



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:44 PM UTC

PDB ID : 2VAK / pdb_00002vak
Title : Crystal structure of the avian reovirus inner capsid protein sigmaA
Authors : Guardado-Calvo, P.; Llamas-Saiz, A.L.; Fox, G.C.; Hermo-Parrado, X.L.;
Vazquez-Iglesias, L.; Martinez-Costas, J.; Benavente, J.; van Raaij, M.J.
Deposited on : 2007-09-01
Resolution : 2.34 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

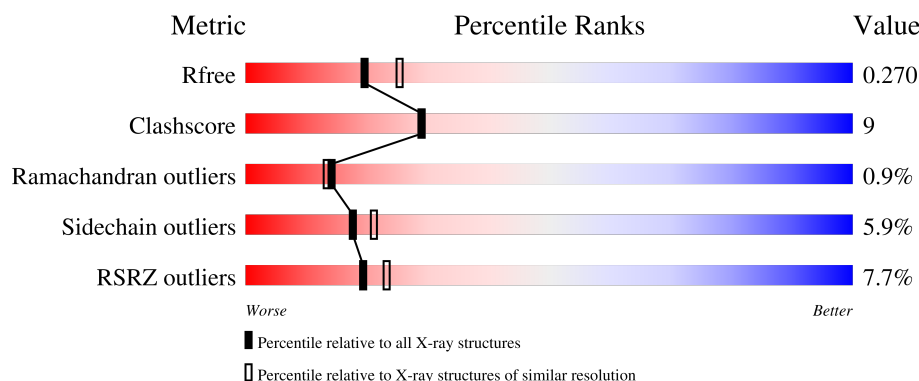
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	423	4% 80% 15% ..
1	B	423	19% 75% 17% ..
1	C	423	8% 73% 20% ..
1	D	423	25% 73% 22% ..
1	E	423	8% 77% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	

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	H	1427	-	-	X	-
2	SO4	J	1427	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41224 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 SIGMA A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			
1	B	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	C	404	Total	C	N	O	S	0	0	0
			3154	1995	553	588	18			
1	D	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	E	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	F	404	Total	C	N	O	S	0	0	0
			3154	1995	553	588	18			
1	G	403	Total	C	N	O	S	0	0	0
			3147	1991	552	586	18			
1	H	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	I	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			
1	J	404	Total	C	N	O	S	0	0	0
			3154	1995	553	588	18			
1	K	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			
1	L	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			

- 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		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

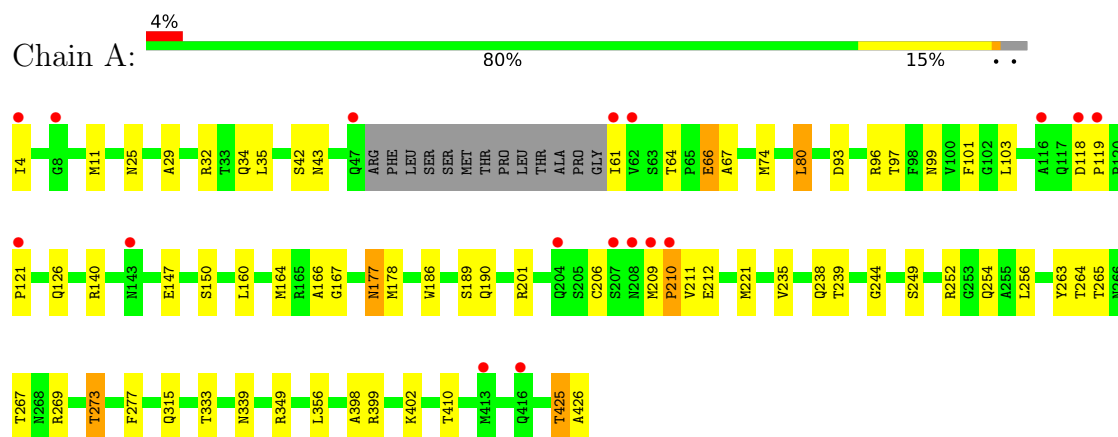
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	262	Total 262	O 262	0	0
3	B	180	Total 180	O 180	0	0
3	C	186	Total 186	O 186	0	0
3	D	160	Total 160	O 160	0	0
3	E	223	Total 223	O 223	0	0
3	F	314	Total 314	O 314	0	0
3	G	305	Total 305	O 305	0	0
3	H	272	Total 272	O 272	0	0
3	I	226	Total 226	O 226	0	0
3	J	247	Total 247	O 247	0	0
3	K	301	Total 301	O 301	0	0
3	L	327	Total 327	O 327	0	0

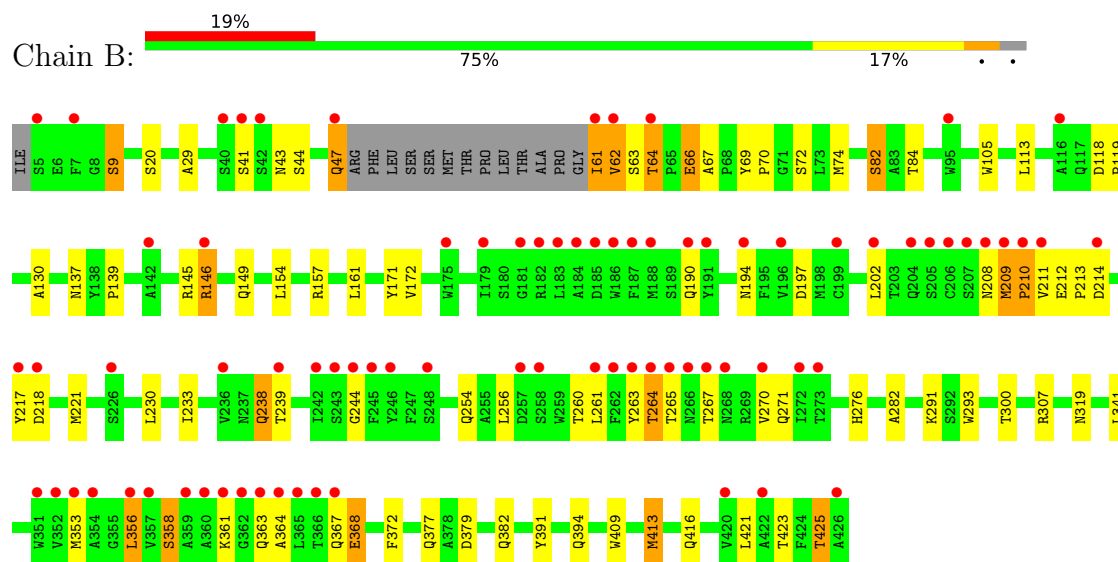
3 Residue-property plots [i](#)

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

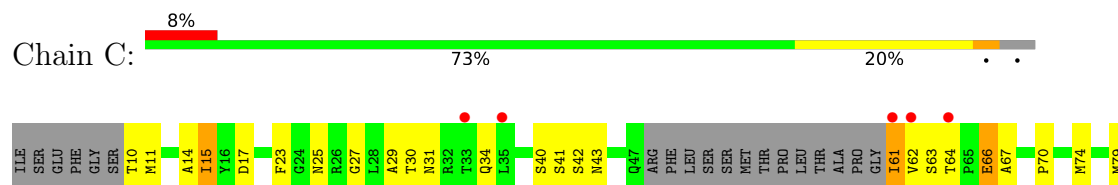
• Molecule 1: SIGMA A

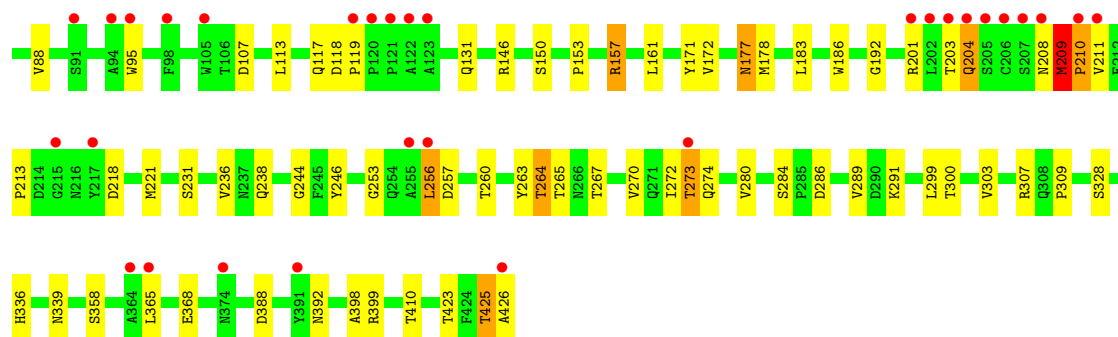


• Molecule 1: SIGMA A

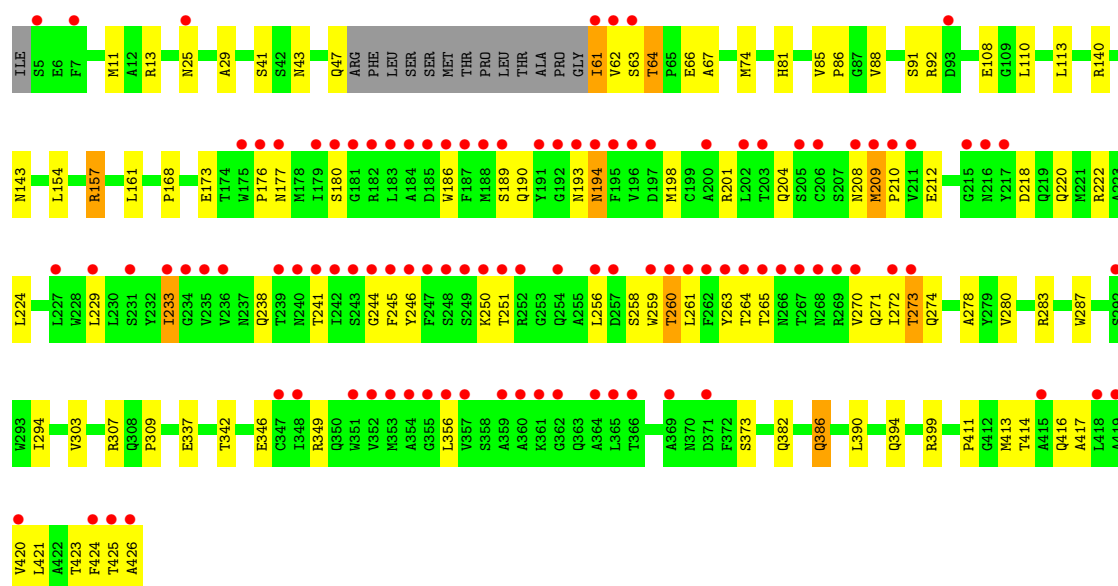


• Molecule 1: SIGMA A

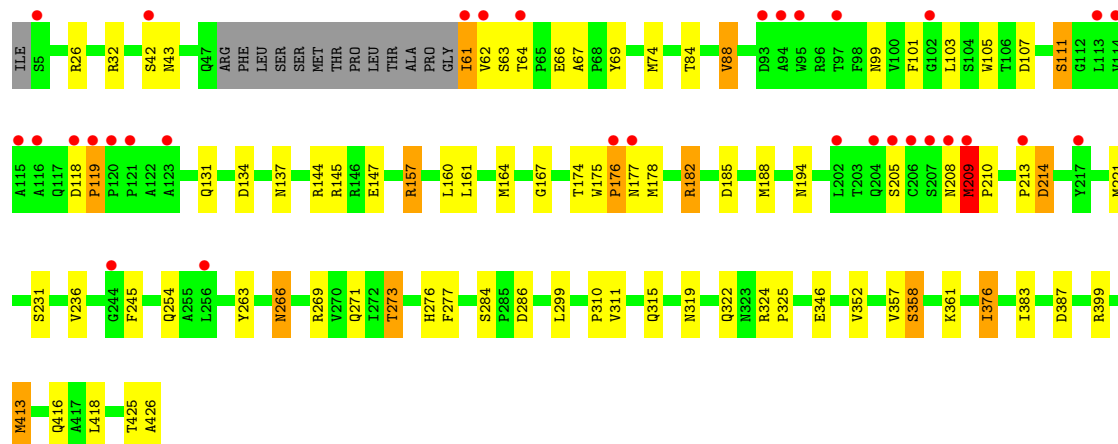
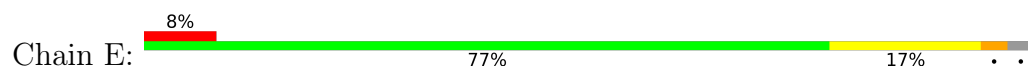




