Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 11:02 pm GMT

PDB ID	:	2VAK
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 (i) 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 (i)) were used in the production of this report:

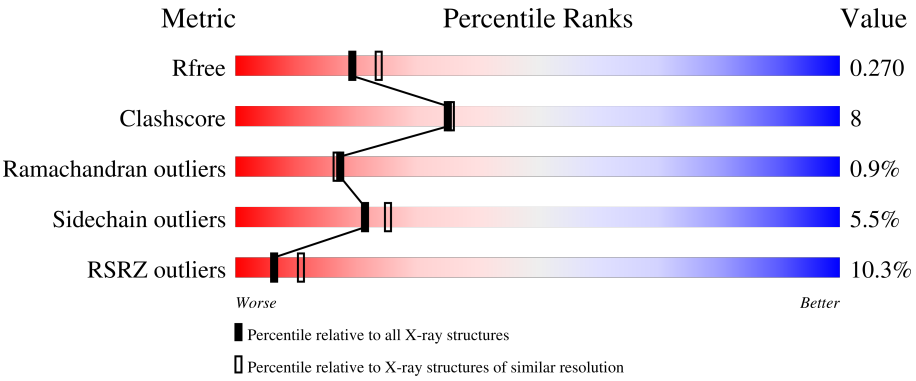
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	8% 82% 13%
1	B	423	17% 75% 18%
1	C	423	12% 76% 18%
1	D	423	27% 74% 20%
1	E	423	11% 79% 16%

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Mol	Chain	Length	Quality of chain
1	F	423	4% 81% 13%
1	G	423	4% 77% 15% 5%
1	H	423	6% 79% 16%
1	I	423	9% 80% 15%
1	J	423	7% 75% 17%
1	K	423	7% 78% 17%
1	L	423	7% 82% 12%

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 (i)

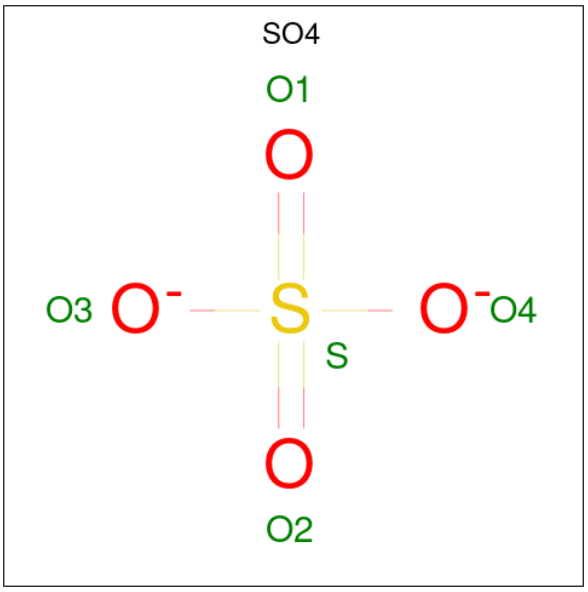
There are 3 unique types of molecules in this entry. The entry contains 41224 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

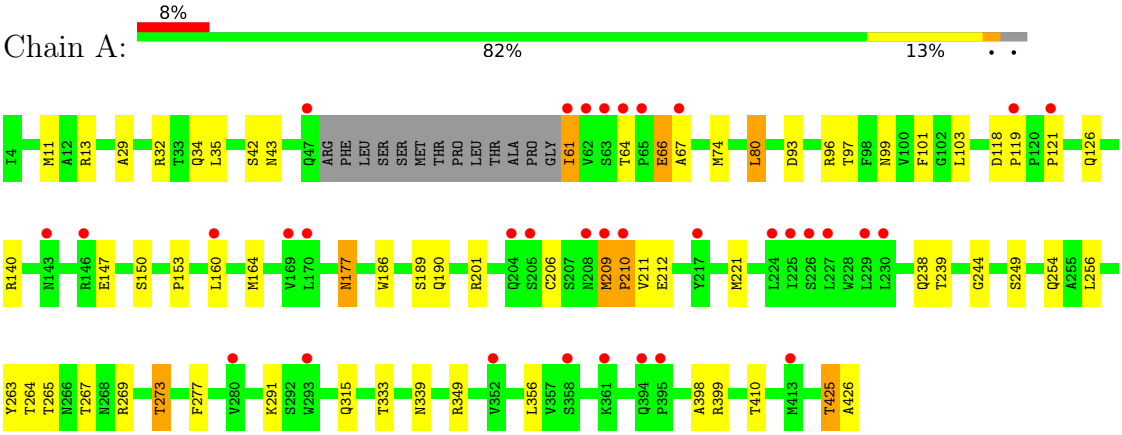
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	262	Total O 262 262	0	0
3	B	180	Total O 180 180	0	0
3	C	186	Total O 186 186	0	0
3	D	160	Total O 160 160	0	0
3	E	223	Total O 223 223	0	0
3	F	314	Total O 314 314	0	0
3	G	305	Total O 305 305	0	0
3	H	272	Total O 272 272	0	0
3	I	226	Total O 226 226	0	0
3	J	247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

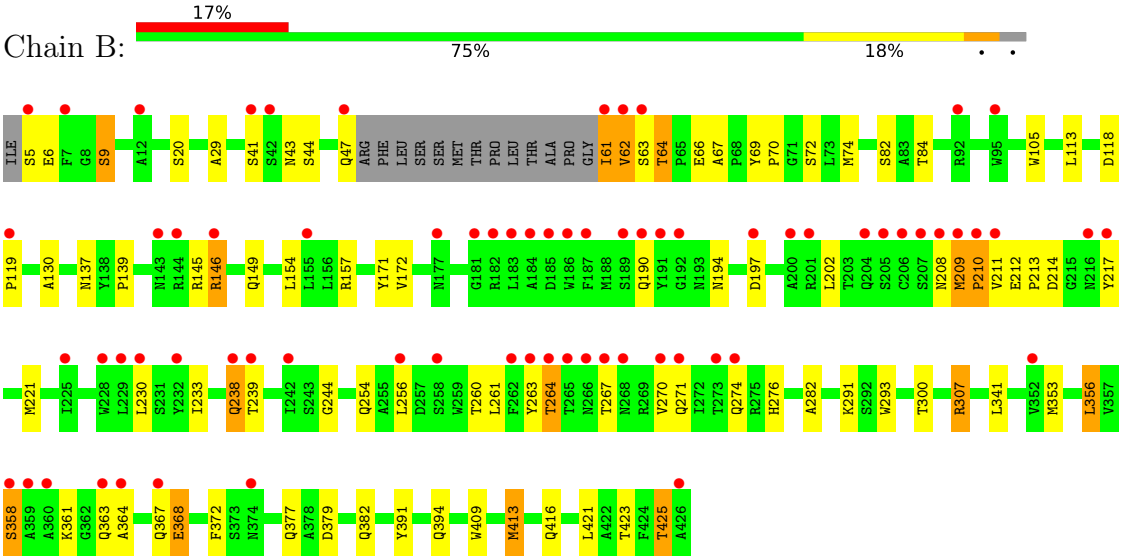
• Molecule 1: SIGMA A

Chain A:



