Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:57 AM 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

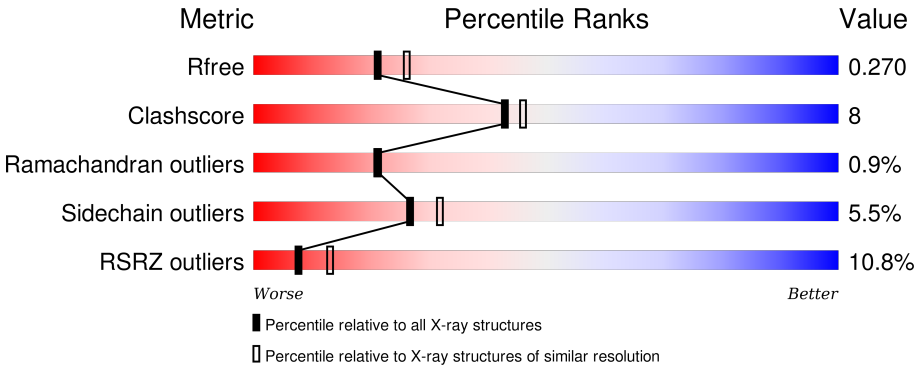
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	9% 82% 13%
1	B	423	17% 75% 18%
1	C	423	13% 76% 18%
1	D	423	28% 74% 20%
1	E	423	12% 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	8% 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	C	1427	-	-	-	X
2	SO4	F	1427	-	-	-	X
2	SO4	H	1427	-	-	X	-
2	SO4	J	1427	-	-	X	-

2 Entry composition (i)

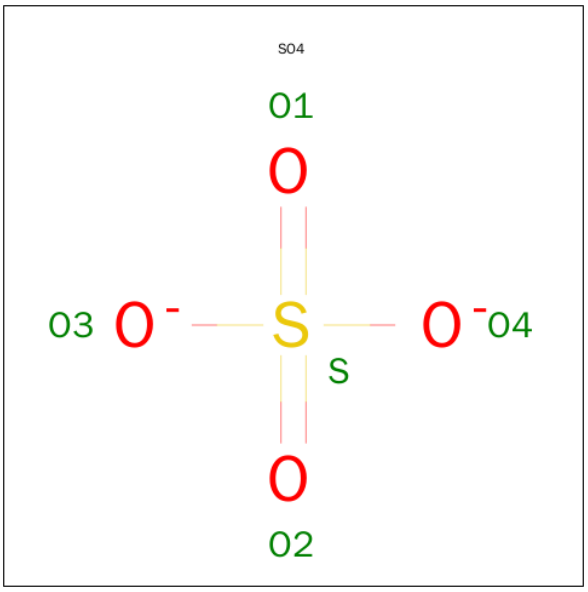
There are 3 unique types of molecules in this entry. The entry contains 41224 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

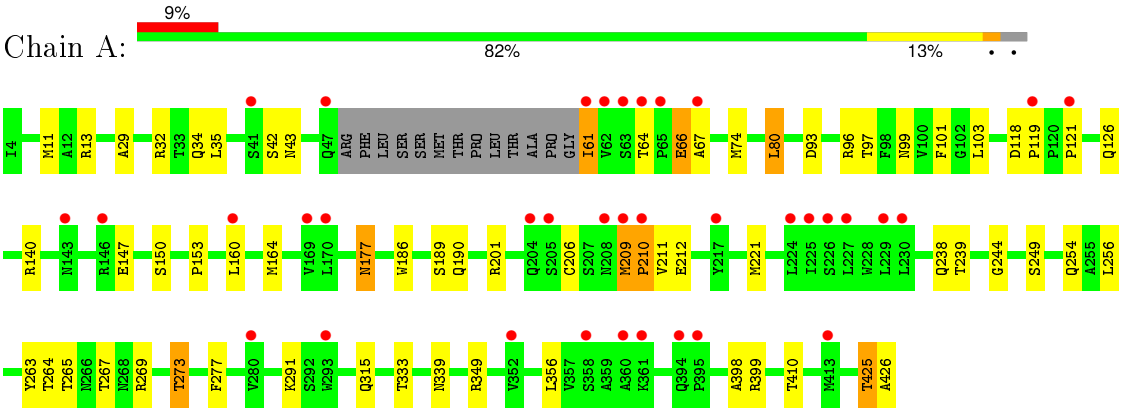
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	262	Total O 262 262	0	0
3	B	180	Total O 180 180	0	0
3	C	186	Total O 186 186	0	0
3	D	160	Total O 160 160	0	0
3	E	223	Total O 223 223	0	0
3	F	314	Total O 314 314	0	0
3	G	305	Total O 305 305	0	0
3	H	272	Total O 272 272	0	0
3	I	226	Total O 226 226	0	0
3	J	247	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

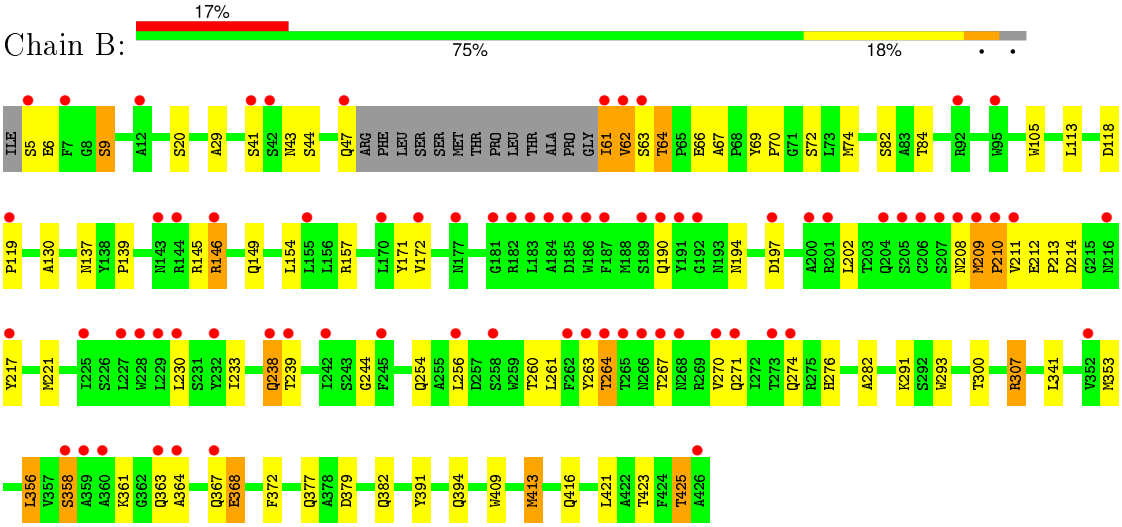
- Molecule 1: SIGMA A

Chain A:



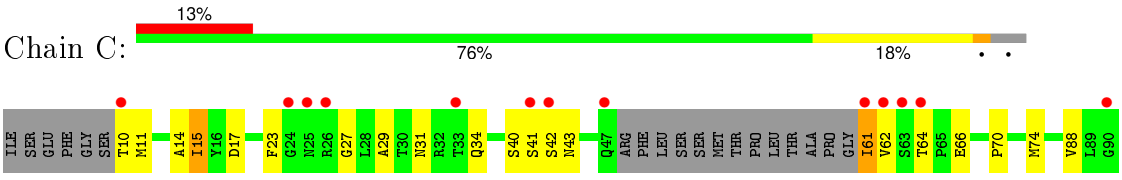
- Molecule 1: SIGMA A

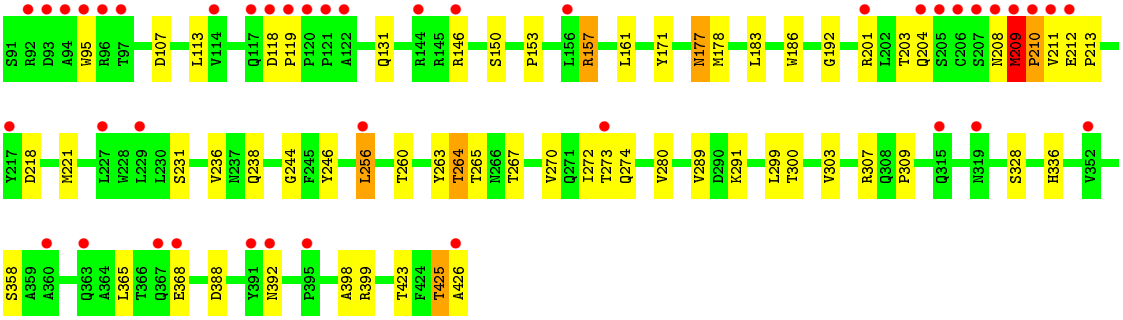
Chain B:



- Molecule 1: SIGMA A

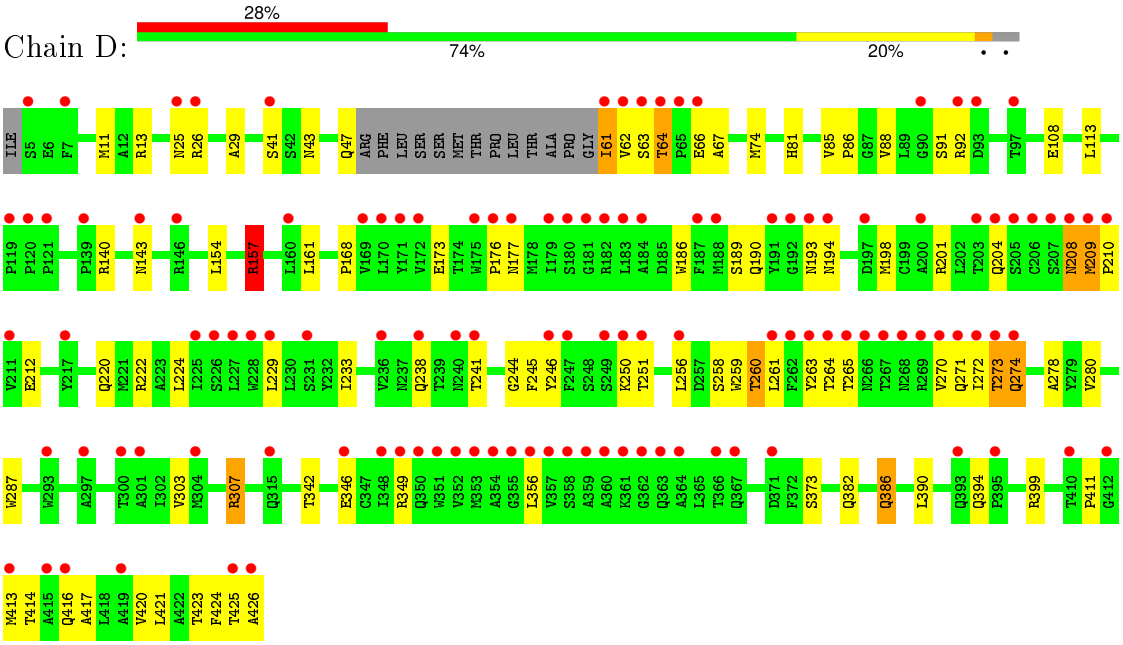
Chain C:





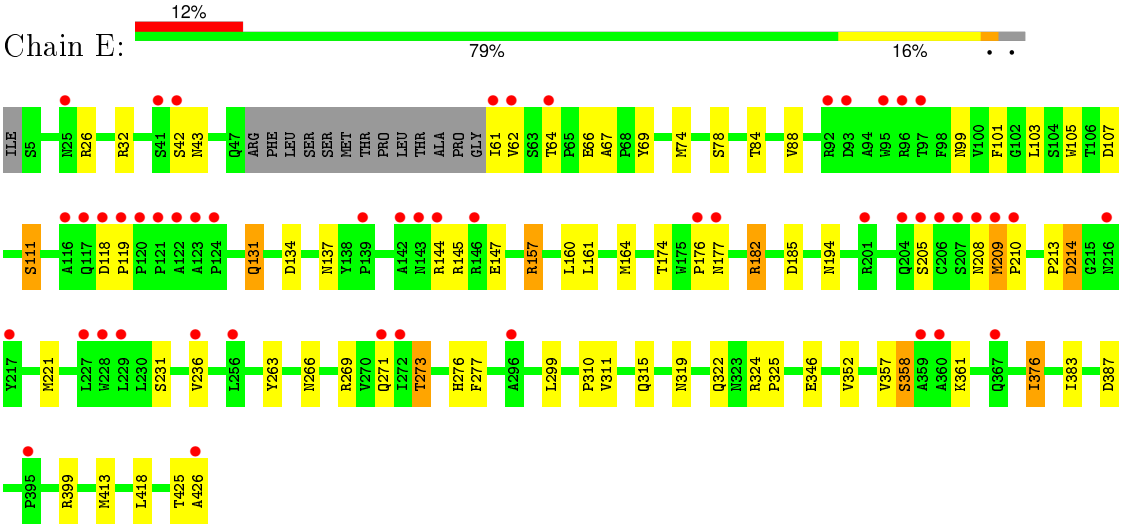
• Molecule 1: SIGMA A

Chain D:



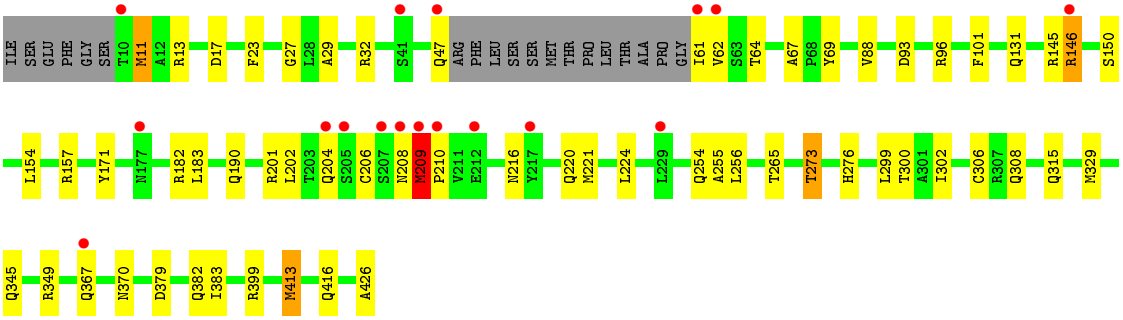
• Molecule 1: SIGMA A

Chain E:



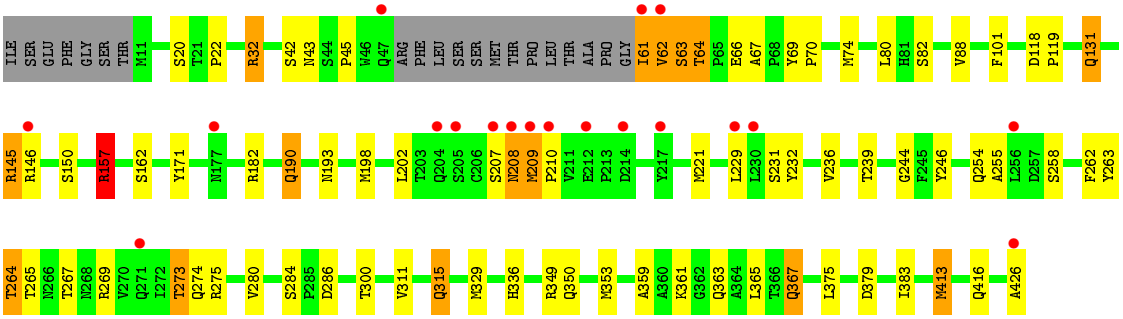
• Molecule 1: SIGMA A

Chain F:



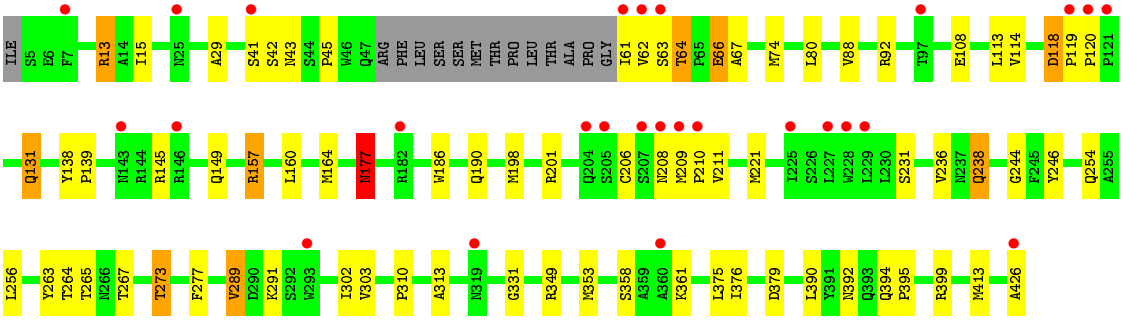
• Molecule 1: SIGMA A

Chain G:



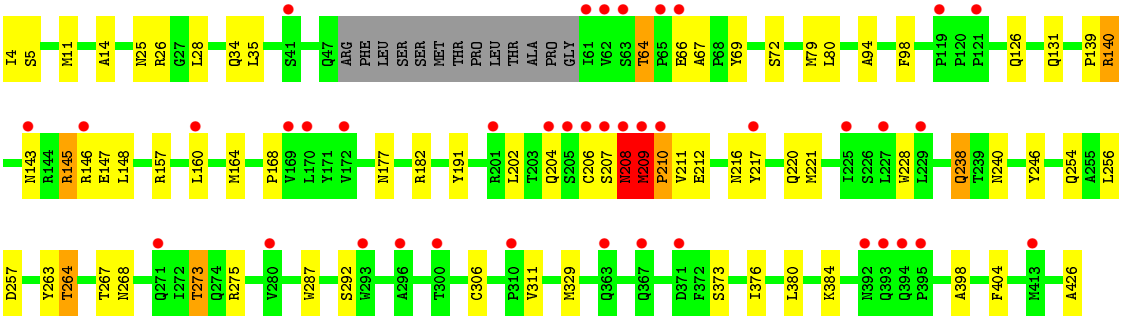
• Molecule 1: SIGMA A

Chain H:



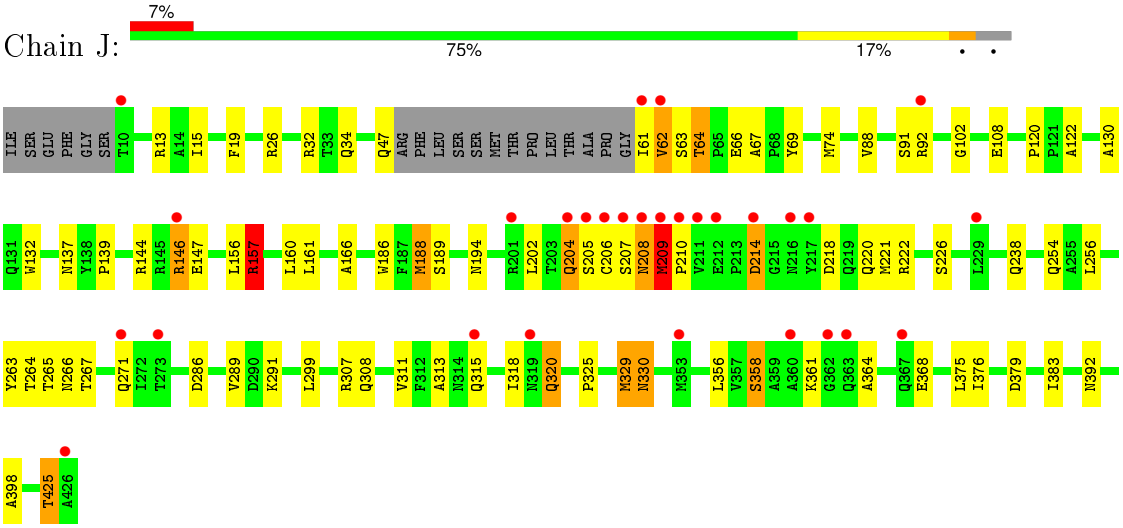
• Molecule 1: SIGMA A

Chain I:



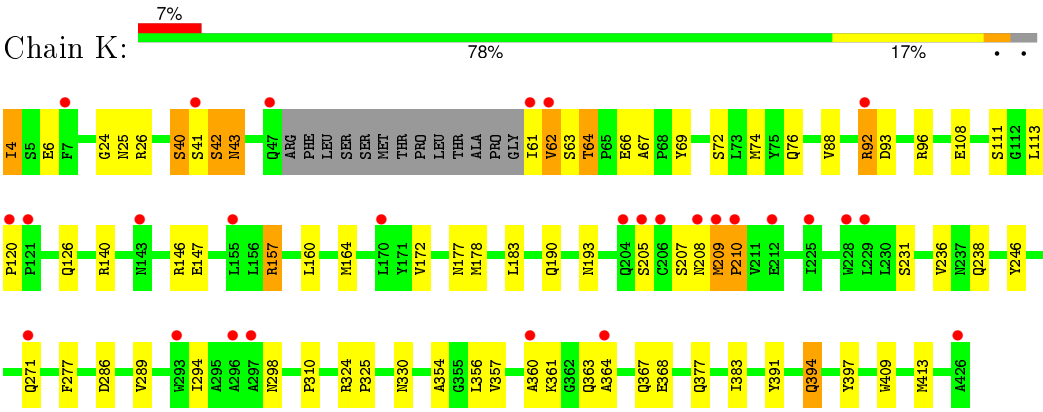
• Molecule 1: SIGMA A

Chain J:



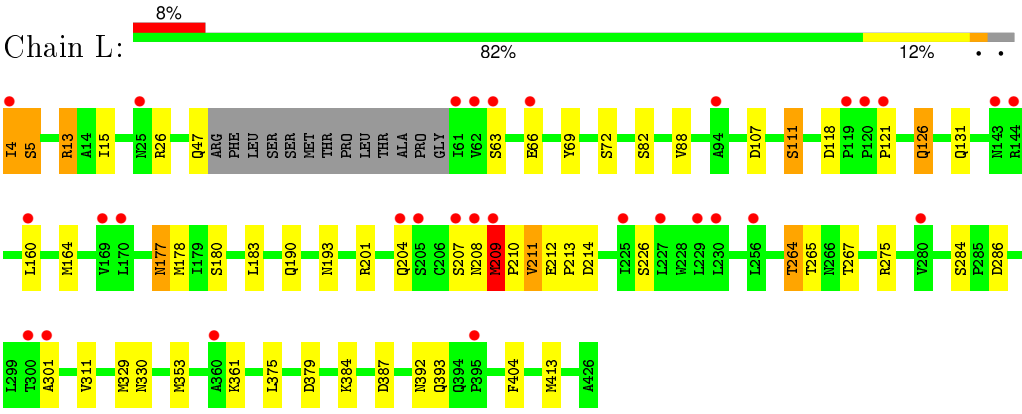
• Molecule 1: SIGMA A

Chain K:



• Molecule 1: SIGMA A

Chain L:



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) 92.3 (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%)	DCC
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 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.38$	Xtriage
Outliers	0 of 282059 reflections	Xtriage
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