• Molecule 1: SIGMA A

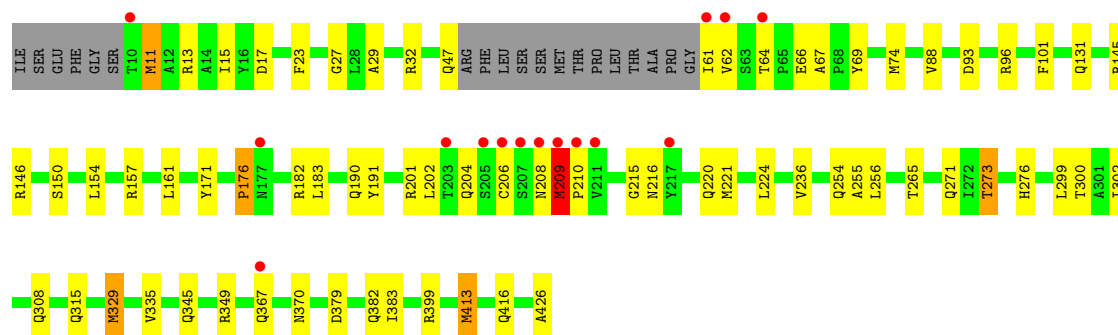


• Molecule 1: SIGMA A



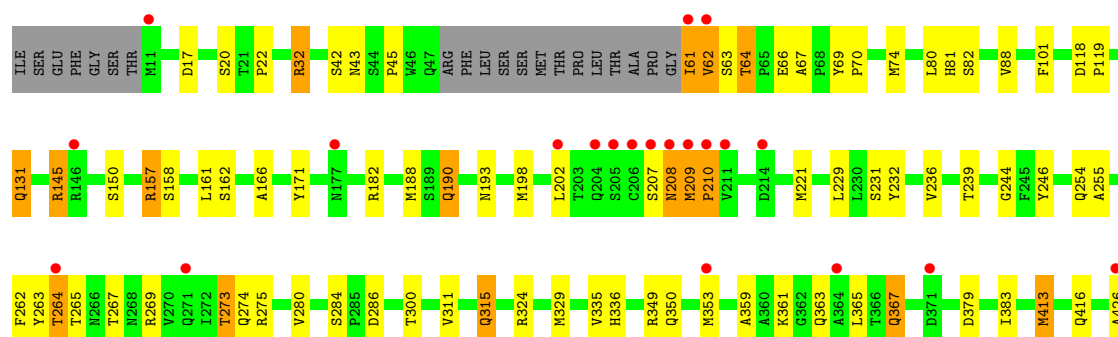
• Molecule 1: SIGMA A

Chain F:  4% 79% 15%



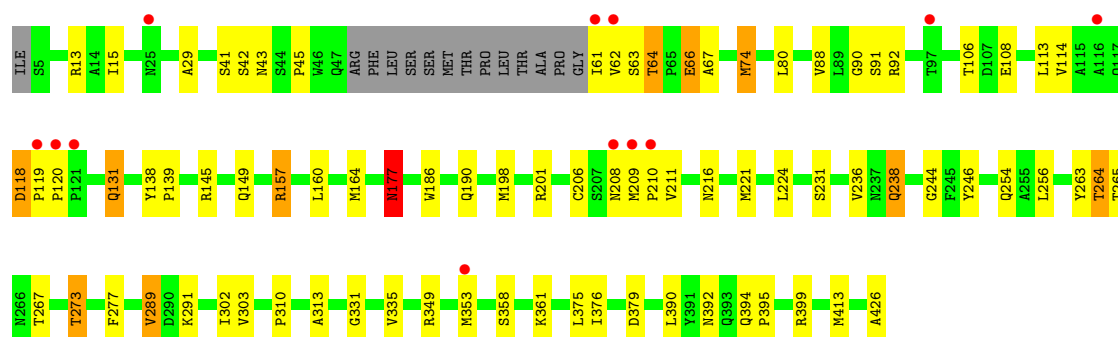
• Molecule 1: SIGMA A

Chain G:  5% 75% 16% 5%



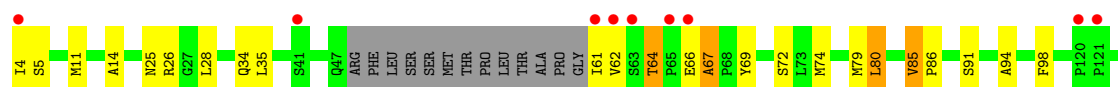
• Molecule 1: SIGMA A

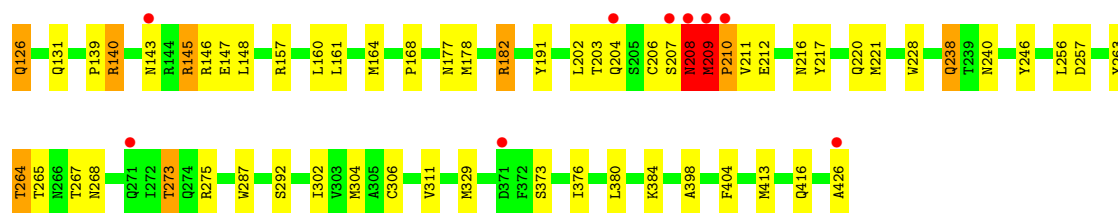
Chain H:  3% 77% 17%



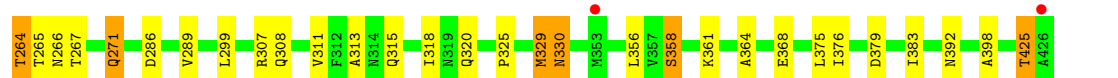
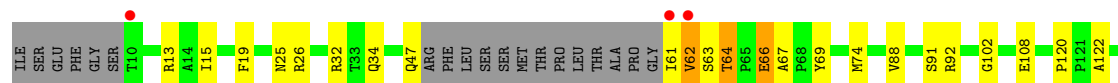
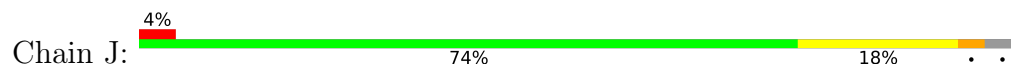
• Molecule 1: SIGMA A

Chain I:  4% 77% 17%

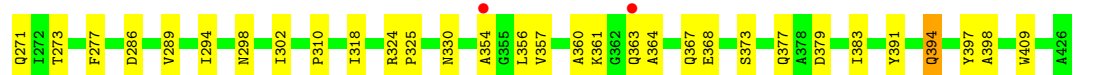
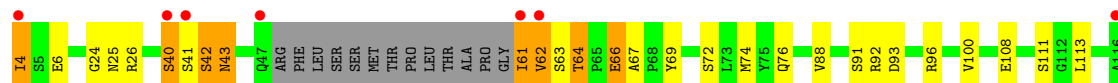
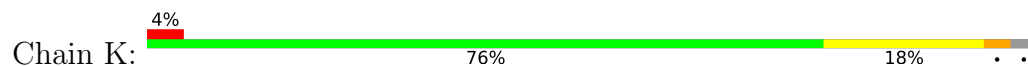




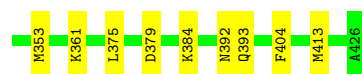
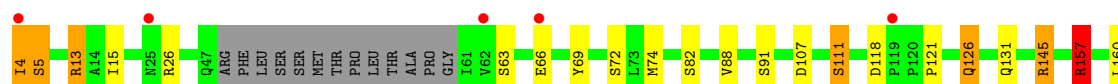
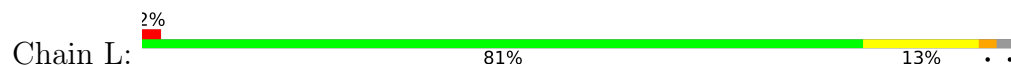
• Molecule 1: SIGMA A



• Molecule 1: SIGMA A



• Molecule 1: SIGMA A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.21Å 129.91Å 144.04Å 93.81° 105.05° 98.16°	Depositor
Resolution (Å)	29.85 – 2.34 29.85 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.85-2.34) 94.0 (29.85-2.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.3.0027	Depositor
R, R_{free}	0.210 , 0.271 0.211 , 0.270	Depositor DCC
R_{free} test set	1383 reflections (0.46%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtrriage
Anisotropy	0.422	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41224	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4877e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.87	0/3282	0.97	5/4478 (0.1%)
1	B	0.81	0/3274	0.95	1/4467 (0.0%)
1	C	0.83	0/3237	0.98	4/4418 (0.1%)
1	D	0.82	1/3274 (0.0%)	0.93	0/4467
1	E	0.86	0/3274	1.00	9/4467 (0.2%)
1	F	0.93	2/3237 (0.1%)	1.02	3/4418 (0.1%)
1	G	0.98	2/3230 (0.1%)	1.02	0/4408
1	H	0.90	1/3274 (0.0%)	1.00	4/4467 (0.1%)
1	I	0.85	0/3282	0.93	6/4478 (0.1%)
1	J	0.86	0/3237	0.96	1/4418 (0.0%)
1	K	0.87	3/3282 (0.1%)	0.98	4/4478 (0.1%)
1	L	0.98	0/3282	1.04	2/4478 (0.0%)
All	All	0.88	9/39165 (0.0%)	0.98	39/53442 (0.1%)

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
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	2
All	All	0	12

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	335	VAL	CA-CB	6.50	1.62	1.53
1	F	335	VAL	CA-CB	5.77	1.60	1.53
1	K	318	ILE	CA-CB	5.74	1.60	1.54
1	K	100	VAL	CA-CB	5.50	1.62	1.54
1	F	236	VAL	CA-CB	5.29	1.60	1.54
1	H	335	VAL	CA-CB	5.17	1.59	1.53
1	D	309	PRO	CA-C	5.15	1.56	1.52
1	K	398	ALA	CA-CB	-5.08	1.46	1.53
1	G	166	ALA	N-CA	-5.01	1.43	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	215	GLY	N-CA-C	-8.10	101.39	112.25
1	L	91	SER	N-CA-C	6.99	118.76	108.14
1	L	157	ARG	N-CA-C	6.68	119.40	111.71
1	J	25	ASN	N-CA-C	6.56	120.14	111.75
1	K	62	VAL	N-CA-C	-6.42	96.00	109.34
1	C	63	SER	N-CA-C	6.29	118.83	110.53
1	A	167	GLY	CA-C-N	6.02	125.78	119.76
1	A	167	GLY	C-N-CA	6.02	125.78	119.76
1	H	91	SER	N-CA-C	5.94	117.29	107.73
1	E	175	TRP	CA-C-N	5.90	127.22	119.84
1	E	175	TRP	C-N-CA	5.90	127.22	119.84
1	I	91	SER	N-CA-C	5.88	117.20	107.73
1	E	119	PRO	CA-C-N	5.72	126.28	120.38
1	E	119	PRO	C-N-CA	5.72	126.28	120.38
1	B	319	ASN	N-CA-C	5.71	118.25	111.33
1	E	167	GLY	CA-C-N	5.68	125.59	119.85
1	E	167	GLY	C-N-CA	5.68	125.59	119.85
1	C	25	ASN	N-CA-C	5.59	118.91	111.75
1	A	25	ASN	N-CA-C	5.48	118.01	111.71
1	A	178	MET	N-CA-C	5.46	117.23	111.28
1	F	176	PRO	CA-C-N	-5.41	115.11	123.17
1	F	176	PRO	C-N-CA	-5.41	115.11	123.17
1	K	373	SER	N-CA-C	5.39	116.84	111.07
1	E	176	PRO	N-CA-C	5.21	123.21	112.47
1	H	216	ASN	N-CA-C	5.19	116.63	111.07
1	I	67	ALA	CA-C-N	5.18	124.98	119.28
1	I	67	ALA	C-N-CA	5.18	124.98	119.28
1	I	304	MET	N-CA-C	5.15	117.63	111.71
1	E	209	MET	CA-C-N	-5.12	113.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	MET	C-N-CA	-5.12	113.44	119.84
1	C	67	ALA	CA-C-N	5.11	124.72	119.56
1	C	67	ALA	C-N-CA	5.11	124.72	119.56
1	K	379	ASP	N-CA-C	5.11	116.53	111.07
1	K	91	SER	N-CA-C	5.08	115.92	107.73
1	I	85	VAL	CA-C-N	-5.03	113.64	119.47
1	I	85	VAL	C-N-CA	-5.03	113.64	119.47
1	H	90	GLY	N-CA-C	5.02	120.41	113.99
1	H	177	ASN	CB-CA-C	5.02	120.41	110.42
1	A	252	ARG	N-CA-C	5.00	116.45	107.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	209	MET	Peptide
1	D	208	ASN	Peptide
1	D	209	MET	Peptide
1	D	61	ILE	Peptide
1	E	209	MET	Peptide
1	F	209	MET	Peptide
1	G	208	ASN	Peptide
1	I	209	MET	Peptide
1	J	209	MET	Peptide
1	K	209	MET	Peptide
1	L	209	MET	Peptide
1	L	63	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	0	3093	34	0
1	B	3190	0	3082	62	0
1	C	3154	0	3054	71	0
1	D	3190	0	3082	57	0
1	E	3190	0	3082	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3154	0	3054	39	0
1	G	3147	0	3047	59	0
1	H	3190	0	3082	68	0
1	I	3198	0	3093	63	0
1	J	3154	0	3054	70	0
1	K	3198	0	3093	61	0
1	L	3198	0	3093	37	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	5	0	0	1	0
2	H	5	0	0	2	0
2	I	5	0	0	0	0
2	J	5	0	0	3	0
2	K	5	0	0	0	0
2	L	5	0	0	1	0
3	A	262	0	0	3	0
3	B	180	0	0	6	0
3	C	186	0	0	10	0
3	D	160	0	0	5	0
3	E	223	0	0	6	0
3	F	314	0	0	5	0
3	G	305	0	0	7	0
3	H	272	0	0	4	0
3	I	226	0	0	4	0
3	J	247	0	0	9	0
3	K	301	0	0	15	0
3	L	327	0	0	10	0
All	All	41224	0	36909	653	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 9.