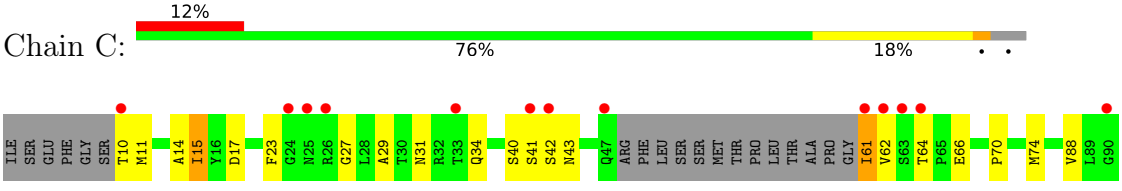
• Molecule 1: SIGMA A

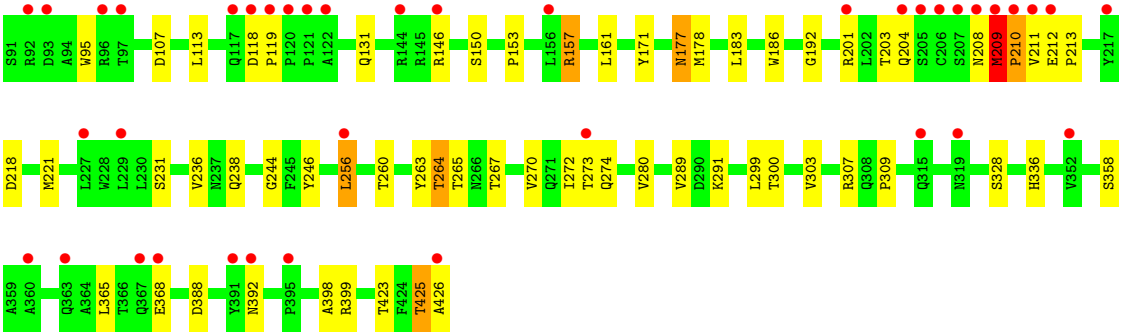
Chain B:



• Molecule 1: SIGMA A

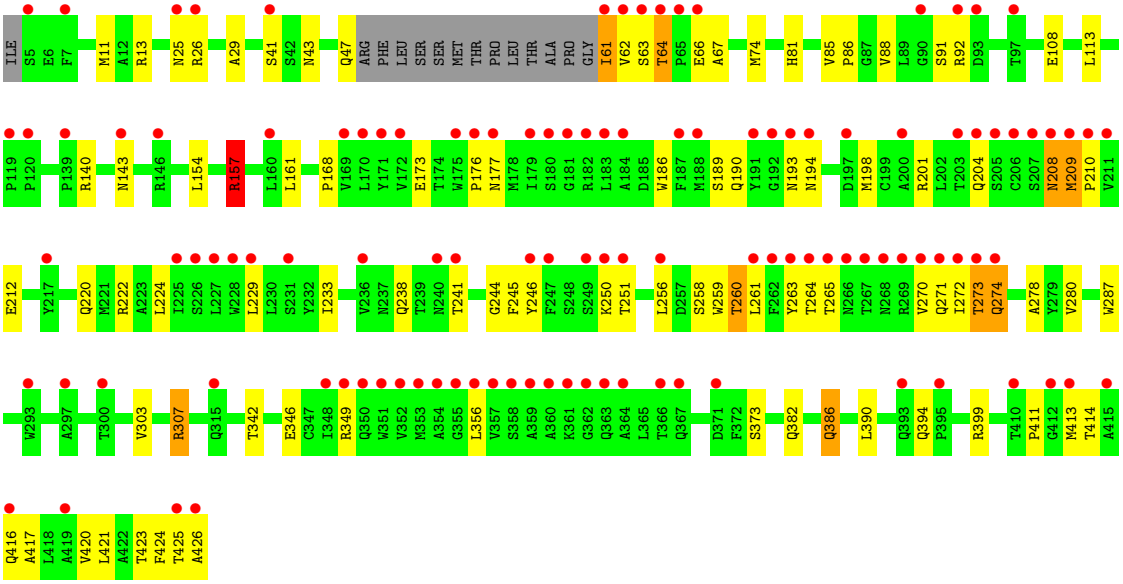
Chain C:





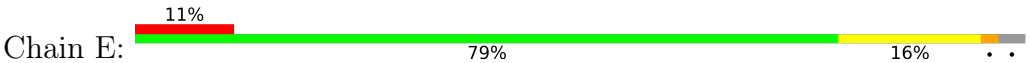
• Molecule 1: SIGMA A

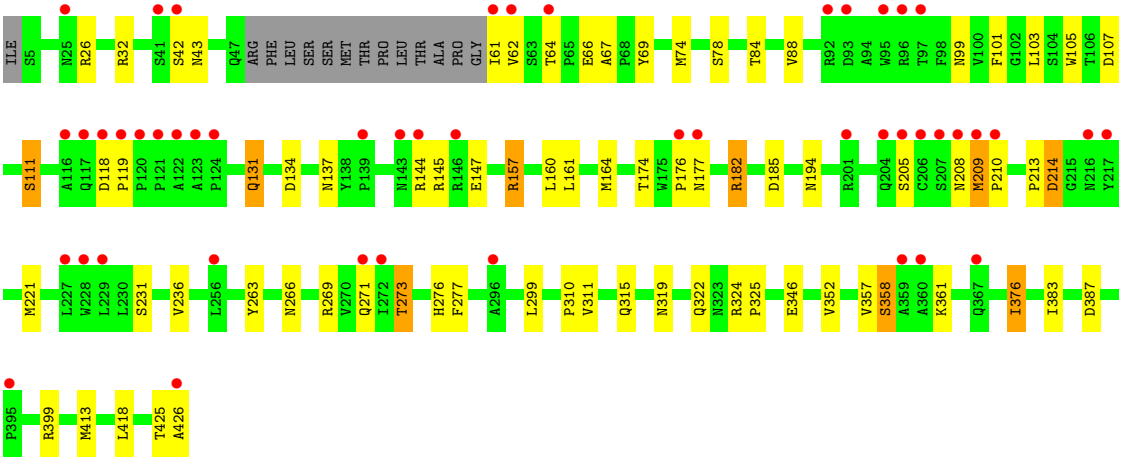
Chain D:



• Molecule 1: SIGMA A

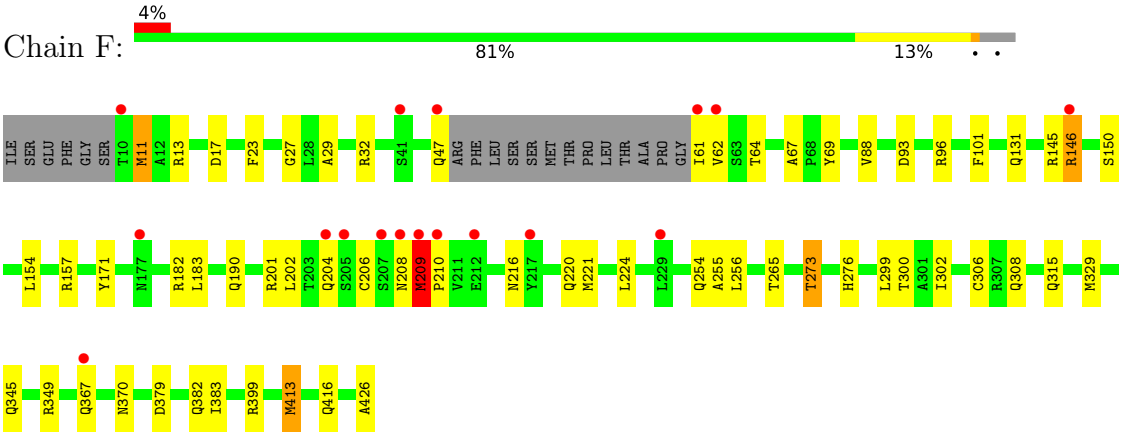
Chain E:





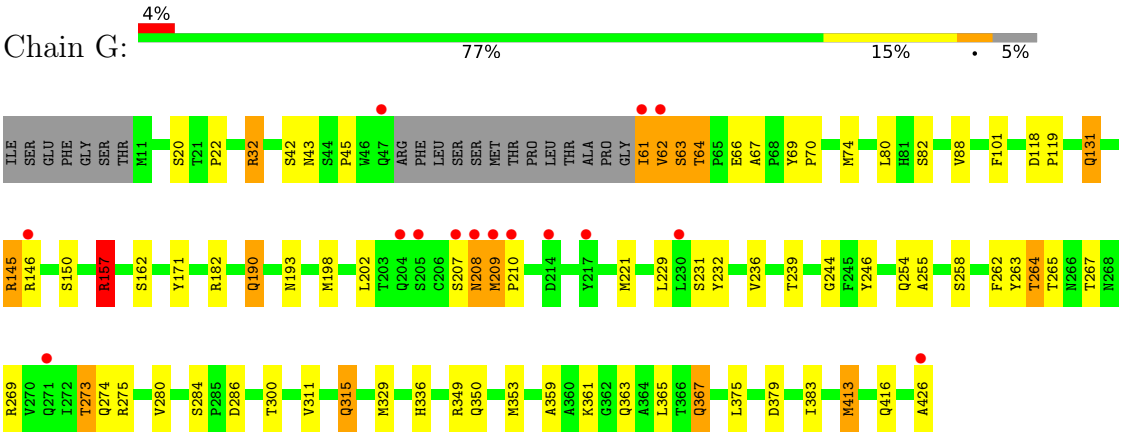
• Molecule 1: SIGMA A

Chain F:



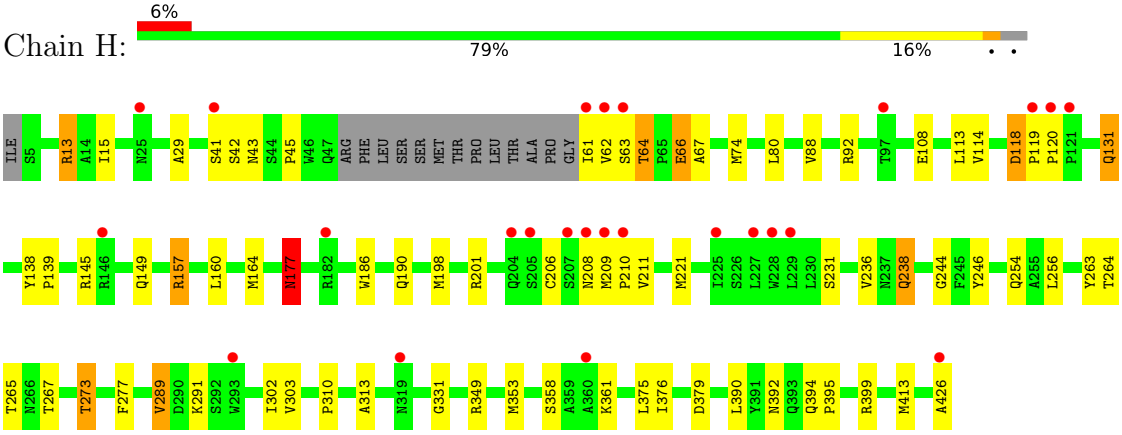
• Molecule 1: SIGMA A

Chain G:



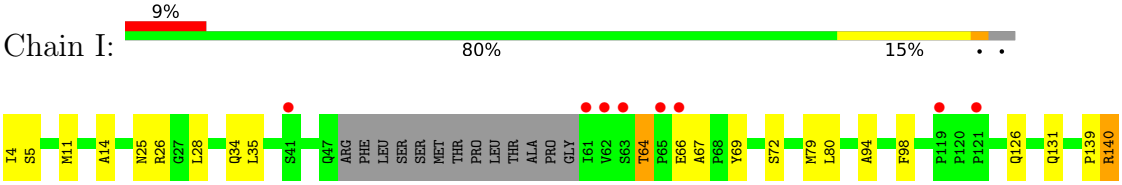
• Molecule 1: SIGMA A

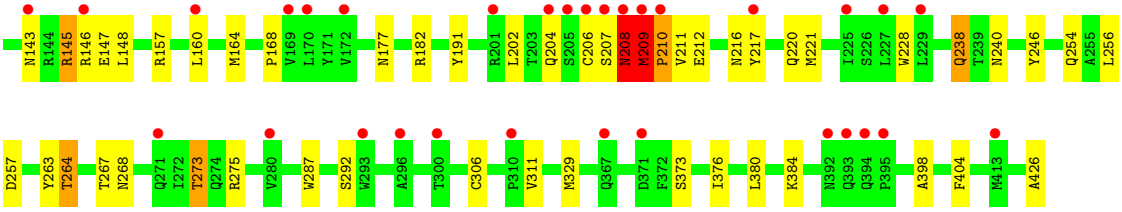
Chain H:



• Molecule 1: SIGMA A

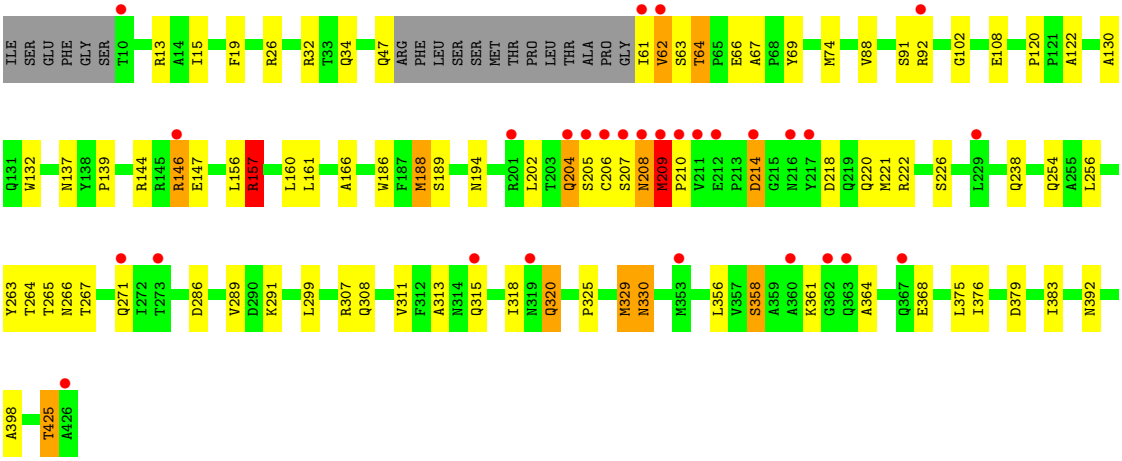
Chain I:





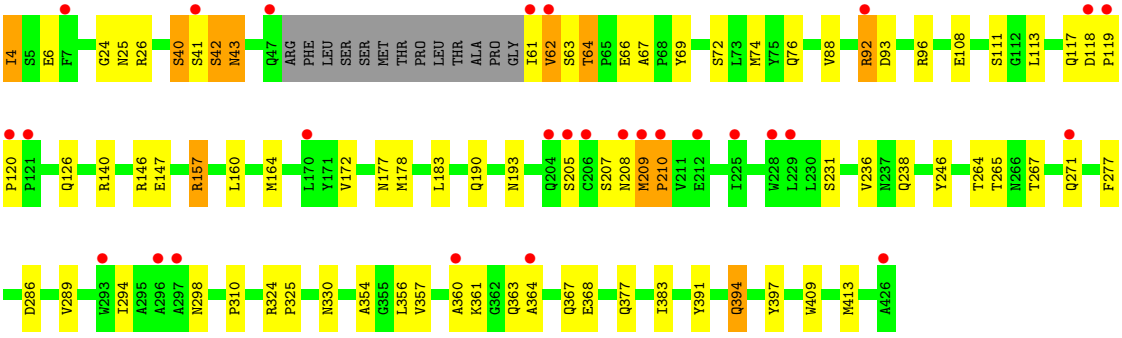
• Molecule 1: SIGMA A

Chain J:



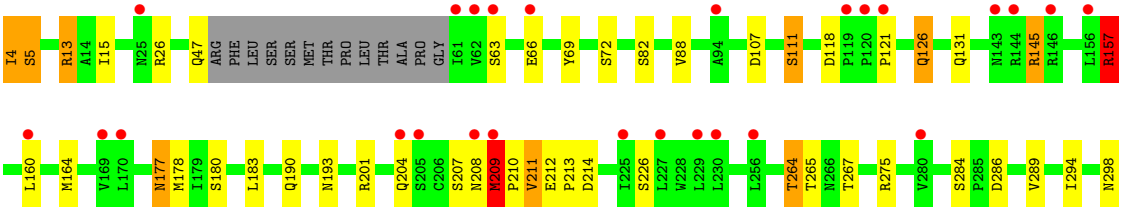
• Molecule 1: SIGMA A

Chain K:



• Molecule 1: SIGMA A

Chain L:




L299
T300
A301
V311
M329
N330
M353
A360
K361
L375
D379
K384
D387
N392
Q393
Q394
P395
F404
M413
A426

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.99 (at 2.34Å)	Xtriage
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 (0.49%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41224	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.69	0/3282	0.65	0/4478
1	B	0.62	0/3274	0.62	0/4467
1	C	0.64	0/3237	0.63	0/4418
1	D	0.63	0/3274	0.64	2/4467 (0.0%)
1	E	0.67	0/3274	0.66	0/4467
1	F	0.73	0/3237	0.70	0/4418
1	G	0.76	0/3230	0.72	3/4408 (0.1%)
1	H	0.71	0/3274	0.69	1/4467 (0.0%)
1	I	0.68	0/3282	0.65	1/4478 (0.0%)
1	J	0.67	0/3237	0.67	2/4418 (0.0%)
1	K	0.69	0/3282	0.69	1/4478 (0.0%)
1	L	0.79	0/3282	0.72	2/4478 (0.0%)
All	All	0.69	0/39165	0.67	12/53442 (0.0%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	J	157	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	J	157	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	D	157	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	157	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	K	62	VAL	N-CA-C	-5.56	96.00	111.00
1	G	157	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	L	157	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	L	387	ASP	CB-CG-OD1	5.20	122.98	118.30
1	G	375	LEU	CA-CB-CG	5.12	127.09	115.30
1	I	157	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	H	177	ASN	CB-CA-C	5.00	120.41	110.40

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3190	0	3082	61	0
1	C	3154	0	3054	64	0
1	D	3190	0	3082	54	0
1	E	3190	0	3082	44	0
1	F	3154	0	3054	37	0
1	G	3147	0	3047	53	0
1	H	3190	0	3082	65	0
1	I	3198	0	3093	57	0
1	J	3154	0	3054	69	0
1	K	3198	0	3093	59	0
1	L	3198	0	3093	34	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	7	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	614	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 8.

