46
1:A:241:TRP:CD1	1:A:241:TRP:C	2.94	0.46
1:D:95:ARG:HG2	1:D:203:TYR:OH	2.16	0.46
1:C:91:GLN:C	1:C:93:GLN:N	2.73	0.46
1:D:217:LYS:CB	1:D:218:PRO:CD	2.94	0.46
1:A:320:LYS:HG2	1:A:322:THR:OG1	2.16	0.46
1:A:217:LYS:HE3	1:A:266:GLN:CD	2.42	0.45
1:C:59:LEU:HG	1:C:60:GLY:N	2.29	0.45
1:D:85:ARG:HA	1:D:205:VAL:HG22	1.97	0.45
1:A:317:HIS:HD2	5:A:349:HOH:O	1.98	0.45
1:D:111:PHE:CE2	1:D:164:LYS:HD3	2.52	0.45
1:D:305:TYR:O	1:D:306:PRO:C	2.58	0.45
1:A:85:ARG:HG2	1:A:203:TYR:O	2.17	0.45
1:A:146:LYS:O	1:A:147:GLY:C	2.59	0.45
1:D:224:ARG:HD2	1:D:234:TYR:CD1	2.51	0.45
1:C:48:VAL:CG1	1:C:49:LYS:CD	2.93	0.45
1:C:170:HIS:CD2	1:C:236:VAL:CG1	2.99	0.45
1:A:51:ASP:OD2	1:A:51:ASP:N	2.45	0.45
1:B:177:HIS:O	1:B:178:ARG:HB2	2.16	0.45
1:C:195:MSE:HE2	1:C:195:MSE:HB2	1.81	0.45
1:C:84:ILE:HD13	1:C:204:LEU:HD12	1.98	0.44
1:C:55:PRO:CG	1:C:56:ILE:H	2.29	0.44
1:C:206:ASP:O	1:C:207:ASP:HB3	2.14	0.44
1:B:70:MSE:CG	1:B:81:VAL:HG11	2.46	0.44
1:B:268:LYS:HG3	5:B:363:HOH:O	2.16	0.44
1:C:85:ARG:HG2	1:C:203:TYR:O	2.17	0.44
1:B:83:ARG:O	1:B:205:VAL:HG23	2.17	0.44
1:A:142:GLN:NE2	1:A:146:LYS:HE2	2.30	0.44
1:B:85:ARG:HA	1:B:205:VAL:HG22	2.00	0.44
1:B:217:LYS:CB	1:B:218:PRO:CD	2.67	0.44
1:C:79:MSE:HE2	1:C:116:TYR:CG	2.52	0.44
1:A:260:TRP:CE3	1:D:320:LYS:HE3	2.53	0.44
1:B:206:ASP:CG	1:B:207:ASP:H	2.26	0.44
1:C:72:HIS:O	1:C:73:VAL:C	2.61	0.44
1:D:318:GLU:O	1:D:318:GLU:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:TYR:HB2	1:B:306:PRO:HD3	2.00	0.43
1:C:220:MSE:HE3	5:C:454:HOH:O	2.17	0.43
1:C:298:ASN:C	1:C:298:ASN:ND2	2.67	0.43
1:B:180:VAL:HB	1:B:242:SER:HB2	2.00	0.43
1:B:72:HIS:C	1:B:74:PRO:HD2	2.43	0.43
1:B:299:SER:HB3	1:B:302:ARG:CZ	2.48	0.43
1:C:304:THR:CB	1:C:306:PRO:HD2	2.49	0.43
1:C:55:PRO:CD	1:C:71:ARG:N	2.81	0.43
1:C:56:ILE:HG22	1:C:57:MSE:O	2.16	0.43
1:B:170:HIS:O	1:B:174:SER:HA	2.19	0.43
1:B:317:HIS:CD2	5:B:347:HOH:O	2.71	0.43
1:D:232:LYS:HB2	1:D:232:LYS:NZ	2.32	0.43
1:B:217:LYS:CD	1:B:266:GLN:OE1	2.60	0.43
1:C:224:ARG:HD3	5:C:462:HOH:O	2.18	0.43
1:C:305:TYR:N	1:C:306:PRO:CD	2.81	0.43
1:D:121:ARG:HH11	1:D:121:ARG:CG	2.23	0.43
1:C:148:GLN:OE1	1:C:330:LEU:HD21	2.18	0.43
1:D:92:GLU:HB3	1:D:203:TYR:HE1	1.84	0.43