All (653) 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:H:264:THR:HG21	1:H:267:THR:OG1	1.50	1.10
1:K:157:ARG:HG2	1:K:157:ARG:HH11	1.11	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ARG:HH11	1:G:157:ARG:HG2	1.19	1.07
1:B:64:THR:HG22	1:B:67:ALA:H	1.20	1.07
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.12	1.06
1:I:140:ARG:HH11	1:I:140:ARG:HG2	1.06	1.06
1:L:264:THR:HG21	1:L:267:THR:OG1	1.56	1.05
1:H:209:MET:HB2	1:H:211:VAL:HG23	1.40	1.02
1:H:43:ASN:HB3	1:H:113:LEU:O	1.60	1.02
1:B:74:MET:HE3	1:B:157:ARG:HD3	1.41	0.99
1:E:157:ARG:HG2	1:E:157:ARG:HH11	1.27	0.98
1:J:64:THR:HG22	1:J:67:ALA:H	1.24	0.98
1:B:44:SER:HB3	1:B:47:GLN:OE1	1.67	0.95
1:I:140:ARG:HH11	1:I:140:ARG:CG	1.79	0.95
1:K:264:THR:HG21	1:K:267:THR:OG1	1.64	0.95
1:H:221:MET:CE	1:H:303:VAL:HG23	1.98	0.94
1:A:64:THR:HG23	1:A:67:ALA:H	1.31	0.94
1:H:221:MET:HE2	1:H:303:VAL:HG23	1.49	0.93
1:H:64:THR:HG22	1:H:67:ALA:H	1.33	0.93
1:A:425:THR:HG21	3:A:2160:HOH:O	1.68	0.93
1:J:311:VAL:HG11	1:J:329:MET:HE3	1.49	0.92
1:L:177:ASN:HB2	3:L:2146:HOH:O	1.71	0.91
1:I:146:ARG:HH21	1:I:210:PRO:CD	1.83	0.90
1:D:157:ARG:HG2	1:D:157:ARG:HH11	1.34	0.90
1:C:15:ILE:HD13	1:J:325:PRO:HB2	1.53	0.89
1:J:92:ARG:HD3	1:J:108:GLU:OE2	1.73	0.88
1:H:390:LEU:CD1	1:I:11:MET:HE1	2.04	0.88
1:H:157:ARG:HG2	1:H:157:ARG:HH11	1.37	0.87
1:K:157:ARG:HG2	1:K:157:ARG:NH1	1.88	0.87
1:C:221:MET:HE2	1:C:299:LEU:HD22	1.57	0.87
1:D:270:VAL:HG13	1:D:425:THR:HG23	1.57	0.85
1:E:64:THR:HG23	1:E:67:ALA:H	1.41	0.85
1:J:188:MET:HE1	1:J:263:TYR:CD2	2.13	0.84
1:I:4:ILE:HA	3:I:2155:HOH:O	1.77	0.84
1:G:64:THR:HG22	1:G:67:ALA:H	1.43	0.83
1:K:64:THR:HG22	1:K:67:ALA:H	1.43	0.83
1:C:157:ARG:HG2	1:C:157:ARG:NH1	1.87	0.83
1:B:264:THR:HB	1:B:267:THR:CG2	2.08	0.82
1:I:140:ARG:NH1	1:I:147:GLU:OE1	2.11	0.82
1:I:264:THR:HG21	1:I:267:THR:OG1	1.80	0.82
1:B:209:MET:C	1:B:211:VAL:H	1.86	0.82
1:I:146:ARG:HH21	1:I:210:PRO:HD3	1.42	0.82
1:K:43:ASN:HB3	1:K:113:LEU:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210:PRO:HD3	3:K:2126:HOH:O	1.80	0.81
1:I:140:ARG:HG2	1:I:140:ARG:NH1	1.88	0.81
1:C:218:ASP:OD1	1:C:307:ARG:NH2	2.14	0.81
1:D:382:GLN:O	1:D:386:GLN:HG2	1.80	0.81
1:I:64:THR:HG22	1:I:67:ALA:H	1.44	0.81
1:D:413:MET:HG3	1:D:416:GLN:NE2	1.96	0.81
1:A:118:ASP:HA	1:A:119:PRO:C	2.05	0.80
1:C:118:ASP:HA	1:C:119:PRO:C	2.07	0.80
1:D:61:ILE:C	1:D:63:SER:H	1.89	0.80
1:A:273:THR:HB	1:A:426:ALA:OXT	1.83	0.79
1:H:221:MET:HE2	1:H:303:VAL:CG2	2.12	0.79
1:B:413:MET:HG3	1:B:416:GLN:NE2	1.98	0.78
1:G:413:MET:HG3	1:G:416:GLN:NE2	1.98	0.78
1:B:64:THR:HG22	1:B:67:ALA:N	1.97	0.78
1:E:221:MET:HE2	1:E:299:LEU:HD22	1.65	0.78
1:J:64:THR:HG22	1:J:67:ALA:N	1.99	0.77
1:H:186:TRP:CZ2	1:H:190:GLN:NE2	2.53	0.77
1:J:264:THR:HG21	1:J:267:THR:OG1	1.85	0.77
1:J:157:ARG:HG2	1:J:157:ARG:HH11	1.50	0.77
1:K:92:ARG:HG2	1:K:108:GLU:OE2	1.87	0.75
1:E:118:ASP:HB2	3:E:2069:HOH:O	1.87	0.74
1:D:303:VAL:HG13	1:D:307:ARG:HH21	1.51	0.74
1:G:315:GLN:HB3	2:G:1427:SO4:O1	1.88	0.73
1:G:244:GLY:HA3	1:G:263:TYR:CE1	2.23	0.73
1:F:146:ARG:HH21	1:F:210:PRO:HD3	1.52	0.73
1:L:157:ARG:HB3	1:L:301:ALA:HB2	1.71	0.73
1:J:358:SER:HB2	1:J:361:LYS:H	1.54	0.72
1:B:271:GLN:HG2	3:B:2106:HOH:O	1.87	0.72
1:D:271:GLN:O	1:D:426:ALA:HB2	1.88	0.72
1:J:364:ALA:O	1:J:368:GLU:HG3	1.90	0.72
1:G:157:ARG:HG2	1:G:157:ARG:NH1	1.96	0.72
1:K:74:MET:HG3	3:K:2064:HOH:O	1.88	0.72
1:H:375:LEU:HD21	3:I:2001:HOH:O	1.90	0.72
1:J:64:THR:HG21	3:J:2015:HOH:O	1.91	0.71
1:J:130:ALA:HB1	1:J:320:GLN:HG3	1.72	0.71
1:E:131:GLN:HG2	3:E:2080:HOH:O	1.91	0.70
1:A:210:PRO:HD2	3:A:2143:HOH:O	1.89	0.70
1:I:74:MET:HE3	1:I:157:ARG:HD3	1.72	0.70
1:B:208:ASN:C	1:B:210:PRO:HD2	2.15	0.70
1:I:146:ARG:HH21	1:I:210:PRO:HD2	1.55	0.70
1:C:61:ILE:HG22	1:C:62:VAL:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:THR:HG22	1:H:67:ALA:N	2.06	0.70
1:B:264:THR:HB	1:B:267:THR:HG22	1.73	0.70
1:C:10:THR:CG2	1:C:213:PRO:HB2	2.22	0.69
1:E:273:THR:HB	1:E:426:ALA:OXT	1.91	0.69
1:F:64:THR:HG23	1:F:67:ALA:H	1.56	0.69
1:C:40:SER:C	1:C:42:SER:H	2.00	0.69
1:H:390:LEU:HD13	1:I:11:MET:HE1	1.74	0.69
1:G:190:GLN:HG3	1:G:193:ASN:OD1	1.92	0.69
1:J:218:ASP:OD1	1:J:307:ARG:NH2	2.26	0.69
1:D:92:ARG:HB2	1:D:108:GLU:OE2	1.92	0.68
1:K:64:THR:HG22	1:K:67:ALA:N	2.08	0.68
1:C:218:ASP:CG	1:C:307:ARG:HH22	2.01	0.68
1:G:64:THR:HG22	1:G:67:ALA:N	2.08	0.68
1:J:137:ASN:O	1:J:139:PRO:HD3	1.93	0.68
1:J:218:ASP:CG	1:J:307:ARG:HH22	2.02	0.68
1:D:423:THR:C	1:D:425:THR:H	2.02	0.68
1:L:209:MET:O	1:L:211:VAL:HG23	1.94	0.67
1:E:263:TYR:OH	1:E:269:ARG:NH2	2.26	0.67
1:H:394:GLN:HG3	1:I:14:ALA:HB1	1.76	0.67
1:G:74:MET:HG3	3:G:2055:HOH:O	1.93	0.67
1:A:209:MET:O	1:A:211:VAL:HG23	1.95	0.67
1:G:64:THR:HG21	3:G:2013:HOH:O	1.95	0.67
1:E:64:THR:CG2	1:E:67:ALA:H	2.07	0.67
1:L:180:SER:HB3	3:L:2146:HOH:O	1.95	0.67
1:B:276:HIS:ND1	3:B:2109:HOH:O	2.29	0.66
1:K:64:THR:HG21	3:K:2023:HOH:O	1.95	0.66
1:C:66:GLU:H	1:C:66:GLU:CD	2.04	0.66
1:B:61:ILE:HD12	1:B:291:LYS:HE3	1.78	0.66
1:G:284:SER:OG	1:G:286:ASP:OD1	2.12	0.65
1:H:264:THR:CG2	1:H:267:THR:H	2.09	0.65
1:I:207:SER:O	1:I:208:ASN:HB3	1.96	0.65
1:I:238:GLN:HG3	1:I:246:TYR:OH	1.96	0.65
1:G:145:ARG:CG	1:G:145:ARG:HH11	2.09	0.65
1:B:209:MET:O	1:B:211:VAL:N	2.28	0.65
1:I:202:LEU:HD13	1:I:221:MET:HG2	1.78	0.65
1:C:61:ILE:HD13	1:C:70:PRO:HD3	1.77	0.65
1:H:206:CYS:O	1:H:209:MET:HB3	1.95	0.65
1:J:64:THR:CG2	1:J:67:ALA:H	2.06	0.65
1:H:64:THR:HG21	3:H:2026:HOH:O	1.96	0.64
1:G:273:THR:HB	1:G:426:ALA:OXT	1.96	0.64
1:E:157:ARG:HG2	1:E:157:ARG:NH1	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ASP:HA	1:H:119:PRO:C	2.23	0.64
1:C:10:THR:HG21	1:C:213:PRO:HB2	1.78	0.64
1:F:221:MET:HE2	1:F:299:LEU:HD22	1.80	0.64
1:D:193:ASN:O	1:D:260:THR:HA	1.97	0.64
1:C:256:LEU:HG	3:C:2111:HOH:O	1.97	0.64
1:D:198:MET:HA	1:D:201:ARG:HH12	1.62	0.64
1:K:330:ASN:HB3	3:K:2226:HOH:O	1.97	0.63
1:D:157:ARG:HG2	1:D:157:ARG:NH1	2.10	0.63
1:K:209:MET:HB2	3:K:2063:HOH:O	1.98	0.63
1:E:188:MET:HE2	1:E:245:PHE:CZ	2.33	0.63
1:I:140:ARG:HH12	1:I:147:GLU:CD	2.07	0.62
1:B:190:GLN:O	1:B:261:LEU:HD23	1.99	0.62
1:H:221:MET:HE1	1:H:302:ILE:HB	1.81	0.62
1:H:145:ARG:O	1:H:149:GLN:HG3	1.98	0.62
1:H:61:ILE:N	1:H:291:LYS:HZ3	1.98	0.62
1:C:192:GLY:O	1:C:260:THR:HG23	1.99	0.62
1:D:61:ILE:HG22	1:D:61:ILE:O	2.00	0.61
1:G:275:ARG:HG3	1:G:275:ARG:HH11	1.65	0.61
1:K:394:GLN:HB2	3:K:2275:HOH:O	2.00	0.61
1:A:264:THR:HG21	1:A:267:THR:OG1	2.00	0.61
1:H:221:MET:HE3	1:H:303:VAL:HG23	1.80	0.61
1:J:209:MET:H	1:J:210:PRO:HD3	1.66	0.61
1:A:150:SER:HA	1:A:209:MET:HG3	1.83	0.61
1:G:274:GLN:HB2	3:G:2203:HOH:O	2.01	0.61
1:C:153:PRO:HG2	1:C:209:MET:HE3	1.83	0.61
1:A:209:MET:O	1:A:210:PRO:C	2.44	0.61
1:F:254:GLN:HG2	1:F:255:ALA:N	2.16	0.61
1:H:42:SER:O	1:H:43:ASN:HB2	2.00	0.61
1:H:210:PRO:HG2	3:H:2142:HOH:O	2.01	0.61
1:H:273:THR:HB	1:H:426:ALA:OXT	2.01	0.61
1:L:311:VAL:HG12	1:L:329:MET:HG2	1.83	0.61
1:K:26:ARG:HD2	3:K:2031:HOH:O	1.99	0.61
1:K:69:TYR:HE1	1:K:383:ILE:CD1	2.14	0.61
1:E:69:TYR:HE1	1:E:383:ILE:HD12	1.66	0.60
1:F:413:MET:HG3	1:F:416:GLN:CD	2.26	0.60
1:E:188:MET:HE2	1:E:245:PHE:HZ	1.67	0.60
1:D:271:GLN:HA	3:D:2102:HOH:O	2.02	0.60
1:D:198:MET:HA	1:D:201:ARG:NH1	2.17	0.60
1:K:190:GLN:O	1:K:193:ASN:HB2	2.02	0.59
1:F:224:LEU:HD23	1:F:299:LEU:HD11	1.84	0.59
1:H:157:ARG:HG2	1:H:157:ARG:NH1	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:130:ALA:CB	1:J:320:GLN:HG3	2.32	0.59
1:K:40:SER:O	1:K:43:ASN:N	2.30	0.59
1:L:107:ASP:OD2	1:L:111:SER:HB2	2.02	0.59
1:J:392:ASN:HB2	3:J:2215:HOH:O	2.03	0.59
1:D:411:PRO:O	1:D:414:THR:OG1	2.15	0.59
1:C:14:ALA:HB1	1:J:308:GLN:HG2	1.85	0.59
1:D:190:GLN:OE1	1:D:198:MET:HG2	2.02	0.59
1:J:214:ASP:HB3	1:J:222:ARG:NH2	2.18	0.59
1:F:190:GLN:OE1	1:F:201:ARG:NH1	2.36	0.59
1:K:64:THR:CG2	1:K:66:GLU:HG2	2.33	0.59
1:A:97:THR:HB	1:A:121:PRO:HB2	1.85	0.58
1:D:251:THR:HG21	1:D:256:LEU:HB2	1.85	0.58
1:F:315:GLN:HG3	2:F:1427:SO4:O3	2.03	0.58
1:J:92:ARG:HD2	3:J:2059:HOH:O	2.04	0.58
1:L:294:ILE:O	1:L:298:ASN:ND2	2.35	0.58
1:J:315:GLN:HG3	2:J:1427:SO4:O4	2.04	0.58
1:C:74:MET:HG2	1:C:161:LEU:HD22	1.86	0.58
1:G:62:VAL:HG22	1:G:62:VAL:O	2.02	0.58
1:I:238:GLN:HG3	1:I:246:TYR:CZ	2.38	0.58
1:H:61:ILE:HG22	1:H:61:ILE:O	2.03	0.58
1:G:413:MET:HG3	1:G:416:GLN:CD	2.27	0.58
1:J:186:TRP:O	1:J:189:SER:OG	2.21	0.58
1:B:367:GLN:OE1	1:B:367:GLN:HA	2.04	0.58
1:I:146:ARG:NH2	1:I:210:PRO:HD3	2.17	0.58
1:C:209:MET:O	1:C:211:VAL:N	2.35	0.58
1:I:273:THR:HB	1:I:426:ALA:OXT	2.04	0.58
1:C:264:THR:HG21	1:C:267:THR:OG1	2.04	0.57
1:C:146:ARG:HG2	3:C:2055:HOH:O	2.02	0.57
1:B:264:THR:HB	1:B:267:THR:HG21	1.84	0.57
1:J:61:ILE:C	1:J:63:SER:H	2.13	0.57
1:E:107:ASP:OD2	1:E:111:SER:HB2	2.04	0.57
1:I:35:LEU:HD22	1:I:80:LEU:HB2	1.86	0.57
1:K:66:GLU:HG3	3:K:2044:HOH:O	2.02	0.57
1:D:88:VAL:HG12	1:D:88:VAL:O	2.02	0.57
1:K:394:GLN:HG2	1:K:397:TYR:HB2	1.85	0.57
1:J:379:ASP:OD2	1:K:4:ILE:HG22	2.04	0.56
1:A:32:ARG:HD2	1:A:101:PHE:O	2.06	0.56
1:C:244:GLY:HA3	1:C:263:TYR:CE1	2.40	0.56
1:H:45:PRO:HB3	1:H:80:LEU:HD21	1.87	0.56
1:C:273:THR:HG21	3:C:2124:HOH:O	2.04	0.56
1:G:190:GLN:HG2	1:G:198:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:188:MET:CE	1:J:263:TYR:CD2	2.88	0.56
1:A:64:THR:CG2	1:A:67:ALA:H	2.12	0.56
1:H:375:LEU:HD11	1:I:4:ILE:HD11	1.88	0.55
1:C:131:GLN:HB3	3:C:2003:HOH:O	2.06	0.55
1:F:69:TYR:HE1	1:F:383:ILE:CD1	2.19	0.55
1:F:221:MET:HE1	1:F:302:ILE:HG21	1.88	0.55
1:C:365:LEU:HA	1:C:368:GLU:OE1	2.06	0.55
1:D:238:GLN:HB3	1:D:356:LEU:HD21	1.88	0.55
1:K:118:ASP:HA	1:K:119:PRO:C	2.31	0.55
1:B:238:GLN:HB3	1:B:356:LEU:HD21	1.88	0.55
1:E:271:GLN:HG2	3:E:2141:HOH:O	2.06	0.55
1:C:291:LYS:HE2	3:C:2136:HOH:O	2.06	0.55
1:E:118:ASP:HA	1:E:119:PRO:C	2.32	0.55