All (614) 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
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:H:221:MET:HE2	1:H:303:VAL:HG23	1.38	1.01
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:A:64:THR:HG23	1:A:67:ALA:H	1.31	0.94
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:H:221:MET:CE	1:H:303:VAL:HG23	1.98	0.93
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:311:VAL:HG11	1:J:329:MET:HE3	1.55	0.89
1:J:92:ARG:HD3	1:J:108:GLU:OE2	1.73	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: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:H:221:MET:HE2	1:H:303:VAL:CG2	2.05	0.85
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:THR:HB	1:A:426:ALA:OXT	1.83	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:B:209:MET:C	1:B:211:VAL:H	1.86	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:E:221:MET:HE2	1:E:299:LEU:HD22	1.66	0.77
1:H:390:LEU:HD13	1:I:11:MET:HE1	1.66	0.77
1:H:390:LEU:CD1	1:I:11:MET:HE1	2.15	0.76
1:A:118:ASP:HA	1:A:119:PRO:C	2.05	0.76
1:C:118:ASP:HA	1:C:119:PRO:C	2.07	0.75
1:D:61:ILE:C	1:D:63:SER:H	1.89	0.75
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:MET:HE2	1:C:299:LEU:HD22	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: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: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:J:188:MET:HE1	1:J:263:TYR:CD2	2.28	0.67
1:B:208:ASN:C	1:B:210:PRO:HD2	2.15	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:K:64:THR:HG21	3:K:2023:HOH:O	1.95	0.66
1:B:61:ILE:HD12	1:B:291:LYS:HE3	1.78	0.66
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
1:C:40:SER:C	1:C:42:SER:H	2.00	0.64
1:C:10:THR:HG21	1:C:213:PRO:HB2	1.78	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:C:218:ASP:CG	1:C:307:ARG:HH22	2.01	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:209:MET:HB2	3:K:2063:HOH:O	1.98	0.63
1:D:423:THR:C	1:D:425:THR:H	2.02	0.63
1:J:218:ASP:CG	1:J:307:ARG:HH22	2.02	0.63
1:B:190:GLN:O	1:B:261:LEU:HD23	1.99	0.62
1:H:145:ARG:O	1:H:149:GLN:HG3	1.98	0.62
1:C:192:GLY:O	1:C:260:THR:HG23	1.99	0.62
1:H:61:ILE:N	1:H:291:LYS:HZ3	1.97	0.62
1:B:276:HIS:ND1	3:B:2109:HOH:O	2.29	0.61
1:D:11:MET:HE1	3:E:2202:HOH:O	2.01	0.61
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:C:66:GLU:H	1:C:66:GLU:CD	2.04	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: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:B:209:MET:C	1:B:211:VAL:N	2.54	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
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:B:74:MET:CE	1:B:157:ARG:HD3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:88:VAL:HG12	1:D:88:VAL:O	2.02	0.58
1:H:118:ASP:HA	1:H:119:PRO:C	2.23	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: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:I:140:ARG:HH12	1:I:147:GLU:CD	2.07	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: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:K:394:GLN:HG2	1:K:397:TYR:HB2	1.85	0.57
1:H:390:LEU:CD1	1:I:11:MET:CE	2.82	0.56
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:A:209:MET:O	1:A:210:PRO:C	2.44	0.56
1:J:188:MET:CE	1:J:263:TYR:CD2	2.88	0.56
1:G:190:GLN:HG2	1:G:198:MET:HG2	1.87	0.56
1:A:64:THR:CG2	1:A:67:ALA:H	2.12	0.56
1:F:413:MET:HG3	1:F:416:GLN:CD	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:64:THR:HG22	1:D:67:ALA:H	1.71	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:F:221:MET:HE2	1:F:299:LEU:HD22	1.87	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:B:74:MET:HE2	1:B:157:ARG:HD3	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:G:413:MET:HG3	1:G:416:GLN:CD	2.27	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:F:11:MET:HE3	1:F:308:GLN:HB2	1.90	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:D:61:ILE:C	1:D:63:SER:N	2.61	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:J:61:ILE:C	1:J:63:SER:H	2.13	0.53
1:J:186:TRP:O	1:J:189:SER:OG	2.21	0.53
1:E:88:VAL:HG21	1:E:105:TRP:NE1	2.24	0.53
1:F:221:MET:HE1	1:F:302:ILE:HG21	1.90	0.53
1:H:61:ILE:O	1:H:61:ILE:CG2	2.57	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:F:202:LEU:HD13	1:F:221:MET:HG2	1.93	0.51
1:G:284:SER:OG	1:G:286:ASP:OD1	2.12	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: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: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:118:ASP:HA	1:K:119:PRO:C	2.31	0.50
1:K:238:GLN:HG3	1:K:246:TYR:OH	2.12	0.50
1:H:66:GLU:H	1:H:66:GLU:CD	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:93:ASP:O	1:K:96:ARG:HG3	2.12	0.49
1:A:66:GLU:H	1:A:66:GLU:CD	2.15	0.49
1:B:202:LEU:HB3	1:B:221:MET:HE2	1.94	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:E:118:ASP:HA	1:E:119:PRO:C	2.32	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: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: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: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: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:L:178:MET:O	1:L:183:LEU:HD23	2.14	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:206:CYS:O	1:F:209:MET:HE2	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:A:61:ILE:N	1:A:291:LYS:HZ1	2.12	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:286:ASP:O	1:L:289:VAL:HG12	2.13	0.47
1:H:277:PHE:CE2	1:H:310:PRO:HG2	2.49	0.47
1:C:40:SER:C	1:C:42:SER:N	2.66	0.47
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: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: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: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:G:350:GLN:HA	1:G:353:MET:HE2	1.96	0.46
1:I:64:THR:HG23	1:I:66:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:423:THR:C	1:B:425:THR:H	2.18	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
1:L:284:SER:OG	1:L:286:ASP:OD1	2.25	0.46
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: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:E:208:ASN:CG	1:E:210:PRO:HD2	2.35	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:H:118:ASP:CA	1:H:119:PRO:C	2.84	0.46
1:B:137:ASN:O	1:B:139:PRO:HD3	2.16	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:H:61:ILE:C	1:H:63:SER:H	2.20	0.45
1:I:207:SER:O	1:I:208:ASN:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:221:MET:HE2	1:J:299:LEU:HD22	1.99	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: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
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: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: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:221:MET:HE1	1:H:302:ILE:HB	2.00	0.44
1:H:349:ARG:O	1:H:353:MET:HG3	2.18	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:J:188:MET:HE1	1:J:263:TYR:CE2	2.53	0.44
1:K:64:THR:HG23	1:K:66:GLU:HG2	1.99	0.44
1:L:353:MET:HE1	3:L:2114:HOH:O	2.18	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:H:221:MET:HE3	1:H:303:VAL:HG23	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:85:VAL:O	1:D:86:PRO:C	2.56	0.43
1:J:205:SER:C	1:J:207:SER:H	2.20	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:C:153:PRO:HG2	1:C:209:MET:CE	2.48	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
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:C:231:SER:HA	1:C:236:VAL:O	2.18	0.43
1:G:42:SER:O	1:G:43:ASN:HB2	2.18	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: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:E:42:SER:O	1:E:43:ASN:HB2	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:L:207:SER:C	1:L:209:MET:H	2.22	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: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:C:208:ASN:C	1:C:210:PRO:HD2	2.40	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:5:SER:OG	1:B:6:GLU:N	2.48	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:J:66:GLU:H	1:J:66:GLU:CD	2.22	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:A:160:LEU:O	1:A:164:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:69:TYR:HE1	1:J:383:ILE:HD12	1.86	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: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: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:256:LEU:O	1:I:257:ASP:C	2.59	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:349:ARG:HG2	1:H:353:MET:HE2	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:423:THR:C	1:C:425:THR:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:62:VAL:HG22	1:J:62:VAL:O	2.21	0.41
1:J:188:MET:HE2	1:J:263:TYR:CG	2.56	0.41
1:L:13:ARG:HD3	1:L:15:ILE:O	2.21	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:A:153:PRO:HG2	1:A:209:MET:HE3	2.02	0.40
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: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:B:74:MET:HE3	1:B:157:ARG:HD3	2.04	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:F:11:MET:HE3	1:F:11:MET:HB3	1.97	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: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 (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	406/423 (96%)	392 (97%)	12 (3%)	2 (0%)	29	31
1	B	405/423 (96%)	376 (93%)	26 (6%)	3 (1%)	22	22
1	C	400/423 (95%)	379 (95%)	17 (4%)	4 (1%)	15	14
1	D	405/423 (96%)	376 (93%)	21 (5%)	8 (2%)	7	4
1	E	405/423 (96%)	382 (94%)	19 (5%)	4 (1%)	15	14
1	F	400/423 (95%)	385 (96%)	13 (3%)	2 (0%)	29	31
1	G	399/423 (94%)	383 (96%)	13 (3%)	3 (1%)	19	20
1	H	405/423 (96%)	386 (95%)	17 (4%)	2 (0%)	29	31
1	I	406/423 (96%)	385 (95%)	18 (4%)	3 (1%)	22	22
1	J	400/423 (95%)	376 (94%)	18 (4%)	6 (2%)	10	7
1	K	406/423 (96%)	385 (95%)	16 (4%)	5 (1%)	13	11
1	L	406/423 (96%)	389 (96%)	13 (3%)	4 (1%)	15	14
All	All	4843/5076 (95%)	4594 (95%)	203 (4%)	46 (1%)	17	17

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 (i)

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%)	24	30
1	B	339/352 (96%)	317 (94%)	22 (6%)	17	19
1	C	335/352 (95%)	320 (96%)	15 (4%)	27	34
1	D	339/352 (96%)	317 (94%)	22 (6%)	17	19
1	E	339/352 (96%)	323 (95%)	16 (5%)	26	33
1	F	335/352 (95%)	316 (94%)	19 (6%)	20	24
1	G	334/352 (95%)	312 (93%)	22 (7%)	16	18
1	H	339/352 (96%)	321 (95%)	18 (5%)	22	27
1	I	340/352 (97%)	326 (96%)	14 (4%)	30	38
1	J	335/352 (95%)	316 (94%)	19 (6%)	20	24
1	K	340/352 (97%)	325 (96%)	15 (4%)	28	35
1	L	340/352 (97%)	317 (93%)	23 (7%)	16	17
All	All	4055/4224 (96%)	3833 (94%)	222 (6%)	21	25

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET
1	A	13	ARG
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	209	MET
1	A	212	GLU
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	61	ILE
1	B	62	VAL
1	B	64	THR

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Mol	Chain	Res	Type
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	274	GLN
1	B	307	ARG
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	157	ARG
1	C	177	ASN
1	C	203	THR
1	C	212	GLU
1	C	256	LEU
1	C	264	THR
1	C	265	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	26	ARG
1	D	41	SER
1	D	47	GLN
1	D	64	THR
1	D	140	ARG
1	D	143	ASN
1	D	157	ARG
1	D	204	GLN

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Mol	Chain	Res	Type
1	D	208	ASN
1	D	212	GLU
1	D	220	GLN
1	D	250	LYS
1	D	258	SER
1	D	260	THR
1	D	265	THR
1	D	274	GLN
1	D	307	ARG
1	D	349	ARG
1	D	373	SER
1	D	386	GLN
1	E	61	ILE
1	E	66	GLU
1	E	78	SER
1	E	111	SER
1	E	131	GLN
1	E	157	ARG
1	E	176	PRO
1	E	177	ASN
1	E	182	ARG
1	E	194	ASN
1	E	214	ASP
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	17	ASP
1	F	47	GLN
1	F	61	ILE
1	F	88	VAL
1	F	131	GLN
1	F	146	ARG
1	F	150	SER
1	F	154	LEU
1	F	157	ARG
1	F	182	ARG
1	F	204	GLN
1	F	265	THR