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, 0.375 respectively for untwinned datasets, and 0.333, 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:HG2	1:G:157:ARG:HH11	1.19	1.07
1:B:64:THR:HG22	1:B:67:ALA:H	1.20	1.07
1:I:140:ARG:HH11	1:I:140:ARG:HG2	1.06	1.06
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.12	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:HH11	1:E:157:ARG:HG2	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:HH11	1:D:157:ARG:HG2	1.34	0.90
1:J:311:VAL:HG11	1:J:329:MET:HE3	1.55	0.89
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: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:H:221:MET:HE2	1:H:303:VAL:CG2	2.05	0.85
1:E:64:THR:HG23	1:E:67:ALA:H	1.41	0.85
1:I:4:ILE:HA	3:I:2155:HOH:O	1.77	0.84
1:K:64:THR:HG22	1:K:67:ALA:H	1.43	0.83
1:G:64:THR:HG22	1:G:67:ALA:H	1.43	0.83
1:C:157:ARG:HG2	1:C:157:ARG:NH1	1.87	0.83
1:I:140:ARG:NH1	1:I:147:GLU:OE1	2.11	0.82
1:B:264:THR:HB	1:B:267:THR:CG2	2.08	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:NH1	1:I:140:ARG:HG2	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:J:364:ALA:O	1:J:368:GLU:HG3	1.90	0.72
1:D:271:GLN:O	1:D:426:ALA:HB2	1.88	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:H:64:THR:HG22	1:H:67:ALA:N	2.06	0.70
1:C:61:ILE:HG22	1:C:62:VAL:H	1.55	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:J:218:ASP:OD1	1:J:307:ARG:NH2	2.26	0.69
1:G:190:GLN:HG3	1:G:193:ASN:OD1	1.92	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:J:188:MET:HE1	1:J:263:TYR:CD2	2.28	0.67
1:H:394:GLN:HG3	1:I:14:ALA:HB1	1.76	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:L:180:SER:HB3	3:L:2146:HOH:O	1.95	0.67
1:E:64:THR:CG2	1:E:67:ALA:H	2.07	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:238:GLN:HG3	1:I:246:TYR:OH	1.96	0.65
1:I:207:SER:O	1:I:208:ASN:HB3	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:H:206:CYS:O	1:H:209:MET:HB3	1.95	0.65
1:C:61:ILE:HD13	1:C:70:PRO:HD3	1.77	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:NH1	1:E:157:ARG:HG2	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:NH1	1:D:157:ARG:HG2	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:H:61:ILE:N	1:H:291:LYS:HZ3	1.97	0.62
1:C:192:GLY:O	1:C:260:THR:HG23	1.99	0.62
1:B:276:HIS:ND1	3:B:2109:HOH:O	2.29	0.61
1:D:61:ILE:O	1:D:61:ILE:HG22	2.00	0.61
1:K:394:GLN:HB2	3:K:2275:HOH:O	2.00	0.61
1:D:11:MET:HE1	3:E:2202:HOH:O	2.01	0.61
1:G:275:ARG:HG3	1:G:275:ARG:HH11	1.65	0.61
1:A:264:THR:HG21	1:A:267:THR:OG1	2.00	0.61
1:J:209:MET:H	1:J:210:PRO:HD3	1.66	0.61
1:C:66:GLU:CD	1:C:66:GLU:H	2.04	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:H:42:SER:O	1:H:43:ASN:HB2	2.00	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:H:210:PRO:HG2	3:H:2142:HOH:O	2.01	0.61
1:F:254:GLN:HG2	1:F:255:ALA:N	2.16	0.61
1:K:69:TYR:HE1	1:K:383:ILE:CD1	2.14	0.61
1:K:26:ARG:HD2	3:K:2031:HOH:O	1.99	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:H:157:ARG:NH1	1:H:157:ARG:HG2	2.12	0.59
1:K:40:SER:O	1:K:43:ASN:N	2.30	0.59
1:J:130:ALA:CB	1:J:320:GLN:HG3	2.32	0.59
1:L:107:ASP:OD2	1:L:111:SER:HB2	2.02	0.59
1:F:224:LEU:HD23	1:F:299:LEU:HD11	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:MET:CE	1:B:157:ARG:HD3	2.33	0.59
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:A:97:THR:HB	1:A:121:PRO:HB2	1.85	0.58
1:D:88:VAL:O	1:D:88:VAL:HG12	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:I:238:GLN:HG3	1:I:246:TYR:CZ	2.38	0.58
1:C:74:MET:HG2	1:C:161:LEU:HD22	1.86	0.58
1:G:62:VAL:O	1:G:62:VAL:HG22	2.02	0.58
1:H:61:ILE:HG22	1:H:61:ILE:O	2.03	0.58
1:I:146:ARG:NH2	1:I:210:PRO:HD3	2.17	0.58
1:B:367:GLN:OE1	1:B:367:GLN:HA	2.04	0.58
1:I:273:THR:HB	1:I:426:ALA:OXT	2.04	0.58
1:C:209:MET:O	1:C:211:VAL:N	2.35	0.58
1:I:140:ARG:HH12	1:I:147:GLU:CD	2.07	0.57
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:I:35:LEU:HD22	1:I:80:LEU:HB2	1.86	0.57
1:E:107:ASP:OD2	1:E:111:SER:HB2	2.04	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:H:45:PRO:HB3	1:H:80:LEU:HD21	1.87	0.56
1:C:244:GLY:HA3	1:C:263:TYR:CE1	2.40	0.56
1:A:32:ARG:HD2	1:A:101:PHE:O	2.06	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:384:LYS:HD3	1:I:404:PHE:CE2	2.43	0.54
1:I:5:SER:O	1:I:275:ARG:HD2	2.07	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: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:C:280:VAL:HG22	1:C:336:HIS:HB2	1.88	0.54
1:I:140:ARG:NH1	1:I:140:ARG:CG	2.51	0.54
1:B:74:MET:HE2	1:B:157:ARG:HD3	1.89	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:G:413:MET:HG3	1:G:416:GLN:CD	2.27	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:F:11:MET:HE3	1:F:308:GLN:HB2	1.90	0.53
1:C:29:ALA:HB1	1:C:399:ARG:HG3	1.91	0.53
1:H:390:LEU:HD13	1:I:11:MET:CE	2.37	0.53
1:D:278:ALA:HA	3:D:2124:HOH:O	2.08	0.53
1:C:88:VAL:O	1:C:88:VAL:HG12	2.07	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:J:61:ILE:C	1:J:63:SER:H	2.13	0.53
1:G:359:ALA:O	1:G:363:GLN:HG2	2.08	0.53
1:J:186:TRP:O	1:J:189:SER:OG	2.21	0.53
1:I:146:ARG:NH2	1:I:210:PRO:CD	2.64	0.53
1:H:61:ILE:CG2	1:H:61:ILE:O	2.57	0.53
1:F:221:MET:HE1	1:F:302:ILE:HG21	1.90	0.53
1:E:88:VAL:HG21	1:E:105:TRP:NE1	2.24	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:K:42:SER:O	1:K:43:ASN:HB2	2.10	0.52
1:F:146:ARG:NH2	1:F:210:PRO:HD3	2.23	0.52
1:H:118:ASP:N	1:H:118:ASP:OD1	2.42	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:D:245:PHE:HB3	1:D:261:LEU:HD11	1.92	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: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:G:361:LYS:O	1:G:365:LEU:HG	2.09	0.51
1:D:189:SER:HB2	3:D:2080:HOH:O	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:L:157:ARG:HB3	1:L:301:ALA:CB	2.38	0.51
1:J:74:MET:HG2	1:J:161:LEU:HD22	1.90	0.51
1:H:42:SER:O	1:H:43:ASN:CB	2.57	0.51
1:G:353:MET:HG3	3:G:2249:HOH:O	2.10	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: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:C:273:THR:HB	1:C:426:ALA:OXT	2.11	0.50
1:B:230:LEU:HD23	1:B:233:ILE:HD11	1.92	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:K:118:ASP:HA	1:K:119:PRO:C	2.31	0.50