1:D:64:THR:HG22	1:D:67:ALA:H	1.71	0.55
1:H:66:GLU:H	1:H:66:GLU:CD	2.15	0.55
1:L:264:THR:HG22	3:L:2200:HOH:O	2.06	0.54
1:L:330:ASN:HA	2:L:1427:SO4:O4	2.07	0.54
1:J:214:ASP:HB3	1:J:222:ARG:HH22	1.72	0.54
1:A:66:GLU:H	1:A:66:GLU:CD	2.15	0.54
1:I:5:SER:O	1:I:275:ARG:HD2	2.07	0.54
1:I:384:LYS:HD3	1:I:404:PHE:CE2	2.43	0.54
1:J:264:THR:HG23	1:J:266:ASN:H	1.73	0.54
1:D:244:GLY:HA3	1:D:263:TYR:CE1	2.43	0.54
1:C:280:VAL:HG22	1:C:336:HIS:HB2	1.88	0.54
1:E:160:LEU:O	1:E:164:MET:HG2	2.08	0.54
1:F:93:ASP:HB3	1:F:96:ARG:HD2	1.89	0.54
1:I:140:ARG:CG	1:I:140:ARG:NH1	2.51	0.54
1:L:126:GLN:HG3	3:L:2096:HOH:O	2.07	0.53
1:H:221:MET:CE	1:H:302:ILE:HB	2.38	0.53
1:J:26:ARG:HD2	3:J:2011:HOH:O	2.08	0.53
1:H:198:MET:HA	1:H:201:ARG:NH1	2.23	0.53
1:C:29:ALA:HB1	1:C:399:ARG:HG3	1.91	0.53
1:C:88:VAL:HG12	1:C:88:VAL:O	2.07	0.53
1:D:278:ALA:HA	3:D:2124:HOH:O	2.08	0.53
1:H:390:LEU:HD13	1:I:11:MET:CE	2.37	0.53
1:C:284:SER:OG	1:C:286:ASP:OD1	2.24	0.53
1:K:277:PHE:CE2	1:K:310:PRO:HG2	2.44	0.53
1:G:359:ALA:O	1:G:363:GLN:HG2	2.08	0.53
1:B:202:LEU:HB3	1:B:221:MET:HE2	1.90	0.53
1:E:88:VAL:HG21	1:E:105:TRP:NE1	2.24	0.53
1:H:61:ILE:O	1:H:61:ILE:CG2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:ARG:NH2	1:I:210:PRO:CD	2.64	0.53
1:C:15:ILE:HG21	1:J:15:ILE:HD11	1.91	0.52
1:E:32:ARG:HB2	1:E:101:PHE:O	2.09	0.52
1:K:360:ALA:HA	1:K:363:GLN:HG2	1.91	0.52
1:K:324:ARG:HD2	1:K:325:PRO:HD2	1.91	0.52
1:C:209:MET:N	1:C:210:PRO:HD2	2.25	0.52
1:H:64:THR:CG2	1:H:67:ALA:H	2.12	0.52
1:L:213:PRO:O	1:L:214:ASP:HB2	2.09	0.52
1:F:146:ARG:NH2	1:F:210:PRO:HD3	2.23	0.52
1:H:118:ASP:OD1	1:H:118:ASP:N	2.42	0.52
1:K:42:SER:O	1:K:43:ASN:HB2	2.10	0.52
1:J:221:MET:HE2	1:J:299:LEU:HD22	1.92	0.52
1:K:146:ARG:HD2	3:K:2126:HOH:O	2.10	0.52
1:K:286:ASP:O	1:K:289:VAL:HG12	2.10	0.52
1:E:315:GLN:HG3	2:E:1427:SO4:O3	2.08	0.52
1:B:43:ASN:HB2	1:B:113:LEU:O	2.10	0.52
1:C:40:SER:C	1:C:42:SER:N	2.66	0.52
1:C:388:ASP:O	1:C:392:ASN:HB2	2.10	0.52
1:D:245:PHE:HB3	1:D:261:LEU:HD11	1.92	0.52
1:B:64:THR:HG21	3:B:2020:HOH:O	2.10	0.52
1:I:208:ASN:O	1:I:209:MET:HB2	2.10	0.52
1:B:209:MET:C	1:B:211:VAL:N	2.54	0.51
1:B:423:THR:C	1:B:425:THR:H	2.18	0.51
1:D:189:SER:HB2	3:D:2080:HOH:O	2.09	0.51
1:G:361:LYS:O	1:G:365:LEU:HG	2.09	0.51
3:A:2002:HOH:O	1:B:394:GLN:HG2	2.10	0.51
1:C:274:GLN:HB2	3:C:2123:HOH:O	2.09	0.51
1:I:221:MET:HE1	1:I:302:ILE:HG22	1.93	0.51
1:J:74:MET:HG2	1:J:161:LEU:HD22	1.90	0.51
1:L:157:ARG:HB3	1:L:301:ALA:CB	2.38	0.51
1:G:353:MET:HG3	3:G:2249:HOH:O	2.10	0.51
1:H:42:SER:O	1:H:43:ASN:CB	2.57	0.51
1:D:425:THR:HG22	1:D:425:THR:O	2.11	0.51
1:K:4:ILE:HG23	3:K:2001:HOH:O	2.10	0.51
1:E:208:ASN:CG	1:E:210:PRO:HD2	2.35	0.51
1:F:202:LEU:HD13	1:F:221:MET:HG2	1.93	0.51
1:F:206:CYS:O	1:F:209:MET:HE2	2.11	0.51
1:B:230:LEU:HD23	1:B:233:ILE:HD11	1.92	0.50
1:C:273:THR:HB	1:C:426:ALA:OXT	2.11	0.50
1:D:61:ILE:HG23	1:D:63:SER:HB3	1.92	0.50
1:E:284:SER:OG	1:E:286:ASP:OD1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:ASN:O	1:J:209:MET:CB	2.58	0.50
1:J:146:ARG:HD2	3:J:2099:HOH:O	2.09	0.50
1:B:66:GLU:HG3	3:B:2022:HOH:O	2.09	0.50
1:H:118:ASP:CA	1:H:119:PRO:C	2.84	0.50
1:A:186:TRP:O	1:A:189:SER:OG	2.24	0.50
1:C:23:PHE:CE2	1:C:27:GLY:HA2	2.47	0.50
1:D:241:THR:HG21	1:D:264:THR:HG22	1.92	0.50
1:K:238:GLN:HG3	1:K:246:TYR:OH	2.12	0.50
1:H:379:ASP:OD2	1:I:4:ILE:HG13	2.12	0.50
1:G:311:VAL:HG11	1:G:329:MET:HB2	1.93	0.50
1:H:61:ILE:C	1:H:63:SER:H	2.20	0.50
1:E:174:THR:OG1	1:E:276:HIS:HB2	2.11	0.50
1:B:364:ALA:O	1:B:368:GLU:HG2	2.11	0.49
1:H:390:LEU:CD1	1:I:11:MET:CE	2.82	0.49
1:K:93:ASP:O	1:K:96:ARG:HG3	2.12	0.49
1:C:150:SER:HA	1:C:209:MET:HG3	1.95	0.49
1:D:423:THR:O	1:D:425:THR:N	2.45	0.49
1:B:210:PRO:HA	3:B:2096:HOH:O	2.12	0.49
1:G:264:THR:HG21	1:G:267:THR:OG1	2.11	0.49
1:G:202:LEU:HD13	1:G:221:MET:HG2	1.95	0.49
1:I:413:MET:HE2	1:I:416:GLN:NE2	2.27	0.49
1:B:29:ALA:HB2	1:B:391:TYR:CE2	2.47	0.49
1:C:270:VAL:HG12	1:C:272:ILE:HG13	1.94	0.49
1:F:254:GLN:HG3	3:F:2191:HOH:O	2.11	0.49
1:C:201:ARG:O	1:C:204:GLN:HB3	2.13	0.49
1:E:387:ASP:HB3	1:E:399:ARG:NH1	2.28	0.49
1:G:64:THR:HG23	1:G:66:GLU:H	1.77	0.49
1:G:188:MET:HE1	1:G:263:TYR:CD2	2.47	0.49
1:I:376:ILE:HG22	1:I:380:LEU:HD12	1.95	0.49
1:C:40:SER:O	1:C:42:SER:N	2.39	0.49
1:G:350:GLN:HA	1:G:353:MET:HE2	1.95	0.49
1:I:216:ASN:O	1:I:220:GLN:HG3	2.13	0.49
1:B:9:SER:HB2	1:B:307:ARG:HE	1.77	0.48
1:C:15:ILE:CD1	1:J:325:PRO:HB2	2.36	0.48
1:D:190:GLN:HB3	1:D:198:MET:HE3	1.94	0.48
1:E:346:GLU:HG3	1:E:418:LEU:HD13	1.95	0.48
1:L:82:SER:HB3	3:L:2099:HOH:O	2.13	0.48
1:A:32:ARG:HB2	1:A:101:PHE:O	2.13	0.48
1:C:274:GLN:CB	3:C:2123:HOH:O	2.61	0.48
1:D:61:ILE:C	1:D:63:SER:N	2.61	0.48
1:L:178:MET:O	1:L:183:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:MET:HE2	1:B:161:LEU:HD22	1.95	0.48
1:E:205:SER:HB3	3:E:2118:HOH:O	2.13	0.48
1:G:32:ARG:HB2	1:G:101:PHE:O	2.14	0.48
1:I:206:CYS:O	1:I:209:MET:HA	2.13	0.48
1:B:146:ARG:HE	1:B:146:ARG:HB2	1.38	0.48
1:C:221:MET:HE2	1:C:299:LEU:CD2	2.37	0.48
1:D:85:VAL:O	1:D:86:PRO:C	2.56	0.48
1:D:280:VAL:HG21	1:D:421:LEU:HD21	1.96	0.48
1:D:342:THR:O	1:D:346:GLU:HG2	2.13	0.48
1:J:205:SER:C	1:J:207:SER:H	2.20	0.48
1:C:186:TRP:HA	3:C:2079:HOH:O	2.13	0.48
1:D:74:MET:HG2	1:D:161:LEU:HD22	1.96	0.48
1:E:231:SER:HA	1:E:236:VAL:O	2.14	0.48
1:I:26:ARG:HD2	3:I:2205:HOH:O	2.13	0.48
1:I:209:MET:O	1:I:211:VAL:HG23	2.14	0.48
1:K:364:ALA:O	1:K:368:GLU:HG3	2.13	0.48
1:L:353:MET:HE3	3:L:2263:HOH:O	2.14	0.48
1:H:43:ASN:OD1	1:H:114:VAL:HG12	2.14	0.48
1:J:144:ARG:HD2	1:J:147:GLU:OE2	2.13	0.48
1:L:264:THR:CG2	1:L:267:THR:H	2.26	0.48
1:A:93:ASP:HB3	1:A:96:ARG:HD2	1.96	0.48
1:E:134:ASP:HB3	1:E:137:ASN:ND2	2.29	0.48
1:G:61:ILE:HD13	1:G:70:PRO:HD3	1.95	0.48
1:F:254:GLN:CG	1:F:255:ALA:N	2.76	0.48
1:J:318:ILE:HD12	1:J:320:GLN:HE21	1.79	0.48
1:B:217:TYR:O	1:B:221:MET:HG2	2.14	0.47
1:G:150:SER:HA	1:G:209:MET:HG3	1.95	0.47
1:C:238:GLN:HG3	1:C:246:TYR:OH	2.14	0.47
1:D:417:ALA:HB2	3:D:2159:HOH:O	2.14	0.47
1:J:204:GLN:O	1:J:207:SER:HB2	2.14	0.47
1:J:313:ALA:HB1	2:J:1427:SO4:O3	2.14	0.47
1:L:311:VAL:CG1	1:L:329:MET:HG2	2.43	0.47
1:E:26:ARG:HD2	3:E:2025:HOH:O	2.15	0.47
1:F:32:ARG:HB2	1:F:101:PHE:O	2.15	0.47
1:H:238:GLN:HG3	1:H:246:TYR:OH	2.13	0.47
1:I:139:PRO:O	1:I:143:ASN:ND2	2.46	0.47
1:L:284:SER:OG	1:L:286:ASP:OD1	2.25	0.47
1:L:286:ASP:O	1:L:289:VAL:HG12	2.13	0.47
1:B:413:MET:HG3	1:B:416:GLN:CD	2.39	0.47
1:H:277:PHE:CE2	1:H:310:PRO:HG2	2.49	0.47
1:H:349:ARG:HG2	1:H:353:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:LEU:O	1:H:164:MET:HG2	2.15	0.47
1:L:4:ILE:HD13	3:L:2212:HOH:O	2.13	0.47
1:C:208:ASN:C	1:C:210:PRO:HD2	2.40	0.47
1:D:43:ASN:HB3	1:D:113:LEU:O	2.15	0.47
1:D:303:VAL:HG13	1:D:307:ARG:NH2	2.26	0.47
1:H:45:PRO:HG3	1:H:113:LEU:HD12	1.97	0.47
1:J:32:ARG:HD2	1:J:102:GLY:HA3	1.97	0.47
1:J:254:GLN:HE21	1:J:256:LEU:HD12	1.79	0.47
1:L:207:SER:C	1:L:209:MET:H	2.22	0.47
1:A:190:GLN:OE1	1:A:201:ARG:NH1	2.48	0.47
1:D:194:ASN:HA	1:D:259:TRP:O	2.15	0.47
1:A:29:ALA:HB1	1:A:399:ARG:HG3	1.97	0.47
1:B:61:ILE:HD13	1:B:61:ILE:N	2.30	0.47
1:D:168:PRO:HD3	1:D:287:TRP:CD2	2.50	0.47
1:D:273:THR:H	1:D:426:ALA:HA	1.79	0.47
1:H:74:MET:HE3	1:H:157:ARG:HD2	1.95	0.47
1:K:294:ILE:O	1:K:298:ASN:ND2	2.46	0.47
1:K:26:ARG:HG3	1:K:391:TYR:O	2.15	0.47
1:L:69:TYR:O	1:L:72:SER:HB2	2.15	0.47
1:B:64:THR:CG2	1:B:66:GLU:HG2	2.45	0.46
1:B:69:TYR:O	1:B:72:SER:HB2	2.15	0.46
1:C:31:ASN:ND2	1:C:398:ALA:HB2	2.30	0.46
1:I:64:THR:HG23	1:I:66:GLU:OE2	2.15	0.46
1:I:148:LEU:HD12	1:I:148:LEU:O	2.15	0.46
1:J:254:GLN:HG3	1:J:256:LEU:H	1.80	0.46
1:L:5:SER:O	1:L:275:ARG:HD2	2.15	0.46
1:C:14:ALA:CB	1:J:308:GLN:HG2	2.44	0.46
1:C:307:ARG:O	1:C:309:PRO:HD3	2.15	0.46
1:G:131:GLN:HG2	3:G:2108:HOH:O	2.14	0.46
1:K:117:GLN:O	1:K:120:PRO:HA	2.15	0.46
1:A:254:GLN:HG2	1:A:256:LEU:H	1.81	0.46
1:B:208:ASN:O	1:B:210:PRO:HD2	2.16	0.46
1:F:183:LEU:HD11	1:F:220:GLN:HA	1.98	0.46
1:F:413:MET:HG3	1:F:416:GLN:NE2	2.30	0.46
1:G:61:ILE:HD12	1:G:63:SER:OG	2.14	0.46
1:G:367:GLN:OE1	1:J:358:SER:HA	2.16	0.46
1:I:168:PRO:HD3	1:I:287:TRP:CD2	2.51	0.46
1:J:330:ASN:HA	2:J:1427:SO4:O1	2.16	0.46
1:L:160:LEU:O	1:L:164:MET:HG2	2.15	0.46
1:F:64:THR:HG23	1:F:67:ALA:N	2.28	0.46
1:F:276:HIS:HD2	3:F:2310:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLN:HA	1:B:372:PHE:CD2	2.50	0.46
1:E:182:ARG:HA	1:E:185:ASP:OD2	2.15	0.46
1:K:231:SER:HA	1:K:236:VAL:O	2.15	0.46
1:C:423:THR:C	1:C:425:THR:H	2.23	0.46
1:E:84:THR:HB	1:E:105:TRP:CZ2	2.50	0.46
1:G:171:TYR:HB2	1:G:300:THR:HG23	1.98	0.46
1:K:42:SER:O	1:K:43:ASN:CB	2.63	0.46
1:K:221:MET:HE1	1:K:302:ILE:HG22	1.98	0.46
1:L:221:MET:HE1	1:L:302:ILE:HG22	1.97	0.46
1:I:256:LEU:O	1:I:257:ASP:C	2.59	0.46
1:J:66:GLU:H	1:J:66:GLU:CD	2.22	0.46
1:C:30:THR:HB	1:C:79:MET:HE3	1.98	0.46
1:F:208:ASN:O	1:F:210:PRO:HD2	2.15	0.46
1:F:273:THR:HB	1:F:426:ALA:OXT	2.16	0.46
1:G:145:ARG:CG	1:G:145:ARG:NH1	2.75	0.46
1:J:254:GLN:NE2	1:J:256:LEU:HD12	2.30	0.46
1:B:137:ASN:O	1:B:139:PRO:HD3	2.16	0.45
1:I:221:MET:HE1	1:I:302:ILE:CG2	2.45	0.45
1:C:178:MET:O	1:C:183:LEU:HD23	2.16	0.45
1:F:216:ASN:O	1:F:220:GLN:HG3	2.17	0.45
1:F:254:GLN:HG2	1:F:256:LEU:H	1.81	0.45
1:J:156:LEU:O	1:J:160:LEU:HG	2.17	0.45
1:H:231:SER:HA	1:H:236:VAL:O	2.17	0.45
1:C:303:VAL:HG13	1:C:307:ARG:HH21	1.82	0.45
1:I:74:MET:HE2	1:I:161:LEU:HD22	1.98	0.45
1:I:207:SER:O	1:I:208:ASN:CB	2.63	0.45
1:J:64:THR:HG23	1:J:66:GLU:H	1.81	0.45
1:L:208:ASN:HB3	3:L:2164:HOH:O	2.17	0.45
1:G:69:TYR:HE1	1:G:383:ILE:CD1	2.30	0.45
1:E:352:VAL:HG22	1:E:357:VAL:HG23	1.99	0.45
1:F:11:MET:HE3	1:F:308:GLN:HB2	1.98	0.45
1:A:42:SER:O	1:A:43:ASN:HB2	2.17	0.45
1:B:282:ALA:HB2	1:B:293:TRP:CE2	2.52	0.45