1:B:142:GLN:O	1:B:146:LYS:HG2	2.19	0.43
1:D:43:MSE:CG	1:D:46:PHE:CD2	2.96	0.43
1:D:154:ILE:HD13	1:D:327:PHE:CD2	2.53	0.43
1:A:309:MSE:HE3	1:A:314:PHE:HZ	1.82	0.43
1:B:52:ASP:O	1:B:53:LEU:CB	2.53	0.43
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.96	0.42
1:B:262:THR:HG23	1:B:264:PHE:H	1.84	0.42
1:A:232:LYS:HB3	1:A:232:LYS:HZ3	1.79	0.42
1:A:252:ILE:C	1:A:253:LEU:HD23	2.40	0.42
1:A:173:LEU:O	1:A:174:SER:HB2	2.19	0.42
1:A:84:ILE:HD12	1:A:125:VAL:HG12	2.00	0.42
1:B:248:ILE:HD12	1:B:295:LEU:CD1	2.49	0.42
1:B:79:MSE:HE2	1:B:79:MSE:HB3	1.90	0.42
1:B:105:ARG:HG3	1:B:106:THR:HG23	2.01	0.42
1:D:182:PRO:CD	1:D:246:THR:HB	2.40	0.42
1:D:226:ASN:N	1:D:227:PRO:HD3	2.34	0.42
1:A:258:ASP:HB3	1:A:260:TRP:CZ3	2.55	0.42
1:A:320:LYS:HG2	1:A:322:THR:HG1	1.85	0.42
1:B:98:MSE:O	1:B:102:ILE:HG12	2.19	0.42
1:B:94:LYS:HA	1:B:97:LEU:HD12	2.02	0.42
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.57	0.42
1:C:50:ALA:HB1	1:C:53:LEU:CD1	2.49	0.42
1:C:152:GLU:OE2	1:C:284:SER:OG	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:HG23	5:D:397:HOH:O	2.20	0.42
1:B:95:ARG:HA	1:B:98:MSE:HG3	2.01	0.42
1:B:240:ILE:HD13	1:B:303:PRO:O	2.19	0.42
1:C:91:GLN:NE2	1:C:92:GLU:HA	2.32	0.42
1:A:298:ASN:HB3	5:A:394:HOH:O	2.20	0.41
1:B:51:ASP:O	1:B:51:ASP:CG	2.62	0.41
1:B:273:GLU:O	1:B:297:LYS:NZ	2.47	0.41
1:C:67:VAL:HG12	1:C:69:LYS:H	1.84	0.41
1:C:148:GLN:HG3	1:C:149:THR:H	1.85	0.41
1:C:317:HIS:O	1:C:318:GLU:C	2.63	0.41
1:D:43:MSE:CB	1:D:46:PHE:HB3	2.45	0.41
1:A:142:GLN:HE21	1:A:146:LYS:CE	2.28	0.41
1:C:55:PRO:HD2	1:C:71:ARG:H	1.84	0.41
1:A:71:ARG:HG2	1:A:78:ILE:HD13	2.01	0.41
1:B:230:ASN:O	1:B:231:GLN:O	2.39	0.41
1:C:262:THR:HB	1:C:263:PRO:CD	2.50	0.41
1:C:278:LEU:HD21	1:C:287:PHE:CE2	2.55	0.41
1:C:307:GLU:O	1:C:310:GLN:HB2	2.20	0.41
1:A:317:HIS:O	1:A:318:GLU:C	2.62	0.41
1:C:177:HIS:HE1	1:C:196:CYS:O	2.02	0.41
1:A:278:LEU:HD12	1:A:278:LEU:HA	1.79	0.41
1:B:306:PRO:O	1:B:310:GLN:HG2	2.20	0.41
1:C:72:HIS:CE1	1:C:75:SER:HB3	2.55	0.41
1:A:72:HIS:HB2	1:A:79:MSE:HE3	2.01	0.41
1:B:63:ALA:O	1:B:64:TYR:CB	2.69	0.41
1:D:232:LYS:NZ	1:D:232:LYS:CB	2.83	0.41
1:C:54:GLU:HA	1:C:55:PRO:HD3	1.84	0.41
1:C:94:LYS:O	1:C:98:MSE:N	2.45	0.41