1:A:186:TRP:O	1:A:189:SER:OG	2.24	0.50
1:D:241:THR:HG21	1:D:264:THR:HG22	1.92	0.50
1:C:23:PHE:CE2	1:C:27:GLY:HA2	2.47	0.50
1:K:238:GLN:HG3	1:K:246:TYR:OH	2.12	0.50
1:H:66:GLU:CD	1:H:66:GLU:H	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:D:423:THR:O	1:D:425:THR:N	2.45	0.49
1:C:150:SER:HA	1:C:209:MET:HG3	1.95	0.49
1:B:202:LEU:HB3	1:B:221:MET:HE2	1.94	0.49
1:A:66:GLU:H	1:A:66:GLU:CD	2.15	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:B:210:PRO:HA	3:B:2096:HOH:O	2.12	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:F:254:GLN:HG3	3:F:2191:HOH:O	2.11	0.49
1:C:270:VAL:HG12	1:C:272:ILE:HG13	1.94	0.49
1:E:387:ASP:HB3	1:E:399:ARG:NH1	2.28	0.49
1:C:201:ARG:O	1:C:204:GLN:HB3	2.13	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: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:B:9:SER:HB2	1:B:307:ARG:HE	1.77	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:I:206:CYS:O	1:I:209:MET:HA	2.13	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: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:B:146:ARG:HE	1:B:146:ARG:HB2	1.38	0.48
1:C:186:TRP:HA	3:C:2079:HOH:O	2.13	0.48
1:I:209:MET:O	1:I:211:VAL:HG23	2.14	0.48
1:I:26:ARG:HD2	3:I:2205:HOH:O	2.13	0.48
1:E:231:SER:HA	1:E:236:VAL:O	2.14	0.48
1:D:74:MET:HG2	1:D:161:LEU:HD22	1.96	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:E:134:ASP:HB3	1:E:137:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ILE:HD13	1:G:70:PRO:HD3	1.95	0.48
1:A:93:ASP:HB3	1:A:96:ARG:HD2	1.96	0.48
1:J:318:ILE:HD12	1:J:320:GLN:HE21	1.79	0.48
1:F:254:GLN:CG	1:F:255:ALA:N	2.76	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:F:206:CYS:O	1:F:209:MET:HE2	2.14	0.47
1:L:311:VAL:CG1	1:L:329:MET:HG2	2.43	0.47
1:J:313:ALA:HB1	2:J:1427:SO4:O3	2.14	0.47
1:J:204:GLN:O	1:J:207:SER:HB2	2.14	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:H:238:GLN:HG3	1:H:246:TYR:OH	2.13	0.47
1:L:286:ASP:O	1:L:289:VAL:HG12	2.13	0.47
1:I:139:PRO:O	1:I:143:ASN:ND2	2.46	0.47
1:F:32:ARG:HB2	1:F:101:PHE:O	2.15	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: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:H:45:PRO:HG3	1:H:113:LEU:HD12	1.97	0.47
1:D:303:VAL:HG13	1:D:307:ARG:NH2	2.26	0.47
1:J:254:GLN:HE21	1:J:256:LEU:HD12	1.79	0.47
1:J:32:ARG:HD2	1:J:102:GLY:HA3	1.97	0.47
1:D:43:ASN:HB3	1:D:113:LEU:O	2.15	0.47
1:D:194:ASN:HA	1:D:259:TRP:O	2.15	0.47
1:A:190:GLN:OE1	1:A:201:ARG:NH1	2.48	0.47
1:D:273:THR:H	1:D:426:ALA:HA	1.79	0.47
1:B:61:ILE:HD13	1:B:61:ILE:N	2.30	0.47
1:K:294:ILE:O	1:K:298:ASN:ND2	2.46	0.47
1:A:29:ALA:HB1	1:A:399:ARG:HG3	1.97	0.47
1:D:168:PRO:HD3	1:D:287:TRP:CD2	2.50	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:I:64:THR:HG23	1:I:66:GLU:OE2	2.15	0.46
1:G:350:GLN:HA	1:G:353:MET:HE2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:TYR:O	1:B:72:SER:HB2	2.15	0.46
1:I:148:LEU:HD12	1:I:148:LEU:O	2.15	0.46
1:C:31:ASN:ND2	1:C:398:ALA:HB2	2.30	0.46
1:C:307:ARG:O	1:C:309:PRO:HD3	2.15	0.46
1:C:14:ALA:CB	1:J:308:GLN:HG2	2.44	0.46
1:B:423:THR:C	1:B:425:THR:H	2.18	0.46
1:K:117:GLN:O	1:K:120:PRO:HA	2.15	0.46
1:G:131:GLN:HG2	3:G:2108:HOH:O	2.14	0.46
1:G:367:GLN:OE1	1:J:358:SER:HA	2.16	0.46
1:B:208:ASN:O	1:B:210:PRO:HD2	2.16	0.46
1:J:330:ASN:HA	2:J:1427:SO4:O1	2.16	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:A:254:GLN:HG2	1:A:256:LEU:H	1.81	0.46
1:I:168:PRO:HD3	1:I:287:TRP:CD2	2.51	0.46
1:F:183:LEU:HD11	1:F:220:GLN:HA	1.98	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:L:284:SER:OG	1:L:286:ASP:OD1	2.25	0.46
1:F:276:HIS:HD2	3:F:2310:HOH:O	1.98	0.46
1:B:254:GLN:HA	1:B:372:PHE:CD2	2.50	0.46
1:K:231:SER:HA	1:K:236:VAL:O	2.15	0.46
1:E:182:ARG:HA	1:E:185:ASP:OD2	2.15	0.46
1:K:42:SER:O	1:K:43:ASN:CB	2.63	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:F:208:ASN:O	1:F:210:PRO:HD2	2.15	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:F:273:THR:HB	1:F:426:ALA:OXT	2.16	0.46
1:E:208:ASN:CG	1:E:210:PRO:HD2	2.35	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:F:254:GLN:HG2	1:F:256:LEU:H	1.81	0.45
1:F:216:ASN:O	1:F:220:GLN:HG3	2.17	0.45
1:C:178:MET:O	1:C:183:LEU:HD23	2.16	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:J:64:THR:HG23	1:J:66:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:207:SER:O	1:I:208:ASN:CB	2.63	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:J:221:MET:HE2	1:J:299:LEU:HD22	1.99	0.45
1:E:352:VAL:HG22	1:E:357:VAL:HG23	1.99	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:42:SER:O	1:A:43:ASN:HB2	2.17	0.45
1:B:358:SER:HB2	1:B:361:LYS:H	1.82	0.45
1:B:282:ALA:HB2	1:B:293:TRP:CE2	2.52	0.45
1:K:160:LEU:O	1:K:164:MET:HG2	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:A:99:ASN:HA	1:A:103:LEU:O	2.17	0.44
1:L:145:ARG:HE	1:L:145:ARG:HB2	1.47	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:A:239:THR:HG23	1:A:356:LEU:HD21	1.99	0.44
1:F:29:ALA:HB1	1:F:399:ARG:HG3	1.99	0.44
1:K:367:GLN:HA	1:K:367:GLN:OE1	2.17	0.44
1:E:352:VAL:CG2	1:E:357:VAL:HG23	2.48	0.44
1:H:221:MET:HE1	1:H:302:ILE:HB	2.00	0.44
1:G:145:ARG:HG2	1:G:145:ARG:HH11	1.82	0.44
1:H:349:ARG:O	1:H:353:MET:HG3	2.18	0.44
1:A:140:ARG:HD3	1:A:147:GLU:OE1	2.17	0.44
1:K:64:THR:HG23	1:K:66:GLU:HG2	1.99	0.44
1:J:188:MET:HE1	1:J:263:TYR:CE2	2.53	0.44
1:L:353:MET:HE1	3:L:2114:HOH:O	2.18	0.44
1:G:349:ARG:NH2	3:G:2248:HOH:O	2.50	0.44
1:G:22:PRO:HD3	1:G:162:SER:HB3	2.00	0.44
1:A:263:TYR:OH	1:A:269:ARG:NH2	2.45	0.44
1:G:231:SER:HA	1:G:236:VAL:O	2.18	0.44
1:H:221:MET:HE3	1:H:303:VAL:HG23	1.93	0.44
1:D:382:GLN:O	1:D:386:GLN:CG	2.61	0.44
1:J:264:THR:HG22	3:J:2150:HOH:O	2.18	0.44
1:C:280:VAL:HA	1:C:336:HIS:O	2.18	0.44
1:J:120:PRO:HB2	1:J:122:ALA:O	2.18	0.44
1:K:238:GLN:HG3	1:K:246:TYR:CZ	2.53	0.44
1:G:145:ARG:HH11	1:G:145:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:254:GLN:NE2	1:H:256:LEU:HD12	2.33	0.44
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:D:85:VAL:O	1:D:86:PRO:C	2.56	0.43
1:G:263:TYR:OH	1:G:269:ARG:NH2	2.43	0.43
1:K:4:ILE:HA	1:K:4:ILE:HD13	1.84	0.43
1:G:280:VAL:HG22	1:G:336:HIS:HB2	1.99	0.43
1:E:144:ARG:HD2	1:E:147:GLU:OE2	2.18	0.43