1:B:358:SER:HB2	1:B:361:LYS:H	1.82	0.45
1:C:253:GLY:H	1:C:257:ASP:CG	2.25	0.45
1:F:64:THR:HG22	1:F:67:ALA:HB3	1.99	0.45
1:F:345:GLN:NE2	1:F:370:ASN:OD1	2.50	0.45
1:A:99:ASN:HA	1:A:103:LEU:O	2.17	0.44
1:H:361:LYS:NZ	3:H:2225:HOH:O	2.50	0.44
1:I:228:TRP:CZ2	1:I:292:SER:HB3	2.52	0.44
1:J:425:THR:HG22	3:J:2246:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:LEU:O	1:K:164:MET:HG2	2.17	0.44
1:L:145:ARG:HE	1:L:145:ARG:HB2	1.47	0.44
1:A:239:THR:HG23	1:A:356:LEU:HD21	1.99	0.44
1:B:218:ASP:CG	1:B:307:ARG:HH12	2.24	0.44
1:C:34:GLN:NE2	1:C:398:ALA:HB1	2.32	0.44
1:D:390:LEU:HD22	1:D:394:GLN:OE1	2.17	0.44
1:H:331:GLY:N	2:H:1427:SO4:O3	2.41	0.44
1:F:29:ALA:HB1	1:F:399:ARG:HG3	1.99	0.44
1:I:85:VAL:O	1:I:86:PRO:C	2.59	0.44
1:K:367:GLN:OE1	1:K:367:GLN:HA	2.17	0.44
1:E:352:VAL:CG2	1:E:357:VAL:HG23	2.48	0.44
1:A:140:ARG:HD3	1:A:147:GLU:OE1	2.17	0.44
1:G:145:ARG:HH11	1:G:145:ARG:HG2	1.82	0.44
1:H:349:ARG:O	1:H:353:MET:HG3	2.18	0.44
1:J:188:MET:HE1	1:J:263:TYR:CE2	2.52	0.44
1:A:263:TYR:OH	1:A:269:ARG:NH2	2.45	0.44
1:G:22:PRO:HD3	1:G:162:SER:HB3	2.00	0.44
1:G:231:SER:HA	1:G:236:VAL:O	2.18	0.44
1:G:349:ARG:NH2	3:G:2248:HOH:O	2.50	0.44
1:K:64:THR:HG23	1:K:66:GLU:HG2	1.99	0.44
1:C:280:VAL:HA	1:C:336:HIS:O	2.18	0.44
1:D:382:GLN:O	1:D:386:GLN:CG	2.61	0.44
1:E:413:MET:HG3	1:E:416:GLN:CD	2.43	0.44
1:J:120:PRO:HB2	1:J:122:ALA:O	2.18	0.44
1:J:264:THR:HG22	3:J:2150:HOH:O	2.18	0.44
1:A:166:ALA:O	1:A:402:LYS:NZ	2.43	0.44
1:G:17:ASP:CG	1:G:324:ARG:HE	2.26	0.44
1:K:238:GLN:HG3	1:K:246:TYR:CZ	2.53	0.44
1:D:11:MET:HG3	3:D:2108:HOH:O	2.17	0.44
1:E:88:VAL:HG21	1:E:105:TRP:HE1	1.81	0.44
1:G:145:ARG:HH11	1:G:145:ARG:HG3	1.82	0.44
1:H:254:GLN:NE2	1:H:256:LEU:HD12	2.33	0.44
1:F:74:MET:HE2	1:F:161:LEU:HD22	2.00	0.43
1:F:329:MET:HB3	1:F:329:MET:HE3	1.75	0.43
1:K:377:GLN:HA	1:K:409:TRP:CZ2	2.53	0.43
1:E:144:ARG:HD2	1:E:147:GLU:OE2	2.18	0.43
1:G:263:TYR:OH	1:G:269:ARG:NH2	2.43	0.43
1:G:280:VAL:HG22	1:G:336:HIS:HB2	1.99	0.43
1:K:4:ILE:HD13	1:K:4:ILE:HA	1.84	0.43
1:I:4:ILE:HD12	3:I:2155:HOH:O	2.17	0.43
1:E:311:VAL:N	1:F:382:GLN:OE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:PRO:HA	1:H:120:PRO:HD2	1.89	0.43
1:I:145:ARG:HA	1:I:145:ARG:HD3	1.58	0.43
1:B:118:ASP:HA	1:B:119:PRO:C	2.43	0.43
1:C:231:SER:HA	1:C:236:VAL:O	2.18	0.43
1:G:188:MET:HE1	1:G:263:TYR:CG	2.53	0.43
1:G:244:GLY:HA2	1:G:264:THR:HG22	2.00	0.43
1:H:190:GLN:OE1	1:H:201:ARG:NH1	2.52	0.43
1:I:211:VAL:O	1:I:306:CYS:HB2	2.18	0.43
1:J:209:MET:H	1:J:210:PRO:CD	2.31	0.43
1:K:64:THR:HG21	1:K:66:GLU:HG2	2.00	0.43
1:B:194:ASN:HB3	1:B:197:ASP:HB2	2.00	0.43
1:B:270:VAL:HG11	1:B:425:THR:OG1	2.19	0.43
1:I:191:TYR:HE1	1:I:263:TYR:H	1.64	0.43
1:J:166:ALA:HA	3:J:2229:HOH:O	2.18	0.43
1:K:172:VAL:O	1:K:277:PHE:HA	2.19	0.43
1:B:379:ASP:O	1:B:382:GLN:HB2	2.19	0.43
1:C:95:TRP:CZ3	1:C:107:ASP:HA	2.53	0.43
1:I:240:ASN:OD1	1:I:268:ASN:ND2	2.51	0.43
1:C:209:MET:C	1:C:211:VAL:N	2.77	0.43
1:J:19:PHE:HB2	1:J:132:TRP:CZ3	2.53	0.43
1:J:202:LEU:HD21	1:J:220:GLN:OE1	2.18	0.43
1:C:153:PRO:HG2	1:C:209:MET:CE	2.48	0.43
1:J:188:MET:CE	1:J:263:TYR:CE2	3.01	0.43
1:K:178:MET:O	1:K:183:LEU:HD23	2.19	0.43
1:D:108:GLU:C	1:D:110:LEU:H	2.27	0.43
1:H:394:GLN:HA	1:H:395:PRO:HD3	1.93	0.43
1:K:354:ALA:HB3	1:K:356:LEU:HD12	2.00	0.43
1:L:190:GLN:OE1	1:L:201:ARG:NH1	2.52	0.43
1:C:43:ASN:HB3	1:C:113:LEU:O	2.18	0.42
1:C:204:GLN:HG3	3:C:2086:HOH:O	2.19	0.42
1:F:23:PHE:CE2	1:F:27:GLY:HA2	2.54	0.42
1:G:74:MET:HE2	1:G:161:LEU:HD22	2.00	0.42
1:B:254:GLN:NE2	1:B:256:LEU:HD12	2.35	0.42
1:C:238:GLN:HG3	1:C:246:TYR:CZ	2.54	0.42
1:G:45:PRO:HB3	1:G:80:LEU:HD21	2.01	0.42
1:J:178:MET:HE3	1:J:178:MET:HB2	1.88	0.42
1:K:157:ARG:NH1	1:K:157:ARG:CG	2.68	0.42
1:K:357:VAL:HB	1:K:361:LYS:HB3	2.01	0.42
1:A:339:ASN:ND2	1:A:410:THR:O	2.50	0.42
1:F:145:ARG:HD3	3:F:2124:HOH:O	2.18	0.42
1:G:42:SER:O	1:G:43:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:GLN:HG2	3:H:2089:HOH:O	2.19	0.42
1:L:190:GLN:O	1:L:193:ASN:HB2	2.19	0.42
1:B:244:GLY:O	1:B:263:TYR:HA	2.19	0.42
1:D:186:TRP:HH2	1:D:224:LEU:HD22	1.85	0.42
1:E:42:SER:O	1:E:43:ASN:HB2	2.18	0.42
1:E:376:ILE:HD13	1:E:376:ILE:HA	1.83	0.42
1:J:64:THR:CG2	1:J:66:GLU:HG2	2.48	0.42
1:L:204:GLN:O	1:L:207:SER:HB2	2.19	0.42
1:E:61:ILE:C	1:E:63:SER:H	2.27	0.42
1:E:74:MET:HG2	1:E:161:LEU:HD22	2.00	0.42
1:F:349:ARG:NH1	1:F:349:ARG:HG2	2.33	0.42
1:H:289:VAL:HG21	1:H:376:ILE:HD12	2.02	0.42
1:I:28:LEU:HD11	1:I:79:MET:HG2	2.02	0.42
1:I:160:LEU:O	1:I:164:MET:HG2	2.19	0.42
1:B:233:ILE:CD1	1:B:421:LEU:HB3	2.50	0.42
1:D:416:GLN:O	1:D:420:VAL:HG23	2.19	0.42
1:I:69:TYR:O	1:I:72:SER:HB2	2.18	0.42
1:B:202:LEU:HB3	1:B:221:MET:CE	2.50	0.42
1:B:213:PRO:O	1:B:214:ASP:HB2	2.20	0.42
1:D:173:GLU:OE1	1:D:222:ARG:HD2	2.20	0.42
1:K:61:ILE:HD12	1:K:63:SER:OG	2.20	0.42
1:B:61:ILE:HB	1:B:63:SER:OG	2.20	0.42
1:C:15:ILE:HD13	1:J:325:PRO:CB	2.38	0.42
1:G:246:TYR:CZ	1:G:262:PHE:HB2	2.55	0.42
1:J:271:GLN:HB2	3:J:2157:HOH:O	2.18	0.42
1:K:205:SER:HA	3:K:2158:HOH:O	2.19	0.42
1:D:81:HIS:CE1	1:D:154:LEU:HG	2.55	0.42
1:B:61:ILE:HG23	1:B:291:LYS:HE2	2.02	0.42
1:D:246:TYR:O	1:D:261:LEU:HD12	2.20	0.42
1:H:29:ALA:HB1	1:H:399:ARG:HG3	2.02	0.42
1:I:126:GLN:HG3	1:K:126:GLN:HB2	2.02	0.42
1:K:66:GLU:CD	1:K:66:GLU:H	2.27	0.42
1:A:160:LEU:O	1:A:164:MET:HG2	2.20	0.41
1:D:29:ALA:HB1	1:D:399:ARG:HG3	2.02	0.41
1:E:361:LYS:O	1:E:361:LYS:HG3	2.20	0.41
1:B:353:MET:HE3	3:B:2136:HOH:O	2.19	0.41
1:D:64:THR:HG22	1:D:66:GLU:N	2.35	0.41
1:D:218:ASP:CG	1:D:307:ARG:HH22	2.28	0.41
1:D:274:GLN:H	1:D:274:GLN:HG3	1.71	0.41
1:G:20:SER:HB2	1:G:82:SER:HB3	2.02	0.41
1:G:209:MET:O	1:G:210:PRO:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:TYR:HE1	1:J:383:ILE:HD12	1.86	0.41
1:A:206:CYS:SG	1:A:221:MET:HE1	2.61	0.41
1:C:171:TYR:HB2	1:C:300:THR:HG23	2.03	0.41
1:H:244:GLY:O	1:H:263:TYR:HA	2.21	0.41
1:K:271:GLN:HG3	3:K:2193:HOH:O	2.19	0.41
1:A:34:GLN:NE2	1:A:398:ALA:HB1	2.35	0.41
1:B:145:ARG:HG2	1:B:149:GLN:OE1	2.19	0.41
1:C:264:THR:O	1:C:264:THR:CG2	2.68	0.41
1:H:198:MET:HE2	1:H:224:LEU:HD13	2.03	0.41
1:J:238:GLN:HB3	1:J:356:LEU:HD21	2.02	0.41
1:K:92:ARG:O	1:K:108:GLU:HG3	2.21	0.41
1:K:119:PRO:HA	3:K:2093:HOH:O	2.20	0.41
1:B:118:ASP:OD2	1:B:119:PRO:HA	2.21	0.41
1:C:131:GLN:HG2	3:C:2001:HOH:O	2.21	0.41
1:F:190:GLN:O	1:F:191:TYR:C	2.63	0.41
1:G:254:GLN:HG2	1:G:255:ALA:H	1.85	0.41
1:I:94:ALA:O	1:I:98:PHE:HB2	2.20	0.41
1:B:20:SER:O	1:B:130:ALA:HA	2.20	0.41
1:B:84:THR:HB	1:B:105:TRP:CZ2	2.55	0.41
1:E:266:ASN:OD1	1:E:266:ASN:N	2.44	0.41
1:E:358:SER:HB2	1:E:361:LYS:H	1.85	0.41
1:I:311:VAL:HG12	1:I:329:MET:HG2	2.03	0.41
1:L:26:ARG:NH1	3:L:2022:HOH:O	2.53	0.41
1:E:99:ASN:HA	1:E:103:LEU:O	2.20	0.41
1:E:324:ARG:HA	1:E:325:PRO:HD3	1.90	0.41
1:F:171:TYR:HB2	1:F:300:THR:HG23	2.02	0.41
1:G:118:ASP:OD1	1:G:119:PRO:HA	2.20	0.41
1:H:66:GLU:CD	1:H:66:GLU:N	2.79	0.41
1:L:74:MET:HE2	1:L:161:LEU:HD22	2.01	0.41
1:A:206:CYS:SG	1:A:221:MET:CE	3.09	0.41
1:B:171:TYR:HB2	1:B:300:THR:HG23	2.02	0.41
1:E:205:SER:CB	3:E:2118:HOH:O	2.67	0.41
1:H:138:TYR:HA	1:H:139:PRO:HD3	1.94	0.41
1:I:208:ASN:ND2	1:I:209:MET:H	2.19	0.41
1:J:286:ASP:O	1:J:289:VAL:HG12	2.21	0.41
1:A:209:MET:O	1:A:211:VAL:N	2.54	0.41
1:A:277:PHE:HE2	1:A:333:THR:HG21	1.86	0.41
1:C:339:ASN:HD22	1:C:410:THR:C	2.28	0.41
1:F:209:MET:HB2	3:F:2128:HOH:O	2.21	0.41
1:F:367:GLN:HA	3:F:2259:HOH:O	2.20	0.41
1:G:254:GLN:HG2	3:G:2191:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:VAL:HG22	1:J:62:VAL:O	2.21	0.41
1:L:13:ARG:HD3	1:L:15:ILE:O	2.21	0.41
1:L:107:ASP:CG	1:L:111:SER:HB2	2.46	0.41
1:B:20:SER:HB2	1:B:82:SER:HB3	2.03	0.41
1:G:229:LEU:O	1:G:232:TYR:HB3	2.21	0.41
1:G:275:ARG:HG3	1:G:275:ARG:NH1	2.33	0.41
1:J:320:GLN:CD	1:J:320:GLN:H	2.28	0.41
1:B:377:GLN:HA	1:B:409:TRP:CZ2	2.56	0.40
1:D:270:VAL:HG12	1:D:272:ILE:HG13	2.03	0.40
1:D:283:ARG:HD2	1:D:337:GLU:CD	2.46	0.40
1:H:186:TRP:CH2	1:H:190:GLN:NE2	2.89	0.40
1:I:34:GLN:NE2	1:I:398:ALA:HB1	2.35	0.40
1:K:72:SER:O	1:K:76:GLN:HG3	2.21	0.40
1:K:140:ARG:HD3	1:K:147:GLU:OE1	2.21	0.40
1:B:61:ILE:HG21	1:B:70:PRO:HG3	2.03	0.40
1:C:15:ILE:HD11	1:C:17:ASP:OD1	2.20	0.40
1:H:13:ARG:HD3	1:H:15:ILE:O	2.22	0.40
1:I:217:TYR:O	1:I:221:MET:HG3	2.21	0.40
1:J:34:GLN:NE2	1:J:398:ALA:HB1	2.36	0.40
1:A:35:LEU:HD22	1:A:80:LEU:HB2	2.02	0.40
1:E:145:ARG:HA	1:E:145:ARG:HD3	1.84	0.40
1:E:277:PHE:CE2	1:E:310:PRO:HG2	2.56	0.40
1:C:10:THR:HG22	1:C:213:PRO:HB2	2.03	0.40
1:D:229:LEU:O	1:D:233:ILE:HG23	2.21	0.40
1:E:319:ASN:HA	1:E:322:GLN:HG3	2.03	0.40
1:G:81:HIS:ND1	1:G:158:SER:OG	2.50	0.40
1:H:64:THR:HG23	1:H:66:GLU:H	1.86	0.40
1:K:24:GLY:HA3	3:K:2030:HOH:O	2.20	0.40
1:K:146:ARG:HG3	3:K:2062:HOH:O	2.20	0.40
1:L:121:PRO:HD2	3:L:2089:HOH:O	2.21	0.40
1:L:384:LYS:HD2	1:L:404:PHE:CE2	2.57	0.40
1:A:244:GLY:HA3	1:A:263:TYR:CE1	2.57	0.40
1:G:145:ARG:NH1	1:G:145:ARG:HG2	2.37	0.40
1:H:92:ARG:O	1:H:108:GLU:HG3	2.21	0.40
1:H:313:ALA:HB1	2:H:1427:SO4:O4	2.21	0.40
1:I:182:ARG:HG3	1:I:182:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/423 (96%)	392 (97%)	12 (3%)	2 (0%)	24	26
1	B	405/423 (96%)	376 (93%)	26 (6%)	3 (1%)	18	18
1	C	400/423 (95%)	379 (95%)	17 (4%)	4 (1%)	12	11
1	D	405/423 (96%)	376 (93%)	21 (5%)	8 (2%)	6	3
1	E	405/423 (96%)	382 (94%)	19 (5%)	4 (1%)	12	11
1	F	400/423 (95%)	385 (96%)	13 (3%)	2 (0%)	24	26
1	G	399/423 (94%)	383 (96%)	13 (3%)	3 (1%)	16	16
1	H	405/423 (96%)	386 (95%)	17 (4%)	2 (0%)	24	26
1	I	406/423 (96%)	385 (95%)	18 (4%)	3 (1%)	18	18
1	J	400/423 (95%)	376 (94%)	18 (4%)	6 (2%)	8	6
1	K	406/423 (96%)	385 (95%)	16 (4%)	5 (1%)	10	8
1	L	406/423 (96%)	389 (96%)	13 (3%)	4 (1%)	12	11
All	All	4843/5076 (95%)	4594 (95%)	203 (4%)	46 (1%)	14	13