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Mol	Chain	Res	Type
1	F	273	THR
1	F	306	CYS
1	F	329	MET
1	F	379	ASP
1	F	413	MET
1	G	32	ARG
1	G	61	ILE
1	G	63	SER
1	G	64	THR
1	G	88	VAL
1	G	131	GLN
1	G	145	ARG
1	G	146	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	258	SER
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	13	ARG
1	H	41	SER
1	H	64	THR
1	H	66	GLU
1	H	74	MET
1	H	88	VAL
1	H	118	ASP
1	H	131	GLN
1	H	157	ARG
1	H	177	ASN
1	H	208	ASN
1	H	238	GLN
1	H	265	THR
1	H	273	THR
1	H	289	VAL

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Mol	Chain	Res	Type
1	H	358	SER
1	H	392	ASN
1	H	413	MET
1	I	25	ASN
1	I	64	THR
1	I	131	GLN
1	I	140	ARG
1	I	145	ARG
1	I	177	ASN
1	I	204	GLN
1	I	208	ASN
1	I	212	GLU
1	I	238	GLN
1	I	254	GLN
1	I	264	THR
1	I	273	THR
1	I	373	SER
1	J	13	ARG
1	J	47	GLN
1	J	64	THR
1	J	88	VAL
1	J	146	ARG
1	J	157	ARG
1	J	188	MET
1	J	194	ASN
1	J	204	GLN
1	J	226	SER
1	J	265	THR
1	J	291	LYS
1	J	320	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

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Mol	Chain	Res	Type
1	K	64	THR
1	K	88	VAL
1	K	92	ARG
1	K	111	SER
1	K	157	ARG
1	K	208	ASN
1	K	265	THR
1	K	394	GLN
1	K	413	MET
1	L	4	ILE
1	L	5	SER
1	L	13	ARG
1	L	47	GLN
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	264	THR
1	L	265	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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	B	406	ASN
1	D	47	GLN
1	D	177	ASN
1	D	271	GLN
1	D	382	GLN

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Mol	Chain	Res	Type
1	E	126	GLN
1	F	276	HIS
1	F	336	HIS
1	G	25	ASN
1	G	131	GLN
1	G	137	ASN
1	G	216	ASN
1	I	374	ASN
1	J	320	GLN
1	J	392	ASN
1	K	43	ASN
1	K	216	ASN
1	K	393	GLN
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 monosaccharides 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	C	1427	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	E	1427	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	D	1427	-	4,4,4	0.22	0	6,6,6	0.41	0
2	SO4	K	1427	-	4,4,4	0.23	0	6,6,6	0.63	0
2	SO4	F	1427	-	4,4,4	0.17	0	6,6,6	0.37	0
2	SO4	L	1427	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	G	1427	-	4,4,4	0.14	0	6,6,6	0.31	0
2	SO4	B	1427	-	4,4,4	0.20	0	6,6,6	0.24	0
2	SO4	H	1427	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	I	1427	-	4,4,4	0.12	0	6,6,6	0.29	0
2	SO4	J	1427	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	A	1427	-	4,4,4	0.15	0	6,6,6	0.21	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	E	1427	SO4	1	0
2	F	1427	SO4	1	0
2	L	1427	SO4	1	0
2	G	1427	SO4	1	0
2	H	1427	SO4	2	0
2	J	1427	SO4	3	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, 95^{th} 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%)	0.33	34 (8%) 11 17	18, 31, 52, 72	0
1	B	409/423 (96%)	0.93	71 (17%) 1 2	21, 46, 89, 102	0
1	C	404/423 (95%)	0.70	52 (12%) 3 6	25, 41, 68, 90	0
1	D	409/423 (96%)	1.12	115 (28%) 0 0	22, 47, 88, 96	0
1	E	409/423 (96%)	0.58	48 (11%) 4 8	19, 38, 66, 84	0
1	F	404/423 (95%)	0.16	17 (4%) 36 47	14, 27, 50, 81	0
1	G	403/423 (95%)	0.17	15 (3%) 41 52	12, 26, 47, 84	0
1	H	409/423 (96%)	0.30	25 (6%) 21 30	15, 30, 51, 77	0
1	I	410/423 (96%)	0.40	39 (9%) 8 13	20, 35, 55, 81	0
1	J	404/423 (95%)	0.27	29 (7%) 15 22	20, 34, 58, 90	0
1	K	410/423 (96%)	0.23	28 (6%) 17 25	15, 30, 54, 76	0
1	L	410/423 (96%)	0.26	29 (7%) 16 23	14, 27, 49, 68	0
All	All	4891/5076 (96%)	0.46	502 (10%) 6 11	12, 34, 70, 102	0

All (502) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	SER	10.1
1	B	205	SER	9.9
1	C	119	PRO	9.3
1	D	208	ASN	8.8
1	B	61	ILE	8.7
1	E	61	ILE	8.3
1	C	62	VAL	8.3
1	D	61	ILE	8.0
1	J	10	THR	7.8
1	D	426	ALA	7.5
1	B	204	GLN	7.3