1:I:4:ILE:HD12	3:I:2155:HOH:O	2.17	0.43
1:C:153:PRO:HG2	1:C:209:MET:CE	2.48	0.43
1:H:119:PRO:HA	1:H:120:PRO:HD2	1.89	0.43
1:E:311:VAL:N	1:F:382:GLN:OE1	2.49	0.43
1:I:145:ARG:HD3	1:I:145:ARG:HA	1.58	0.43
1:K:64:THR:HG21	1:K:66:GLU:HG2	2.00	0.43
1:H:190:GLN:OE1	1:H:201:ARG:NH1	2.52	0.43
1:G:244:GLY:HA2	1:G:264:THR:HG22	2.00	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: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:K:172:VAL:O	1:K:277:PHE:HA	2.19	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:B:194:ASN:HB3	1:B:197:ASP:HB2	2.00	0.43
1:J:166:ALA:HA	3:J:2229:HOH:O	2.18	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:B:379:ASP:O	1:B:382:GLN:HB2	2.19	0.43
1:J:202:LEU:HD21	1:J:220:GLN:OE1	2.18	0.43
1:J:19:PHE:HB2	1:J:132:TRP:CZ3	2.53	0.43
1:J:188:MET:CE	1:J:263:TYR:CE2	3.01	0.43
1:E:42:SER:O	1:E:43:ASN:HB2	2.18	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:L:190:GLN:OE1	1:L:201:ARG:NH1	2.52	0.43
1:K:354:ALA:HB3	1:K:356:LEU:HD12	2.00	0.43
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:C:43:ASN:HB3	1:C:113:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:ARG:CG	1:K:157:ARG:NH1	2.68	0.42
1:C:238:GLN:HG3	1:C:246:TYR:CZ	2.54	0.42
1:B:254:GLN:NE2	1:B:256:LEU:HD12	2.35	0.42
1:G:45:PRO:HB3	1:G:80:LEU:HD21	2.01	0.42
1:K:357:VAL:HB	1:K:361:LYS:HB3	2.01	0.42
1:L:207:SER:C	1:L:209:MET:H	2.22	0.42
1:L:190:GLN:O	1:L:193:ASN:HB2	2.19	0.42
1:F:145:ARG:HD3	3:F:2124:HOH:O	2.18	0.42
1:A:339:ASN:ND2	1:A:410:THR:O	2.50	0.42
1:H:131:GLN:HG2	3:H:2089:HOH:O	2.19	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: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:C:208:ASN:C	1:C:210:PRO:HD2	2.40	0.42
1:I:28:LEU:HD11	1:I:79:MET:HG2	2.02	0.42
1:E:74:MET:HG2	1:E:161:LEU:HD22	2.00	0.42
1:I:160:LEU:O	1:I:164:MET:HG2	2.19	0.42
1:H:289:VAL:HG21	1:H:376:ILE:HD12	2.02	0.42
1:F:349:ARG:NH1	1:F:349:ARG:HG2	2.33	0.42
1:D:416:GLN:O	1:D:420:VAL:HG23	2.19	0.42
1:B:233:ILE:CD1	1:B:421:LEU:HB3	2.50	0.42
1:B:5:SER:OG	1:B:6:GLU:N	2.48	0.42
1:I:69:TYR:O	1:I:72:SER:HB2	2.18	0.42
1:J:66:GLU:H	1:J:66:GLU:CD	2.22	0.42
1:B:202:LEU:HB3	1:B:221:MET:CE	2.50	0.42
1:K:61:ILE:HD12	1:K:63:SER:OG	2.20	0.42
1:D:173:GLU:OE1	1:D:222:ARG:HD2	2.20	0.42
1:B:213:PRO:O	1:B:214:ASP:HB2	2.20	0.42
1:C:15:ILE:HD13	1:J:325:PRO:CB	2.38	0.42
1:B:61:ILE:HB	1:B:63:SER:OG	2.20	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:I:126:GLN:HG3	1:K:126:GLN:HB2	2.02	0.42
1:H:29:ALA:HB1	1:H:399:ARG:HG3	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:D:64:THR:HG22	1:D:66:GLU:N	2.35	0.41
1:G:20:SER:HB2	1:G:82:SER:HB3	2.02	0.41
1:B:353:MET:HE3	3:B:2136:HOH:O	2.19	0.41
1:D:274:GLN:H	1:D:274:GLN:HG3	1.71	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:K:92:ARG:O	1:K:108:GLU:HG3	2.21	0.41
1:C:264:THR:O	1:C:264:THR:CG2	2.68	0.41
1:K:119:PRO:HA	3:K:2093:HOH:O	2.20	0.41
1:B:145:ARG:HG2	1:B:149:GLN:OE1	2.19	0.41
1:A:34:GLN:NE2	1:A:398:ALA:HB1	2.35	0.41
1:J:238:GLN:HB3	1:J:356:LEU:HD21	2.02	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:118:ASP:OD2	1:B:119:PRO:HA	2.21	0.41
1:E:358:SER:HB2	1:E:361:LYS:H	1.85	0.41
1:L:26:ARG:NH1	3:L:2022:HOH:O	2.53	0.41
1:I:311:VAL:HG12	1:I:329:MET:HG2	2.03	0.41
1:I:256:LEU:O	1:I:257:ASP:C	2.59	0.41
1:E:266:ASN:OD1	1:E:266:ASN:N	2.44	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:H:349:ARG:HG2	1:H:353:MET:HE2	2.01	0.41
1:E:99:ASN:HA	1:E:103:LEU:O	2.20	0.41
1:F:171:TYR:HB2	1:F:300:THR:HG23	2.02	0.41
1:E:324:ARG:HA	1:E:325:PRO:HD3	1.90	0.41
1:G:118:ASP:OD1	1:G:119:PRO:HA	2.20	0.41
1:I:208:ASN:ND2	1:I:209:MET:H	2.19	0.41
1:E:205:SER:CB	3:E:2118:HOH:O	2.67	0.41
1:B:171:TYR:HB2	1:B:300:THR:HG23	2.02	0.41
1:A:206:CYS:SG	1:A:221:MET:CE	3.09	0.41
1:J:286:ASP:O	1:J:289:VAL:HG12	2.21	0.41
1:H:138:TYR:HA	1:H:139:PRO:HD3	1.94	0.41
1:A:209:MET:O	1:A:211:VAL:N	2.54	0.41
1:J:188:MET:HE2	1:J:263:TYR:CG	2.56	0.41
1:F:209:MET:HB2	3:F:2128:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:GLN:HG2	3:G:2191:HOH:O	2.20	0.41
1:A:277:PHE:HE2	1:A:333:THR:HG21	1.86	0.41
1:F:367:GLN:HA	3:F:2259:HOH:O	2.20	0.41
1:C:423:THR:C	1:C:425:THR:H	2.23	0.41
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:G:275:ARG:HG3	1:G:275:ARG:NH1	2.33	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: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:A:153:PRO:HG2	1:A:209:MET:HE3	2.02	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:I:34:GLN:NE2	1:I:398:ALA:HB1	2.35	0.40
1:B:377:GLN:HA	1:B:409:TRP:CZ2	2.56	0.40
1:C:15:ILE:HD11	1:C:17:ASP:OD1	2.20	0.40
1:B:61:ILE:HG21	1:B:70:PRO:HG3	2.03	0.40
1:I:217:TYR:O	1:I:221:MET:HG3	2.21	0.40
1:B:74:MET:HE3	1:B:157:ARG:HD3	2.04	0.40
1:J:34:GLN:NE2	1:J:398:ALA:HB1	2.36	0.40
1:H:13:ARG:HD3	1:H:15:ILE:O	2.22	0.40
1:F:11:MET:HE3	1:F:11:MET:HB3	1.97	0.40
1:A:35:LEU:HD22	1:A:80:LEU:HB2	2.02	0.40
1:E:277:PHE:CE2	1:E:310:PRO:HG2	2.56	0.40
1:E:145:ARG:HD3	1:E:145:ARG:HA	1.84	0.40
1:H:64:THR:HG23	1:H:66:GLU:H	1.86	0.40
1:K:146:ARG:HG3	3:K:2062:HOH:O	2.20	0.40
1:C:10:THR:HG22	1:C:213:PRO:HB2	2.03	0.40
1:L:384:LYS:HD2	1:L:404:PHE:CE2	2.57	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:L:121:PRO:HD2	3:L:2089:HOH:O	2.21	0.40
1:K:24:GLY:HA3	3:K:2030:HOH:O	2.20	0.40
1:G:145:ARG:HG2	1:G:145:ARG:NH1	2.37	0.40
1:H:313:ALA:HB1	2:H:1427:SO4:O4	2.21	0.40
1:A:244:GLY:HA3	1:A:263:TYR:CE1	2.57	0.40
1:H:92:ARG:O	1:H:108:GLU:HG3	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%)	34	37
1	B	405/423 (96%)	376 (93%)	26 (6%)	3 (1%)	26	28
1	C	400/423 (95%)	379 (95%)	17 (4%)	4 (1%)	19	18
1	D	405/423 (96%)	376 (93%)	21 (5%)	8 (2%)	9	6
1	E	405/423 (96%)	382 (94%)	19 (5%)	4 (1%)	19	18
1	F	400/423 (95%)	385 (96%)	13 (3%)	2 (0%)	34	37
1	G	399/423 (94%)	383 (96%)	13 (3%)	3 (1%)	24	25
1	H	405/423 (96%)	386 (95%)	17 (4%)	2 (0%)	34	37
1	I	406/423 (96%)	385 (95%)	18 (4%)	3 (1%)	26	28
1	J	400/423 (95%)	376 (94%)	18 (4%)	6 (2%)	13	10
1	K	406/423 (96%)	385 (95%)	16 (4%)	5 (1%)	16	14
1	L	406/423 (96%)	389 (96%)	13 (3%)	4 (1%)	19	18
All	All	4843/5076 (95%)	4594 (95%)	203 (4%)	46 (1%)	21	21