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PRO
1	C	210	PRO
1	D	210	PRO
1	E	214	ASP
1	I	208	ASN
1	I	209	MET
1	J	208	ASN
1	J	209	MET
1	J	214	ASP
1	K	62	VAL
1	K	177	ASN
1	K	210	PRO

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Mol	Chain	Res	Type
1	L	209	MET
1	L	210	PRO
1	A	177	ASN
1	B	210	PRO
1	C	41	SER
1	D	91	SER
1	D	177	ASN
1	D	209	MET
1	D	424	PHE
1	E	62	VAL
1	E	209	MET
1	F	62	VAL
1	F	209	MET
1	G	208	ASN
1	H	62	VAL
1	J	62	VAL
1	B	209	MET
1	C	177	ASN
1	C	209	MET
1	D	62	VAL
1	G	210	PRO
1	H	177	ASN
1	I	210	PRO
1	J	91	SER
1	K	43	ASN
1	L	177	ASN
1	L	211	VAL
1	J	206	CYS
1	K	207	SER
1	B	62	VAL
1	D	176	PRO
1	D	273	THR
1	E	213	PRO
1	G	62	VAL

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	340/352 (97%)	323 (95%)	17 (5%)	22	27
1	B	339/352 (96%)	315 (93%)	24 (7%)	13	14
1	C	335/352 (95%)	316 (94%)	19 (6%)	18	23
1	D	339/352 (96%)	317 (94%)	22 (6%)	15	17
1	E	339/352 (96%)	321 (95%)	18 (5%)	20	25
1	F	335/352 (95%)	314 (94%)	21 (6%)	16	19
1	G	334/352 (95%)	315 (94%)	19 (6%)	18	23
1	H	339/352 (96%)	320 (94%)	19 (6%)	19	23
1	I	340/352 (97%)	319 (94%)	21 (6%)	16	19
1	J	335/352 (95%)	316 (94%)	19 (6%)	18	23
1	K	340/352 (97%)	322 (95%)	18 (5%)	20	25
1	L	340/352 (97%)	316 (93%)	24 (7%)	13	14
All	All	4055/4224 (96%)	3814 (94%)	241 (6%)	18	21