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Mol	Chain	Res	Type	RSRZ
1	E	205	SER	7.3
1	D	352	VAL	7.2
1	C	256	LEU	7.2
1	D	268	ASN	7.2
1	G	208	ASN	7.1
1	B	62	VAL	6.8
1	I	62	VAL	6.8
1	D	266	ASN	6.8
1	C	204	GLN	6.8
1	K	204	GLN	6.8
1	K	61	ILE	6.7
1	E	120	PRO	6.7
1	B	207	SER	6.6
1	D	357	VAL	6.4
1	E	62	VAL	6.4
1	F	61	ILE	6.4
1	D	360	ALA	6.3
1	B	217	TYR	6.3
1	E	123	ALA	6.2
1	D	62	VAL	6.2
1	D	210	PRO	6.1
1	D	217	TYR	6.1
1	E	119	PRO	6.1
1	H	61	ILE	6.1
1	B	208	ASN	5.9
1	B	206	CYS	5.9
1	C	118	ASP	5.8
1	F	207	SER	5.8
1	I	205	SER	5.8
1	G	210	PRO	5.8
1	D	209	MET	5.8
1	H	62	VAL	5.7
1	D	271	GLN	5.7
1	E	209	MET	5.7
1	H	120	PRO	5.6
1	F	62	VAL	5.6
1	B	266	ASN	5.5
1	B	426	ALA	5.5
1	J	207	SER	5.5
1	J	62	VAL	5.5
1	G	62	VAL	5.5
1	D	177	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	209	MET	5.4
1	C	208	ASN	5.4
1	D	206	CYS	5.4
1	B	42	SER	5.4
1	G	61	ILE	5.3
1	D	204	GLN	5.3
1	D	182	ARG	5.3
1	J	210	PRO	5.2
1	B	41	SER	5.2
1	C	207	SER	5.2
1	B	239	THR	5.2
1	K	41	SER	5.1
1	I	61	ILE	5.1
1	I	204	GLN	5.1
1	D	267	THR	5.1
1	D	270	VAL	5.1
1	D	351	TRP	5.0
1	H	209	MET	5.0
1	K	210	PRO	4.9
1	B	256	LEU	4.9
1	A	204	GLN	4.9
1	B	363	GLN	4.9
1	F	204	GLN	4.8
1	D	191	TYR	4.8
1	E	121	PRO	4.8
1	B	182	ARG	4.8
1	A	209	MET	4.8
1	J	209	MET	4.8
1	E	256	LEU	4.8
1	L	62	VAL	4.7
1	G	204	GLN	4.7
1	E	217	TYR	4.7
1	J	205	SER	4.7
1	C	41	SER	4.6
1	C	121	PRO	4.6
1	D	205	SER	4.6
1	E	42	SER	4.6
1	H	119	PRO	4.6
1	B	7	PHE	4.6
1	A	62	VAL	4.6
1	K	62	VAL	4.5
1	E	118	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	186	TRP	4.4
1	E	360	ALA	4.4
1	A	121	PRO	4.4
1	I	209	MET	4.3
1	C	61	ILE	4.3
1	B	185	ASP	4.3
1	L	209	MET	4.3
1	I	63	SER	4.3
1	E	206	CYS	4.3
1	E	41	SER	4.3
1	H	208	ASN	4.2
1	H	210	PRO	4.2
1	J	426	ALA	4.2
1	B	229	LEU	4.2
1	I	65	PRO	4.2
1	A	119	PRO	4.2
1	J	204	GLN	4.2
1	D	207	SER	4.1
1	G	426	ALA	4.1
1	L	119	PRO	4.1
1	C	146	ARG	4.1
1	I	207	SER	4.1
1	I	208	ASN	4.0
1	E	210	PRO	4.0
1	D	273	THR	4.0
1	B	360	ALA	4.0
1	I	121	PRO	4.0
1	D	359	ALA	4.0
1	C	209	MET	4.0
1	D	197	ASP	4.0
1	C	426	ALA	4.0
1	A	63	SER	4.0
1	D	356	LEU	3.9
1	D	348	ILE	3.9
1	C	206	CYS	3.9
1	K	209	MET	3.9
1	E	204	GLN	3.9
1	K	229	LEU	3.9
1	H	204	GLN	3.9
1	G	207	SER	3.8
1	F	208	ASN	3.8
1	D	349	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	393	GLN	3.8
1	D	7	PHE	3.8
1	B	225	ILE	3.8
1	D	192	GLY	3.8
1	D	176	PRO	3.8
1	B	191	TYR	3.8
1	D	364	ALA	3.7
1	B	263	TYR	3.7
1	E	359	ALA	3.7
1	D	175	TRP	3.7
1	A	64	THR	3.7
1	E	93	ASP	3.6
1	E	122	ALA	3.6
1	D	194	ASN	3.6
1	B	210	PRO	3.6
1	C	120	PRO	3.6
1	C	47	GLN	3.6
1	A	229	LEU	3.6
1	H	97	THR	3.6
1	C	217	TYR	3.6
1	F	10	THR	3.6
1	C	212	GLU	3.5
1	E	207	SER	3.5
1	B	364	ALA	3.5
1	E	144	ARG	3.5
1	L	204	GLN	3.5
1	D	225	ILE	3.5
1	B	264	THR	3.5
1	B	267	THR	3.4
1	B	181	GLY	3.4
1	B	216	ASN	3.4
1	B	92	ARG	3.4
1	D	355	GLY	3.4
1	B	358	SER	3.4
1	E	117	GLN	3.4
1	D	419	ALA	3.4
1	B	265	THR	3.4
1	D	264	THR	3.4
1	D	187	PHE	3.4
1	I	229	LEU	3.4
1	J	217	TYR	3.3
1	I	271	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	170	LEU	3.3
1	D	172	VAL	3.3
1	B	63	SER	3.3
1	I	41	SER	3.3
1	D	184	ALA	3.3
1	D	229	LEU	3.3
1	A	208	ASN	3.3
1	K	228	TRP	3.3
1	F	205	SER	3.2
1	B	144	ARG	3.2
1	I	169	VAL	3.2
1	L	208	ASN	3.2
1	J	208	ASN	3.2
1	D	63	SER	3.2
1	B	177	ASN	3.2
1	D	169	VAL	3.2
1	B	359	ALA	3.2
1	H	229	LEU	3.2
1	A	217	TYR	3.2
1	E	208	ASN	3.2
1	B	273	THR	3.2
1	A	395	PRO	3.2
1	F	210	PRO	3.2
1	K	208	ASN	3.2
1	D	367	GLN	3.1
1	D	416	GLN	3.1
1	C	10	THR	3.1
1	D	211	VAL	3.1
1	H	121	PRO	3.1
1	D	263	TYR	3.1
1	D	274	GLN	3.1
1	B	47	GLN	3.1
1	D	293	TRP	3.1
1	D	180	SER	3.1
1	I	395	PRO	3.1
1	B	200	ALA	3.1
1	C	211	VAL	3.0
1	D	188	MET	3.0
1	A	210	PRO	3.0
1	J	211	VAL	3.0
1	K	205	SER	3.0
1	B	143	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	201	ARG	3.0
1	J	363	GLN	3.0
1	J	61	ILE	3.0
1	I	225	ILE	3.0
1	B	271	GLN	3.0
1	I	66	GLU	3.0
1	E	116	ALA	3.0
1	L	66	GLU	3.0
1	C	367	GLN	3.0
1	D	251	THR	3.0
1	C	319	ASN	2.9
1	C	273	THR	2.9
1	K	225	ILE	2.9
1	I	172	VAL	2.9
1	K	170	LEU	2.9
1	D	171	TYR	2.9
1	L	395	PRO	2.9
1	E	97	THR	2.9
1	J	229	LEU	2.9
1	C	360	ALA	2.9
1	C	210	PRO	2.9
1	I	119	PRO	2.9
1	B	183	LEU	2.9
1	I	413	MET	2.9
1	D	300	THR	2.8
1	E	64	THR	2.8
1	D	183	LEU	2.8
1	J	92	ARG	2.8
1	E	395	PRO	2.8
1	E	228	TRP	2.8
1	I	217	TYR	2.8
1	A	225	ILE	2.8
1	D	119	PRO	2.8
1	D	41	SER	2.8
1	H	205	SER	2.8
1	D	64	THR	2.8
1	L	225	ILE	2.8
1	E	229	LEU	2.8
1	L	229	LEU	2.8
1	E	143	ASN	2.8
1	A	205	SER	2.8
1	F	41	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	232	TYR	2.8
1	L	25	ASN	2.8
1	B	268	ASN	2.8
1	D	139	PRO	2.8
1	K	119	PRO	2.8
1	C	26	ARG	2.8
1	J	367	GLN	2.8
1	H	228	TRP	2.8
1	B	192	GLY	2.7
1	D	358	SER	2.7
1	C	25	ASN	2.7
1	E	25	ASN	2.7