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%)	30	37
1	B	339/352 (96%)	317 (94%)	22 (6%)	21	24
1	C	335/352 (95%)	320 (96%)	15 (4%)	34	42
1	D	339/352 (96%)	317 (94%)	22 (6%)	21	24
1	E	339/352 (96%)	323 (95%)	16 (5%)	32	40
1	F	335/352 (95%)	316 (94%)	19 (6%)	25	30
1	G	334/352 (95%)	312 (93%)	22 (7%)	21	23
1	H	339/352 (96%)	321 (95%)	18 (5%)	28	34
1	I	340/352 (97%)	326 (96%)	14 (4%)	37	47
1	J	335/352 (95%)	316 (94%)	19 (6%)	25	30
1	K	340/352 (97%)	325 (96%)	15 (4%)	35	44
1	L	340/352 (97%)	317 (93%)	23 (7%)	20	22
All	All	4055/4224 (96%)	3833 (94%)	222 (6%)	27	32

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

Some 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	A	1427	-	4,4,4	0.33	0	6,6,6	0.23	0
2	SO4	B	1427	-	4,4,4	0.41	0	6,6,6	0.20	0
2	SO4	C	1427	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	D	1427	-	4,4,4	0.32	0	6,6,6	0.38	0
2	SO4	E	1427	-	4,4,4	0.56	0	6,6,6	0.17	0
2	SO4	F	1427	-	4,4,4	0.31	0	6,6,6	0.41	0
2	SO4	G	1427	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	H	1427	-	4,4,4	0.43	0	6,6,6	0.25	0
2	SO4	I	1427	-	4,4,4	0.30	0	6,6,6	0.37	0
2	SO4	J	1427	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	K	1427	-	4,4,4	0.47	0	6,6,6	0.38	0
2	SO4	L	1427	-	4,4,4	0.41	0	6,6,6	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	L	1427	-	-	0/0/0/0	0/0/0/0

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	G	1427	SO4	1	0
2	H	1427	SO4	2	0
2	J	1427	SO4	3	0
2	L	1427	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.39	36 (8%) 12 19	18, 31, 52, 72	0
1	B	409/423 (96%)	0.99	74 (18%) 2 3	21, 46, 89, 102	0
1	C	404/423 (95%)	0.77	55 (13%) 4 8	25, 41, 68, 90	0
1	D	409/423 (96%)	1.21	120 (29%) 1 1	22, 47, 88, 96	0
1	E	409/423 (96%)	0.63	50 (12%) 5 9	19, 38, 66, 84	0
1	F	404/423 (95%)	0.21	17 (4%) 40 52	14, 27, 50, 81	0
1	G	403/423 (95%)	0.23	19 (4%) 35 48	12, 26, 47, 84	0
1	H	409/423 (96%)	0.36	27 (6%) 22 32	15, 30, 51, 77	0
1	I	410/423 (96%)	0.46	40 (9%) 10 16	20, 35, 55, 81	0
1	J	404/423 (95%)	0.32	29 (7%) 18 27	20, 34, 58, 90	0
1	K	410/423 (96%)	0.27	30 (7%) 18 27	15, 30, 54, 76	0
1	L	410/423 (96%)	0.32	32 (7%) 16 24	14, 27, 49, 68	0
All	All	4891/5076 (96%)	0.51	529 (10%) 8 13	12, 34, 70, 102	0

All (529) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	SER	10.6
1	B	205	SER	10.2
1	C	119	PRO	9.6
1	D	208	ASN	9.3
1	B	61	ILE	8.9
1	C	62	VAL	8.5
1	E	61	ILE	8.4
1	D	61	ILE	8.3
1	J	10	THR	8.2
1	D	426	ALA	7.7
1	D	352	VAL	7.6