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	11	MET
1	A	61	ILE
1	A	66	GLU
1	A	74	MET
1	A	80	LEU
1	A	126	GLN
1	A	177	ASN
1	A	212	GLU
1	A	235	VAL
1	A	238	GLN
1	A	249	SER
1	A	265	THR
1	A	273	THR
1	A	315	GLN
1	A	349	ARG
1	A	425	THR
1	B	9	SER
1	B	41	SER
1	B	47	GLN
1	B	61	ILE
1	B	62	VAL

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Mol	Chain	Res	Type
1	B	64	THR
1	B	66	GLU
1	B	82	SER
1	B	146	ARG
1	B	154	LEU
1	B	172	VAL
1	B	212	GLU
1	B	238	GLN
1	B	239	THR
1	B	260	THR
1	B	264	THR
1	B	265	THR
1	B	341	LEU
1	B	356	LEU
1	B	358	SER
1	B	363	GLN
1	B	368	GLU
1	B	413	MET
1	B	425	THR
1	C	11	MET
1	C	15	ILE
1	C	61	ILE
1	C	64	THR
1	C	66	GLU
1	C	117	GLN
1	C	157	ARG
1	C	172	VAL
1	C	177	ASN
1	C	203	THR
1	C	204	GLN
1	C	256	LEU
1	C	264	THR
1	C	265	THR
1	C	273	THR
1	C	289	VAL
1	C	328	SER
1	C	358	SER
1	C	425	THR
1	D	13	ARG
1	D	25	ASN
1	D	41	SER
1	D	47	GLN

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Mol	Chain	Res	Type
1	D	64	THR
1	D	140	ARG
1	D	143	ASN
1	D	157	ARG
1	D	180	SER
1	D	194	ASN
1	D	204	GLN
1	D	212	GLU
1	D	220	GLN
1	D	233	ILE
1	D	250	LYS
1	D	258	SER
1	D	260	THR
1	D	265	THR
1	D	294	ILE
1	D	349	ARG
1	D	373	SER
1	D	386	GLN
1	E	61	ILE
1	E	66	GLU
1	E	88	VAL
1	E	111	SER
1	E	157	ARG
1	E	176	PRO
1	E	177	ASN
1	E	178	MET
1	E	182	ARG
1	E	194	ASN
1	E	214	ASP
1	E	254	GLN
1	E	266	ASN
1	E	273	THR
1	E	358	SER
1	E	376	ILE
1	E	413	MET
1	E	425	THR
1	F	11	MET
1	F	13	ARG
1	F	15	ILE
1	F	17	ASP
1	F	47	GLN
1	F	61	ILE

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Mol	Chain	Res	Type
1	F	66	GLU
1	F	88	VAL
1	F	131	GLN
1	F	150	SER
1	F	154	LEU
1	F	157	ARG
1	F	176	PRO
1	F	182	ARG
1	F	204	GLN
1	F	265	THR
1	F	271	GLN
1	F	273	THR
1	F	329	MET
1	F	379	ASP
1	F	413	MET
1	G	32	ARG
1	G	61	ILE
1	G	64	THR
1	G	88	VAL
1	G	131	GLN
1	G	145	ARG
1	G	157	ARG
1	G	182	ARG
1	G	190	GLN
1	G	207	SER
1	G	209	MET
1	G	239	THR
1	G	264	THR
1	G	265	THR
1	G	273	THR
1	G	315	GLN
1	G	367	GLN
1	G	379	ASP
1	G	413	MET
1	H	41	SER
1	H	64	THR
1	H	66	GLU
1	H	74	MET
1	H	88	VAL
1	H	106	THR
1	H	118	ASP
1	H	131	GLN

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Mol	Chain	Res	Type
1	H	157	ARG
1	H	177	ASN
1	H	208	ASN
1	H	238	GLN
1	H	264	THR
1	H	265	THR
1	H	273	THR
1	H	289	VAL
1	H	358	SER
1	H	392	ASN
1	H	413	MET
1	I	25	ASN
1	I	61	ILE
1	I	62	VAL
1	I	64	THR
1	I	80	LEU
1	I	126	GLN
1	I	131	GLN
1	I	140	ARG
1	I	145	ARG
1	I	177	ASN
1	I	178	MET
1	I	182	ARG
1	I	203	THR
1	I	204	GLN
1	I	208	ASN
1	I	212	GLU
1	I	238	GLN
1	I	264	THR
1	I	265	THR
1	I	273	THR
1	I	373	SER
1	J	13	ARG
1	J	47	GLN
1	J	64	THR
1	J	66	GLU
1	J	88	VAL
1	J	157	ARG
1	J	194	ASN
1	J	204	GLN
1	J	226	SER
1	J	239	THR

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Mol	Chain	Res	Type
1	J	264	THR
1	J	265	THR
1	J	271	GLN
1	J	329	MET
1	J	330	ASN
1	J	358	SER
1	J	375	LEU
1	J	376	ILE
1	J	425	THR
1	K	4	ILE
1	K	6	GLU
1	K	25	ASN
1	K	40	SER
1	K	41	SER
1	K	42	SER
1	K	61	ILE
1	K	64	THR
1	K	66	GLU
1	K	88	VAL
1	K	111	SER
1	K	157	ARG
1	K	208	ASN
1	K	235	VAL
1	K	264	THR
1	K	265	THR
1	K	273	THR
1	K	394	GLN
1	L	4	ILE
1	L	5	SER
1	L	13	ARG
1	L	66	GLU
1	L	88	VAL
1	L	111	SER
1	L	118	ASP
1	L	126	GLN
1	L	131	GLN
1	L	145	ARG
1	L	157	ARG
1	L	209	MET
1	L	212	GLU
1	L	226	SER
1	L	254	GLN

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Mol	Chain	Res	Type
1	L	264	THR
1	L	265	THR
1	L	273	THR
1	L	361	LYS
1	L	375	LEU
1	L	379	ASP
1	L	392	ASN
1	L	393	GLN
1	L	413	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	208	ASN
1	A	288	ASN
1	A	336	HIS
1	A	394	GLN
1	B	194	ASN
1	B	216	ASN
1	B	288	ASN
1	B	315	GLN
1	B	330	ASN
1	B	336	HIS
1	C	268	ASN
1	C	336	HIS
1	D	47	GLN
1	D	194	ASN
1	D	220	GLN
1	D	240	ASN
1	D	271	GLN
1	D	382	GLN
1	E	137	ASN
1	E	330	ASN
1	E	336	HIS
1	E	345	GLN
1	E	370	ASN
1	E	394	GLN
1	E	406	ASN
1	F	254	GLN
1	F	276	HIS
1	F	288	ASN