1:C:142:GLN:O	1:C:146:LYS:HG2	2.21	0.41
1:D:232:LYS:HE2	1:D:232:LYS:HB3	1.80	0.41
1:D:296:LYS:O	1:D:297:LYS:C	2.62	0.41
1:B:298:ASN:OD1	1:B:299:SER:N	2.54	0.40
1:C:72:HIS:ND1	1:C:75:SER:CB	2.85	0.40
1:A:47:GLU:OE2	1:A:120:PHE:CD1	2.69	0.40
1:C:61:ARG:HH11	1:C:61:ARG:CB	2.35	0.40
1:C:149:THR:HG22	1:C:150:ILE:N	2.35	0.40
1:D:231:GLN:HG2	1:D:232:LYS:C	2.46	0.40
1:C:138:LYS:O	1:C:139:PHE:C	2.64	0.40
1:B:148:GLN:HG2	5:B:351:HOH:O	2.19	0.40
1:C:48:VAL:CG1	1:C:49:LYS:CG	2.96	0.40
1:D:46:PHE:HD1	1:D:104:MSE:HE1	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:CD2	1:A:46:PHE:C	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	275/316 (87%)	264 (96%)	10 (4%)	1 (0%)	30	34
1	B	264/316 (84%)	247 (94%)	14 (5%)	3 (1%)	11	11
1	C	269/316 (85%)	244 (91%)	17 (6%)	8 (3%)	3	2
1	D	278/316 (88%)	261 (94%)	14 (5%)	3 (1%)	11	11
All	All	1086/1264 (86%)	1016 (94%)	55 (5%)	15 (1%)	9	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	GLN
1	C	49	LYS
1	C	51	ASP
1	C	55	PRO
1	C	56	ILE
1	C	107	VAL
1	C	207	ASP
1	A	233	GLY
1	C	174	SER
1	C	284	SER
1	D	44	GLU
1	D	231	GLN
1	D	258	ASP
1	B	60	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	122	GLU

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	250/269 (93%)	222 (89%)	28 (11%)	6	5
1	B	245/269 (91%)	212 (86%)	33 (14%)	4	3
1	C	247/269 (92%)	216 (87%)	31 (13%)	4	4
1	D	253/269 (94%)	221 (87%)	32 (13%)	4	4
All	All	995/1076 (92%)	871 (88%)	124 (12%)	4	4

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	54	GLU
1	A	58	GLU
1	A	61	ARG
1	A	98	MSE
1	A	121	ARG
1	A	138	LYS
1	A	149	THR
1	A	172	LYS
1	A	175	VAL
1	A	186	LEU
1	A	204	LEU
1	A	217	LYS
1	A	220	MSE
1	A	223	GLU
1	A	228	GLU
1	A	229	LEU
1	A	231	GLN
1	A	232	LYS
1	A	235	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	253	LEU
1	A	262	THR
1	A	271	VAL
1	A	278	LEU
1	A	291	THR
1	A	292	SER
1	A	308	LEU
1	A	310	GLN
1	B	51	ASP
1	B	53	LEU
1	B	57	MSE
1	B	58	GLU
1	B	67	VAL
1	B	88	VAL
1	B	98	MSE
1	B	102	ILE
1	B	109	CYS
1	B	121	ARG
1	B	134	THR
1	B	140	TYR
1	B	148	GLN
1	B	167	GLU
1	B	172	LYS
1	B	179	ASP
1	B	186	LEU
1	B	204	LEU
1	B	207	ASP
1	B	217	LYS
1	B	220	MSE
1	B	223	GLU
1	B	224	ARG
1	B	229	LEU