1	L	360	ALA	2.7
1	L	61	ILE	2.7
1	I	210	PRO	2.7
1	L	121	PRO	2.7
1	B	190	GLN	2.7
1	D	256	LEU	2.7
1	D	236	VAL	2.7
1	I	170	LEU	2.7
1	D	249	SER	2.7
1	D	395	PRO	2.7
1	H	182	ARG	2.7
1	D	246	TYR	2.7
1	C	42	SER	2.6
1	E	216	ASN	2.6
1	G	209	MET	2.6
1	H	207	SER	2.6
1	D	200	ALA	2.6
1	K	364	ALA	2.6
1	F	146	ARG	2.6
1	B	230	LEU	2.6
1	B	270	VAL	2.6
1	G	217	TYR	2.6
1	K	271	GLN	2.6
1	B	228	TRP	2.6
1	E	92	ARG	2.6
1	C	229	LEU	2.6
1	C	352	VAL	2.6
1	I	201	ARG	2.6
1	H	426	ALA	2.6
1	D	265	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	271	GLN	2.6
1	B	184	ALA	2.6
1	C	392	ASN	2.6
1	H	25	ASN	2.6
1	F	47	GLN	2.5
1	K	118	ASP	2.5
1	K	360	ALA	2.5
1	G	146	ARG	2.5
1	D	203	THR	2.5
1	D	353	MET	2.5
1	D	415	ALA	2.5
1	C	63	SER	2.5
1	B	367	GLN	2.5
1	E	271	GLN	2.5
1	L	120	PRO	2.5
1	D	90	GLY	2.5
1	J	216	ASN	2.5
1	K	206	CYS	2.5
1	D	371	ASP	2.5
1	J	319	ASN	2.5
1	D	228	TRP	2.5
1	L	280	VAL	2.5
1	B	12	ALA	2.5
1	G	214	ASP	2.5
1	C	96	ARG	2.5
1	A	230	LEU	2.5
1	I	293	TRP	2.5
1	I	227	LEU	2.5
1	B	189	SER	2.4
1	A	169	VAL	2.4
1	B	146	ARG	2.4
1	I	392	ASN	2.4
1	D	393	GLN	2.4
1	L	205	SER	2.4
1	D	247	PHE	2.4
1	C	33	THR	2.4
1	C	395	PRO	2.4
1	H	225	ILE	2.4
1	H	360	ALA	2.4
1	H	146	ARG	2.4
1	D	231	SER	2.4
1	H	63	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	160	LEU	2.4
1	A	352	VAL	2.4
1	I	371	ASP	2.4
1	D	143	ASN	2.4
1	D	193	ASN	2.4
1	D	363	GLN	2.4
1	C	93	ASP	2.4
1	B	262	PHE	2.4
1	L	169	VAL	2.4
1	B	238	GLN	2.4
1	D	5	SER	2.4
1	D	93	ASP	2.4
1	J	353	MET	2.4
1	C	64	THR	2.4
1	C	97	THR	2.4
1	D	425	THR	2.4
1	B	274	GLN	2.4
1	B	258	SER	2.4
1	E	95	TRP	2.3
1	E	227	LEU	2.3
1	L	227	LEU	2.3
1	D	97	THR	2.3
1	D	413	MET	2.3
1	E	367	GLN	2.3
1	J	212	GLU	2.3
1	C	122	ALA	2.3
1	E	426	ALA	2.3
1	D	261	LEU	2.3
1	I	146	ARG	2.3
1	D	262	PHE	2.3
1	C	117	GLN	2.3
1	C	315	GLN	2.3
1	D	412	GLY	2.3
1	E	176	PRO	2.3
1	J	206	CYS	2.3
1	L	230	LEU	2.3
1	A	226	SER	2.3
1	A	413	MET	2.3
1	B	187	PHE	2.3
1	C	201	ARG	2.3
1	A	143	ASN	2.3
1	D	315	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	144	ARG	2.3
1	L	146	ARG	2.3
1	D	25	ASN	2.3
1	D	250	LYS	2.3
1	A	170	LEU	2.2
1	A	227	LEU	2.2
1	C	227	LEU	2.2
1	D	227	LEU	2.2
1	E	96	ARG	2.2
1	B	352	VAL	2.2
1	K	293	TRP	2.2
1	K	47	GLN	2.2
1	B	242	ILE	2.2
1	J	201	ARG	2.2
1	J	360	ALA	2.2
1	C	90	GLY	2.2
1	J	214	ASP	2.2
1	C	363	GLN	2.2
1	A	65	PRO	2.2
1	D	179	ILE	2.2
1	D	354	ALA	2.2
1	D	366	THR	2.2
1	D	410	THR	2.2
1	D	240	ASN	2.2
1	H	227	LEU	2.2
1	D	350	GLN	2.2
1	A	146	ARG	2.2
1	D	26	ARG	2.2
1	I	310	PRO	2.2
1	K	7	PHE	2.2
1	B	95	TRP	2.2
1	L	156	LEU	2.2
1	D	361	LYS	2.2
1	J	362	GLY	2.2
1	I	160	LEU	2.2
1	B	119	PRO	2.2
1	K	120	PRO	2.2
1	C	391	TYR	2.2
1	D	226	SER	2.2
1	G	205	SER	2.2
1	I	367	GLN	2.2
1	A	361	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	206	CYS	2.2
1	A	293	TRP	2.2
1	G	230	LEU	2.2
1	C	368	GLU	2.2
1	D	66	GLU	2.2
1	E	124	PRO	2.2
1	A	47	GLN	2.2
1	A	67	ALA	2.1
1	L	94	ALA	2.1
1	B	155	LEU	2.1
1	B	197	ASP	2.1
1	K	121	PRO	2.1
1	D	362	GLY	2.1
1	C	144	ARG	2.1
1	A	160	LEU	2.1
1	E	177	ASN	2.1
1	I	143	ASN	2.1
1	H	293	TRP	2.1
1	D	241	THR	2.1
1	F	367	GLN	2.1
1	D	146	ARG	2.1
1	D	65	PRO	2.1
1	E	272	ILE	2.1
1	L	170	LEU	2.1
1	J	315	GLN	2.1
1	K	296	ALA	2.1
1	L	300	THR	2.1
1	D	92	ARG	2.1
1	C	24	GLY	2.1
1	E	139	PRO	2.1
1	H	41	SER	2.1
1	A	61	ILE	2.1
1	F	177	ASN	2.1
1	H	319	ASN	2.1
1	D	181	GLY	2.1
1	D	120	PRO	2.1
1	C	156	LEU	2.1
1	D	272	ILE	2.1
1	A	394	GLN	2.1
1	I	394	GLN	2.1
1	F	212	GLU	2.1
1	D	297	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	358	SER	2.1
1	I	280	VAL	2.1
1	K	212	GLU	2.0
1	D	269	ARG	2.0
1	E	201	ARG	2.0
1	F	229	LEU	2.0
1	B	374	ASN	2.0
1	F	209	MET	2.0
1	E	296	ALA	2.0
1	L	63	SER	2.0
1	B	211	VAL	2.0
1	G	47	GLN	2.0
1	C	92	ARG	2.0
1	E	146	ARG	2.0
1	F	217	TYR	2.0
1	A	224	LEU	2.0
1	L	256	LEU	2.0
1	J	271	GLN	2.0
1	J	273	THR	2.0
1	B	5	SER	2.0
1	J	146	ARG	2.0
1	A	280	VAL	2.0
1	L	143	ASN	2.0
1	D	160	LEU	2.0
1	I	300	THR	2.0
1	K	92	ARG	2.0
1	I	296	ALA	2.0
1	K	297	ALA	2.0
1	K	426	ALA	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 monosaccharides 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, 95^{th} 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	D	1427	5/5	0.94	0.26	63,66,67,68	0
2	SO4	J	1427	5/5	0.94	0.25	74,75,75,76	0
2	SO4	F	1427	5/5	0.95	0.23	63,63,66,66	0
2	SO4	C	1427	5/5	0.95	0.37	85,85,85,86	0
2	SO4	G	1427	5/5	0.97	0.15	67,67,68,68	0
2	SO4	I	1427	5/5	0.97	0.17	55,56,57,58	0
2	SO4	B	1427	5/5	0.97	0.21	63,63,64,65	0
2	SO4	K	1427	5/5	0.98	0.20	49,49,51,52	0
2	SO4	A	1427	5/5	0.99	0.15	48,49,49,50	0
2	SO4	E	1427	5/5	0.99	0.18	49,50,51,52	0
2	SO4	H	1427	5/5	0.99	0.14	42,44,45,46	0
2	SO4	L	1427	5/5	0.99	0.17	46,47,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.