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Mol	Chain	Res	Type
1	F	363	GLN
1	G	25	ASN
1	G	117	GLN
1	G	126	GLN
1	G	194	ASN
1	G	208	ASN
1	G	336	HIS
1	H	194	ASN
1	H	254	GLN
1	H	336	HIS
1	I	194	ASN
1	I	274	GLN
1	J	99	ASN
1	J	238	GLN
1	J	268	ASN
1	J	320	GLN
1	J	394	GLN
1	K	43	ASN
1	K	194	ASN
1	K	216	ASN
1	L	99	ASN
1	L	194	ASN
1	L	240	ASN
1	L	268	ASN
1	L	274	GLN
1	L	330	ASN
1	L	336	HIS
1	L	367	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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	K	1427	-	4,4,4	0.29	0	6,6,6	0.63	0
2	SO4	G	1427	-	4,4,4	0.22	0	6,6,6	0.33	0
2	SO4	A	1427	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	H	1427	-	4,4,4	0.23	0	6,6,6	0.25	0
2	SO4	E	1427	-	4,4,4	0.22	0	6,6,6	0.25	0
2	SO4	F	1427	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	B	1427	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	J	1427	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	D	1427	-	4,4,4	0.31	0	6,6,6	0.33	0
2	SO4	C	1427	-	4,4,4	0.24	0	6,6,6	0.30	0
2	SO4	L	1427	-	4,4,4	0.29	0	6,6,6	0.29	0
2	SO4	I	1427	-	4,4,4	0.19	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1427	SO4	1	0
2	H	1427	SO4	2	0
2	E	1427	SO4	1	0
2	F	1427	SO4	1	0
2	J	1427	SO4	3	0
2	L	1427	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	410/423 (96%)	0.16	17 (4%) 41 47	18, 31, 52, 72	0
1	B	409/423 (96%)	1.04	80 (19%) 3 3	21, 46, 89, 102	0
1	C	404/423 (95%)	0.68	35 (8%) 16 19	25, 41, 68, 90	0
1	D	409/423 (96%)	1.18	104 (25%) 1 1	22, 47, 88, 96	0
1	E	409/423 (96%)	0.54	32 (7%) 19 23	19, 38, 66, 84	0
1	F	404/423 (95%)	0.02	15 (3%) 45 51	14, 27, 50, 81	0
1	G	403/423 (95%)	0.05	21 (5%) 33 39	12, 26, 47, 84	0
1	H	409/423 (96%)	0.11	12 (2%) 53 60	15, 30, 51, 77	0
1	I	410/423 (96%)	0.27	18 (4%) 39 45	20, 35, 55, 81	0
1	J	404/423 (95%)	0.30	15 (3%) 45 51	20, 34, 58, 90	0
1	K	410/423 (96%)	0.11	19 (4%) 37 43	15, 30, 54, 76	0
1	L	410/423 (96%)	0.05	7 (1%) 69 73	14, 27, 49, 68	0
All	All	4891/5076 (96%)	0.38	375 (7%) 19 23	12, 34, 70, 102	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	6.9
1	D	61	ILE	6.8
1	E	61	ILE	5.7
1	C	119	PRO	5.6
1	B	205	SER	5.6
1	J	62	VAL	5.4
1	K	204	GLN	5.3
1	H	62	VAL	5.2
1	D	184	ALA	5.1
1	D	270	VAL	5.0
1	D	351	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	61	ILE	4.9
1	C	61	ILE	4.9
1	B	354	ALA	4.8
1	E	209	MET	4.7
1	D	208	ASN	4.7
1	I	62	VAL	4.7
1	B	272	ILE	4.6
1	D	356	LEU	4.6
1	C	94	ALA	4.6
1	I	209	MET	4.5
1	D	175	TRP	4.5
1	E	123	ALA	4.5
1	F	61	ILE	4.4
1	D	241	THR	4.4
1	D	357	VAL	4.4
1	D	5	SER	4.4
1	B	183	LEU	4.4
1	A	209	MET	4.3
1	B	209	MET	4.3
1	J	209	MET	4.3
1	B	62	VAL	4.3
1	E	62	VAL	4.3
1	D	267	THR	4.3
1	A	61	ILE	4.3
1	G	61	ILE	4.3
1	J	10	THR	4.2
1	D	263	TYR	4.2
1	D	179	ILE	4.2
1	I	61	ILE	4.2
1	D	181	GLY	4.1
1	D	233	ILE	4.1
1	D	246	TYR	4.1
1	E	208	ASN	4.1
1	D	194	ASN	4.1
1	D	240	ASN	4.1
1	B	264	THR	4.0
1	C	205	SER	4.0
1	D	236	VAL	4.0
1	F	203	THR	4.0
1	D	209	MET	4.0
1	C	62	VAL	3.9
1	C	256	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	208	ASN	3.9
1	H	210	PRO	3.9
1	D	247	PHE	3.8
1	E	119	PRO	3.8
1	K	61	ILE	3.8
1	B	211	VAL	3.8
1	D	186	TRP	3.8
1	B	363	GLN	3.8
1	D	269	ARG	3.8
1	C	210	PRO	3.8
1	B	270	VAL	3.7
1	C	122	ALA	3.7
1	B	186	TRP	3.7
1	D	244	GLY	3.7
1	A	62	VAL	3.7
1	B	184	ALA	3.7
1	C	121	PRO	3.7
1	D	261	LEU	3.7
1	E	120	PRO	3.7
1	H	209	MET	3.6
1	F	207	SER	3.6
1	J	61	ILE	3.6
1	B	357	VAL	3.6
1	J	217	TYR	3.6
1	J	210	PRO	3.6
1	F	205	SER	3.6
1	D	256	LEU	3.6
1	D	176	PRO	3.6
1	K	4	ILE	3.5
1	D	187	PHE	3.5
1	D	364	ALA	3.5
1	D	180	SER	3.5
1	D	191	TYR	3.5
1	D	251	THR	3.5
1	C	206	CYS	3.5
1	B	179	ILE	3.5
1	H	61	ILE	3.5
1	B	352	VAL	3.5
1	D	354	ALA	3.5
1	I	207	SER	3.5
1	D	272	ILE	3.5
1	D	348	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	202	LEU	3.5
1	D	245	PHE	3.5
1	H	120	PRO	3.4
1	D	196	VAL	3.4
1	B	217	TYR	3.4
1	F	62	VAL	3.4
1	B	426	ALA	3.4
1	J	214	ASP	3.4
1	D	7	PHE	3.4
1	L	209	MET	3.4
1	D	353	MET	3.4
1	F	10	THR	3.4
1	I	271	GLN	3.4
1	D	188	MET	3.3
1	B	267	THR	3.3
1	B	273	THR	3.3
1	D	419	ALA	3.3
1	C	215	GLY	3.3
1	G	214	ASP	3.3
1	D	262	PHE	3.3
1	E	95	TRP	3.3
1	G	206	CYS	3.2
1	D	248	SER	3.2
1	B	364	ALA	3.2
1	D	193	ASN	3.2
1	B	202	LEU	3.2
1	C	120	PRO	3.2
1	J	205	SER	3.2
1	D	217	TYR	3.2
1	B	263	TYR	3.1
1	D	365	LEU	3.1
1	D	242	ILE	3.1
1	B	42	SER	3.1
1	B	208	ASN	3.1
1	J	208	ASN	3.1
1	B	365	LEU	3.1
1	B	239	THR	3.1
1	B	5	SER	3.1
1	E	114	VAL	3.1
1	E	256	LEU	3.1
1	D	366	THR	3.1
1	K	41	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	192	GLY	3.1
1	D	426	ALA	3.1
1	L	4	ILE	3.0
1	B	265	THR	3.0
1	D	273	THR	3.0
1	E	64	THR	3.0
1	B	226	SER	3.0
1	B	268	ASN	3.0
1	G	210	PRO	3.0
1	D	420	VAL	3.0
1	G	211	VAL	3.0
1	G	208	ASN	3.0
1	B	210	PRO	3.0
1	B	242	ILE	3.0
1	L	62	VAL	2.9
1	D	239	THR	2.9
1	B	181	GLY	2.9
1	B	262	PHE	2.9
1	K	209	MET	2.9
1	A	8	GLY	2.9
1	D	177	ASN	2.9
1	A	121	PRO	2.9
1	F	211	VAL	2.9
1	G	62	VAL	2.9
1	C	203	THR	2.9
1	D	265	THR	2.9
1	I	66	GLU	2.9
1	F	208	ASN	2.9
1	D	359	ALA	2.9
1	A	413	MET	2.9
1	I	4	ILE	2.9
1	K	62	VAL	2.8
1	B	175	TRP	2.8
1	D	25	ASN	2.8
1	D	243	SER	2.8
1	D	355	GLY	2.8
1	F	210	PRO	2.8
1	A	204	GLN	2.8
1	C	204	GLN	2.8
1	B	353	MET	2.8
1	D	231	SER	2.8
1	B	185	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	364	ALA	2.8
1	D	424	PHE	2.8
1	D	264	THR	2.7
1	D	197	ASP	2.7
1	E	121	PRO	2.7
1	B	261	LEU	2.7
1	E	113	LEU	2.7
1	C	426	ALA	2.7
1	B	236	VAL	2.7
1	B	146	ARG	2.7
1	D	360	ALA	2.7
1	K	47	GLN	2.7
1	B	366	THR	2.7
1	G	177	ASN	2.7
1	B	95	TRP	2.7
1	E	115	ALA	2.7
1	B	191	TYR	2.7
1	D	268	ASN	2.7
1	F	177	ASN	2.7
1	J	211	VAL	2.7
1	H	97	THR	2.7
1	G	209	MET	2.7
1	B	245	PHE	2.6
1	B	266	ASN	2.6
1	D	211	VAL	2.6
1	E	177	ASN	2.6
1	I	208	ASN	2.6
1	A	119	PRO	2.6
1	A	210	PRO	2.6
1	H	119	PRO	2.6
1	F	209	MET	2.6
1	J	353	MET	2.6
1	A	116	ALA	2.6
1	B	360	ALA	2.6
1	A	118	ASP	2.6
1	B	362	GLY	2.6
1	C	64	THR	2.6
1	D	362	GLY	2.6
1	B	204	GLN	2.6
1	B	199	CYS	2.6
1	C	211	VAL	2.6
1	D	215	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	95	TRP	2.6
1	D	425	THR	2.6
1	D	205	SER	2.6
1	C	123	ALA	2.5
1	C	255	ALA	2.5
1	E	206	CYS	2.5
1	I	143	ASN	2.5
1	L	25	ASN	2.5
1	E	118	ASP	2.5
1	K	210	PRO	2.5
1	D	259	TRP	2.5
1	D	254	GLN	2.5
1	K	40	SER	2.5
1	L	66	GLU	2.5
1	B	218	ASP	2.5
1	H	208	ASN	2.5
1	D	210	PRO	2.5
1	A	207	SER	2.5
1	B	187	PHE	2.5
1	B	359	ALA	2.5
1	G	204	GLN	2.5
1	D	195	PHE	2.4
1	D	249	SER	2.4
1	D	352	VAL	2.4
1	B	351	TRP	2.4
1	D	202	LEU	2.4
1	D	229	LEU	2.4
1	B	367	GLN	2.4
1	H	116	ALA	2.4
1	I	121	PRO	2.4
1	I	210	PRO	2.4
1	G	264	THR	2.4
1	B	206	CYS	2.4
1	J	206	CYS	2.4
1	B	356	LEU	2.4
1	K	202	LEU	2.4
1	C	201	ARG	2.4
1	D	216	ASN	2.4
1	B	243	SER	2.4
1	E	202	LEU	2.4
1	B	246	TYR	2.4
1	B	194	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	143	ASN	2.3
1	D	257	ASP	2.3
1	H	121	PRO	2.3
1	G	364	ALA	2.3
1	E	5	SER	2.3
1	B	7	PHE	2.3
1	D	235	VAL	2.3
1	B	47	GLN	2.3
1	C	35	LEU	2.3
1	B	257	ASP	2.3
1	K	143	ASN	2.3
1	D	234	GLY	2.3
1	D	203	THR	2.3
1	E	97	THR	2.3
1	C	207	SER	2.3
1	D	418	LEU	2.3
1	E	93	ASP	2.3
1	B	258	SER	2.3
1	E	42	SER	2.3
1	K	205	SER	2.3
1	K	211	VAL	2.3
1	B	214	ASP	2.3
1	L	208	ASN	2.3
1	E	244	GLY	2.3
1	D	415	ALA	2.3
1	E	116	ALA	2.3
1	D	260	THR	2.3
1	D	63	SER	2.3
1	E	207	SER	2.3
1	A	4	ILE	2.3
1	D	183	LEU	2.2
1	D	347	CYS	2.2
1	B	182	ARG	2.2
1	G	146	ARG	2.2
1	E	94	ALA	2.2
1	J	426	ALA	2.2
1	D	371	ASP	2.2
1	E	102	GLY	2.2
1	A	47	GLN	2.2
1	E	205	SER	2.2
1	I	41	SER	2.2
1	G	202	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	196	VAL	2.2
1	B	188	MET	2.2
1	E	213	PRO	2.2
1	G	353	MET	2.2
1	F	367	GLN	2.2
1	B	142	ALA	2.2
1	K	354	ALA	2.2
1	D	189	SER	2.2
1	F	217	TYR	2.2
1	C	365	LEU	2.2
1	D	227	LEU	2.2
1	D	252	ARG	2.2
1	H	25	ASN	2.2
1	K	118	ASP	2.2
1	I	120	PRO	2.2
1	B	244	GLY	2.2
1	I	204	GLN	2.2
1	D	206	CYS	2.2
1	B	41	SER	2.2
1	B	207	SER	2.2
1	B	422	ALA	2.2
1	D	369	ALA	2.2
1	G	207	SER	2.2
1	K	116	ALA	2.2
1	D	185	ASP	2.1
1	G	271	GLN	2.1
1	J	204	GLN	2.1
1	B	64	THR	2.1
1	C	33	THR	2.1
1	C	91	SER	2.1
1	I	63	SER	2.1
1	I	426	ALA	2.1
1	C	391	TYR	2.1
1	E	217	TYR	2.1
1	D	361	LYS	2.1
1	A	208	ASN	2.1
1	D	93	ASP	2.1
1	B	40	SER	2.1
1	D	292	SER	2.1
1	B	361	LYS	2.1
1	H	353	MET	2.1
1	C	217	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	119	PRO	2.1
1	C	105	TRP	2.1
1	J	186	TRP	2.1
1	F	206	CYS	2.1
1	B	116	ALA	2.1
1	D	200	ALA	2.1
1	D	250	LYS	2.1
1	G	426	ALA	2.1
1	B	190	GLN	2.1
1	I	371	ASP	2.1
1	C	98	PHE	2.1
1	B	248	SER	2.0
1	C	273	THR	2.0
1	G	11	MET	2.0
1	K	363	GLN	2.0
1	C	374	ASN	2.0
1	D	266	ASN	2.0
1	G	371	ASP	2.0
1	E	176	PRO	2.0
1	L	119	PRO	2.0
1	B	420	VAL	2.0
1	D	182	ARG	2.0
1	F	64	THR	2.0
1	G	205	SER	2.0
1	K	122	ALA	2.0
1	A	416	GLN	2.0
1	E	204	GLN	2.0
1	I	65	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1427	5/5	0.87	0.18	63,66,67,68	0
2	SO4	C	1427	5/5	0.89	0.13	85,85,85,86	0
2	SO4	J	1427	5/5	0.89	0.12	74,75,75,76	0
2	SO4	F	1427	5/5	0.91	0.14	63,63,66,66	0
2	SO4	I	1427	5/5	0.94	0.13	55,56,57,58	0
2	SO4	G	1427	5/5	0.94	0.10	67,67,68,68	0
2	SO4	B	1427	5/5	0.95	0.10	63,63,64,65	0
2	SO4	K	1427	5/5	0.97	0.15	49,49,51,52	0
2	SO4	L	1427	5/5	0.97	0.11	46,47,48,48	0
2	SO4	E	1427	5/5	0.98	0.10	49,50,51,52	0
2	SO4	H	1427	5/5	0.98	0.07	42,44,45,46	0
2	SO4	A	1427	5/5	0.98	0.09	48,49,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.