1	B	230	ASN
1	B	231	GLN
1	B	232	LYS
1	B	262	THR
1	B	271	VAL
1	B	298	ASN
1	B	308	LEU
1	B	318	GLU
1	B	329	LYS
1	C	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	56	ILE
1	C	57	MSE
1	C	58	GLU
1	C	61	ARG
1	C	69	LYS
1	C	77	GLN
1	C	91	GLN
1	C	95	ARG
1	C	98	MSE
1	C	109	CYS
1	C	119	LEU
1	C	134	THR
1	C	148	GLN
1	C	149	THR
1	C	179	ASP
1	C	186	LEU
1	C	195	MSE
1	C	204	LEU
1	C	217	LYS
1	C	224	ARG
1	C	229	LEU
1	C	259	SER
1	C	269	GLN
1	C	271	VAL
1	C	281	ASP
1	C	284	SER
1	C	291	THR
1	C	300	LYS
1	C	310	GLN
1	C	319	SER
1	D	57	MSE
1	D	58	GLU
1	D	59	LEU
1	D	61	ARG
1	D	78	ILE
1	D	102	ILE
1	D	105	ARG
1	D	109	CYS
1	D	121	ARG
1	D	131	LEU
1	D	146	LYS
1	D	149	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	182	PRO
1	D	186	LEU
1	D	204	LEU
1	D	207	ASP
1	D	217	LYS
1	D	220	MSE
1	D	223	GLU
1	D	229	LEU
1	D	231	GLN
1	D	232	LYS
1	D	246	THR
1	D	248	ILE
1	D	259	SER
1	D	262	THR
1	D	271	VAL
1	D	278	LEU
1	D	308	LEU
1	D	319	SER
1	D	329	LYS
1	D	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	77	GLN
1	A	93	GLN
1	A	142	GLN
1	A	170	HIS
1	A	177	HIS
1	A	184	ASN
1	A	230	ASN
1	A	265	GLN
1	B	72	HIS
1	B	93	GLN
1	B	142	GLN
1	B	184	ASN
1	B	265	GLN
1	B	269	GLN
1	B	277	GLN
1	C	77	GLN
1	C	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	170	HIS
1	C	177	HIS
1	C	184	ASN
1	C	269	GLN
1	C	298	ASN
1	D	72	HIS
1	D	91	GLN
1	D	93	GLN
1	D	184	ASN
1	D	265	GLN
1	D	269	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	SO4	C	3	-	4,4,4	0.31	0	6,6,6	0.22	0
2	SO4	B	4	-	4,4,4	0.41	0	6,6,6	0.33	0
3	GOL	A	1	-	5,5,5	0.50	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	1	-	4,4,4	0.37	0	6,6,6	1.11	0
2	SO4	A	2	-	4,4,4	0.24	0	6,6,6	0.80	0
4	EDO	B	1	-	3,3,3	0.48	0	2,2,2	0.88	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
4	EDO	B	1	-	-	0/1/1/1	-
3	GOL	A	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	GOL	C1-C2-C3-O3
3	A	1	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	SO4	1	0
2	B	4	SO4	5	0
3	A	1	GOL	7	0
2	A	2	SO4	1	0
4	B	1	EDO	7	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	268/316 (84%)	0.52	13 (4%) 35 41	47, 56, 67, 73	0
1	B	260/316 (82%)	1.20	46 (17%) 4 4	23, 56, 69, 79	4 (1%)
1	C	264/316 (83%)	0.69	26 (9%) 13 15	42, 57, 68, 76	1 (0%)
1	D	270/316 (85%)	0.50	8 (2%) 52 59	44, 57, 65, 79	0
All	All	1062/1264 (84%)	0.73	93 (8%) 15 18	23, 57, 68, 79	5 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	LEU	8.0
1	C	62	GLY	5.7
1	C	260	TRP	5.5
1	C	208	VAL	5.1
1	B	90	SER	4.7
1	D	229	LEU	4.6
1	B	143	VAL	4.4
1	B	150	ILE	4.0
1	A	207	ASP	3.9
1	B	229	LEU	3.9
1	B	208	VAL	3.8
1	B	205	VAL	3.8
1	B	105	ARG	3.5
1	B	147	GLY	3.5
1	D	45	ASN	3.5
1	B	101	ASP	3.4
1	C	59	LEU	3.4
1	B	260	TRP	3.3
1	B	106	THR	3.3
1	C	333	ALA	3.3
1	C	60	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	ASP	3.2
1	B	49	LYS	3.2
1	B	117	GLY	3.1
1	C	230	ASN	3.1
1	C	108	ASP	3.1
1	A	143	VAL	3.0
1	D	231	GLN	2.9
1	B	298	ASN	2.9
1	C	235	SER	2.9
1	A	74	PRO	2.9
1	B	169	LEU	2.8
1	B	88	VAL	2.8
1	B	175	VAL	2.8
1	B	86	ALA	2.8
1	C	175	VAL	2.8
1	C	97	LEU	2.8
1	A	330	LEU	2.8
1	D	333	ALA	2.8
1	B	116	TYR	2.7
1	B	328	VAL	2.7
1	B	171	SER	2.7
1	A	231	GLN	2.7
1	B	107	VAL	2.7
1	B	77	GLN	2.6
1	A	73	VAL	2.6
1	B	230	ASN	2.6
1	C	102	ILE	2.6
1	C	50	ALA	2.6
1	C	48	VAL	2.6
1	A	259	SER	2.6
1	C	171	SER	2.6
1	C	259	SER	2.6
1	C	143	VAL	2.5
1	D	74	PRO	2.5
1	B	149	THR	2.5
1	B	60	GLY	2.5
1	B	183	SER	2.4
1	C	176	ILE	2.4
1	A	260	TRP	2.4
1	B	140	TYR	2.4
1	C	105	ARG	2.4
1	B	235	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	331	ILE	2.4
1	A	229	LEU	2.4
1	A	140	TYR	2.3
1	B	206	ASP	2.3
1	B	137	ASP	2.3
1	B	146	LYS	2.3
1	B	232	LYS	2.3
1	B	332	LEU	2.3
1	D	59	LEU	2.3
1	B	62	GLY	2.3
1	B	110	PRO	2.2
1	B	97	LEU	2.2
1	D	207	ASP	2.2
1	A	217	LYS	2.2
1	B	173	LEU	2.2
1	B	231	GLN	2.2
1	C	150	ILE	2.2
1	C	93	GLN	2.2
1	C	231	GLN	2.2
1	C	153	ASP	2.1
1	B	72	HIS	2.1
1	A	61	ARG	2.1
1	B	141	LYS	2.1
1	A	141	LYS	2.1
1	C	258	ASP	2.1
1	C	147	GLY	2.1
1	B	138	LYS	2.0
1	D	258	ASP	2.0
1	B	217	LYS	2.0
1	C	49	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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
2	SO4	B	4	5/5	0.57	0.15	125,125,126,127	0
3	GOL	A	1	6/6	0.73	0.20	66,73,75,75	0
4	EDO	B	1	4/4	0.86	0.41	49,49,54,56	0
2	SO4	D	1	5/5	0.91	0.15	72,73,74,74	0
2	SO4	C	3	5/5	0.92	0.23	97,97,99,99	0
2	SO4	A	2	5/5	0.96	0.14	64,66,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.