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Mol	Chain	Res	Type	RSRZ
1	E	205	SER	7.5
1	B	204	GLN	7.5
1	G	208	ASN	7.5
1	D	268	ASN	7.3
1	C	256	LEU	7.3
1	B	62	VAL	7.2
1	I	62	VAL	7.1
1	D	266	ASN	7.0
1	E	120	PRO	6.9
1	C	204	GLN	6.9
1	K	204	GLN	6.9
1	B	207	SER	6.8
1	K	61	ILE	6.7
1	F	61	ILE	6.7
1	E	62	VAL	6.6
1	D	357	VAL	6.6
1	B	217	TYR	6.6
1	D	62	VAL	6.5
1	D	360	ALA	6.5
1	D	210	PRO	6.4
1	D	217	TYR	6.4
1	E	123	ALA	6.4
1	E	119	PRO	6.3
1	H	61	ILE	6.2
1	B	208	ASN	6.1
1	B	206	CYS	6.1
1	D	209	MET	6.1
1	F	207	SER	6.0
1	G	210	PRO	6.0
1	D	271	GLN	6.0
1	I	205	SER	5.9
1	C	118	ASP	5.9
1	F	62	VAL	5.9
1	H	62	VAL	5.8
1	D	177	ASN	5.8
1	J	207	SER	5.8
1	G	62	VAL	5.7
1	D	206	CYS	5.7
1	J	62	VAL	5.7
1	E	209	MET	5.7
1	C	208	ASN	5.7
1	H	120	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	266	ASN	5.6
1	B	426	ALA	5.6
1	D	204	GLN	5.5
1	B	209	MET	5.5
1	B	42	SER	5.5
1	J	210	PRO	5.5
1	G	61	ILE	5.4
1	I	61	ILE	5.4
1	C	207	SER	5.4
1	B	239	THR	5.4
1	B	41	SER	5.4
1	D	267	THR	5.4
1	D	270	VAL	5.4
1	D	182	ARG	5.3
1	D	351	TRP	5.2
1	K	41	SER	5.2
1	I	204	GLN	5.1
1	B	363	GLN	5.1
1	E	121	PRO	5.1
1	H	209	MET	5.0
1	D	191	TYR	5.0
1	B	182	ARG	4.9
1	K	210	PRO	4.9
1	F	204	GLN	4.9
1	G	204	GLN	4.9
1	A	204	GLN	4.9
1	E	256	LEU	4.9
1	J	209	MET	4.9
1	A	209	MET	4.9
1	D	205	SER	4.9
1	J	205	SER	4.9
1	L	62	VAL	4.9
1	B	256	LEU	4.8
1	E	217	TYR	4.8
1	C	41	SER	4.8
1	E	42	SER	4.7
1	A	62	VAL	4.7
1	H	119	PRO	4.7
1	B	186	TRP	4.7
1	E	360	ALA	4.7
1	B	7	PHE	4.6
1	C	121	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	118	ASP	4.6
1	A	121	PRO	4.6
1	K	62	VAL	4.5
1	I	209	MET	4.5
1	I	63	SER	4.5
1	B	185	ASP	4.5
1	E	206	CYS	4.5
1	C	61	ILE	4.5
1	D	207	SER	4.5
1	I	65	PRO	4.4
1	L	209	MET	4.4
1	H	210	PRO	4.4
1	B	229	LEU	4.4
1	D	273	THR	4.3
1	H	208	ASN	4.3
1	A	119	PRO	4.3
1	E	41	SER	4.3
1	J	204	GLN	4.3
1	C	146	ARG	4.3
1	E	210	PRO	4.3
1	D	359	ALA	4.3
1	L	119	PRO	4.2
1	G	426	ALA	4.2
1	J	426	ALA	4.2
1	D	348	ILE	4.2
1	B	360	ALA	4.2
1	C	209	MET	4.2
1	I	121	PRO	4.2
1	I	208	ASN	4.1
1	C	426	ALA	4.1
1	C	206	CYS	4.1
1	A	63	SER	4.1
1	D	356	LEU	4.1
1	D	197	ASP	4.0
1	K	229	LEU	4.0
1	G	207	SER	4.0
1	I	207	SER	4.0
1	D	176	PRO	4.0
1	E	359	ALA	4.0
1	H	204	GLN	4.0
1	B	225	ILE	4.0
1	D	349	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	204	GLN	3.9
1	I	393	GLN	3.9
1	K	209	MET	3.9
1	D	192	GLY	3.9
1	F	208	ASN	3.9
1	E	122	ALA	3.9
1	D	364	ALA	3.9
1	D	7	PHE	3.9
1	B	210	PRO	3.9
1	B	191	TYR	3.8
1	A	64	THR	3.8
1	D	175	TRP	3.8
1	C	47	GLN	3.8
1	F	10	THR	3.8
1	H	97	THR	3.8
1	E	93	ASP	3.8
1	D	225	ILE	3.7
1	L	204	GLN	3.7
1	A	229	LEU	3.7
1	B	263	TYR	3.7
1	C	217	TYR	3.7
1	D	419	ALA	3.7
1	D	194	ASN	3.7
1	C	120	PRO	3.7
1	B	267	THR	3.6
1	B	181	GLY	3.6
1	E	207	SER	3.6
1	D	187	PHE	3.6
1	C	212	GLU	3.6
1	E	144	ARG	3.6
1	B	358	SER	3.6
1	B	264	THR	3.5
1	D	264	THR	3.5
1	B	364	ALA	3.5
1	B	216	ASN	3.5
1	J	217	TYR	3.5
1	I	271	GLN	3.5
1	I	229	LEU	3.5
1	I	41	SER	3.5
1	B	92	ARG	3.5
1	B	265	THR	3.5
1	B	177	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	117	GLN	3.5
1	B	63	SER	3.4
1	D	170	LEU	3.4
1	D	355	GLY	3.4
1	L	208	ASN	3.4
1	D	184	ALA	3.4
1	D	172	VAL	3.4
1	A	208	ASN	3.4
1	D	229	LEU	3.4
1	H	229	LEU	3.4
1	F	205	SER	3.4
1	B	359	ALA	3.4
1	F	210	PRO	3.4
1	D	211	VAL	3.4
1	I	169	VAL	3.4
1	D	367	GLN	3.4
1	D	63	SER	3.3
1	A	395	PRO	3.3
1	B	144	ARG	3.3
1	K	228	TRP	3.3
1	J	208	ASN	3.3
1	D	169	VAL	3.3
1	C	211	VAL	3.3
1	J	211	VAL	3.3
1	D	416	GLN	3.3
1	E	208	ASN	3.3
1	A	217	TYR	3.3
1	D	263	TYR	3.3
1	A	210	PRO	3.2
1	D	180	SER	3.2
1	D	293	TRP	3.2
1	K	208	ASN	3.2
1	B	273	THR	3.2
1	H	121	PRO	3.2
1	C	10	THR	3.2
1	D	188	MET	3.2
1	I	225	ILE	3.1
1	B	200	ALA	3.1
1	D	274	GLN	3.1
1	B	143	ASN	3.1
1	B	47	GLN	3.1
1	B	271	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	395	PRO	3.1
1	K	205	SER	3.1
1	C	210	PRO	3.1
1	L	395	PRO	3.1
1	J	61	ILE	3.1
1	C	360	ALA	3.1
1	E	116	ALA	3.1
1	D	183	LEU	3.1
1	C	319	ASN	3.1
1	C	367	GLN	3.1
1	D	251	THR	3.1
1	D	171	TYR	3.1
1	B	201	ARG	3.1
1	K	225	ILE	3.0
1	E	97	THR	3.0
1	I	172	VAL	3.0
1	I	66	GLU	3.0
1	L	66	GLU	3.0
1	B	183	LEU	3.0
1	C	273	THR	3.0
1	I	413	MET	3.0
1	J	229	LEU	3.0
1	D	300	THR	3.0
1	J	363	GLN	3.0
1	I	119	PRO	3.0
1	L	225	ILE	3.0
1	K	170	LEU	3.0
1	D	358	SER	3.0
1	F	41	SER	3.0
1	J	92	ARG	3.0
1	E	143	ASN	2.9
1	I	217	TYR	2.9
1	A	225	ILE	2.9
1	E	228	TRP	2.9
1	B	232	TYR	2.9
1	E	229	LEU	2.9
1	I	210	PRO	2.9
1	L	229	LEU	2.9
1	H	205	SER	2.9
1	D	64	THR	2.9
1	D	119	PRO	2.9
1	B	268	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	228	TRP	2.9
1	J	367	GLN	2.9
1	D	139	PRO	2.9
1	E	64	THR	2.9
1	D	41	SER	2.9
1	D	246	TYR	2.9
1	L	360	ALA	2.8
1	K	119	PRO	2.8
1	C	25	ASN	2.8
1	G	209	MET	2.8
1	L	25	ASN	2.8
1	E	395	PRO	2.8
1	B	230	LEU	2.8
1	C	26	ARG	2.8
1	B	192	GLY	2.8
1	C	352	VAL	2.8
1	A	205	SER	2.8
1	B	228	TRP	2.8
1	L	121	PRO	2.8
1	B	184	ALA	2.8
1	E	25	ASN	2.8
1	H	182	ARG	2.8
1	D	236	VAL	2.8
1	C	229	LEU	2.8
1	D	395	PRO	2.8
1	H	426	ALA	2.8
1	C	42	SER	2.7
1	H	207	SER	2.7
1	D	256	LEU	2.7
1	I	170	LEU	2.7
1	L	61	ILE	2.7
1	G	217	TYR	2.7
1	K	271	GLN	2.7
1	E	92	ARG	2.7
1	B	270	VAL	2.7
1	D	265	THR	2.7
1	D	228	TRP	2.7
1	B	190	GLN	2.7
1	K	364	ALA	2.7
1	D	249	SER	2.7
1	D	200	ALA	2.7
1	D	415	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	203	THR	2.7
1	E	216	ASN	2.7
1	B	367	GLN	2.7
1	G	214	ASP	2.7
1	F	146	ARG	2.6
1	I	201	ARG	2.6
1	E	271	GLN	2.6
1	H	360	ALA	2.6
1	K	360	ALA	2.6
1	C	33	THR	2.6
1	J	216	ASN	2.6
1	L	280	VAL	2.6
1	I	293	TRP	2.6
1	G	271	GLN	2.6
1	D	143	ASN	2.6
1	H	25	ASN	2.6
1	B	189	SER	2.6
1	C	63	SER	2.6
1	K	206	CYS	2.6
1	A	230	LEU	2.6
1	D	353	MET	2.6
1	D	371	ASP	2.6
1	C	392	ASN	2.6
1	G	146	ARG	2.6
1	J	319	ASN	2.6
1	C	395	PRO	2.6
1	C	96	ARG	2.6
1	D	90	GLY	2.6
1	B	12	ALA	2.6
1	A	169	VAL	2.6
1	L	169	VAL	2.6
1	H	225	ILE	2.6
1	E	227	LEU	2.5
1	L	120	PRO	2.5
1	L	205	SER	2.5
1	C	93	ASP	2.5
1	I	227	LEU	2.5
1	L	160	LEU	2.5
1	F	47	GLN	2.5
1	D	193	ASN	2.5
1	K	118	ASP	2.5
1	D	413	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	146	ARG	2.5
1	D	231	SER	2.5
1	D	247	PHE	2.5
1	I	392	ASN	2.5
1	D	363	GLN	2.5
1	E	95	TRP	2.5
1	C	64	THR	2.5
1	D	425	THR	2.5
1	A	352	VAL	2.5
1	B	146	ARG	2.5
1	C	97	THR	2.5
1	D	5	SER	2.5
1	A	413	MET	2.5
1	C	315	GLN	2.5
1	D	93	ASP	2.5
1	B	262	PHE	2.5
1	D	97	THR	2.4
1	H	63	SER	2.4
1	J	206	CYS	2.4
1	D	393	GLN	2.4
1	E	176	PRO	2.4
1	I	371	ASP	2.4
1	B	238	GLN	2.4
1	C	201	ARG	2.4
1	L	227	LEU	2.4
1	B	242	ILE	2.4
1	C	90	GLY	2.4
1	A	143	ASN	2.4
1	L	156	LEU	2.4
1	L	230	LEU	2.4
1	D	315	GLN	2.4
1	E	367	GLN	2.4
1	E	426	ALA	2.4
1	D	227	LEU	2.4
1	J	353	MET	2.4
1	L	144	ARG	2.4
1	L	146	ARG	2.4
1	D	412	GLY	2.4
1	A	226	SER	2.4
1	B	187	PHE	2.4
1	C	122	ALA	2.4
1	J	212	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	2.4
1	C	227	LEU	2.4
1	G	205	SER	2.4
1	D	262	PHE	2.4
1	A	65	PRO	2.4
1	B	274	GLN	2.4
1	J	201	ARG	2.4
1	C	368	GLU	2.3
1	D	261	LEU	2.3
1	K	47	GLN	2.3
1	J	214	ASP	2.3
1	D	240	ASN	2.3
1	D	226	SER	2.3
1	C	117	GLN	2.3
1	C	363	GLN	2.3
1	D	366	THR	2.3
1	D	362	GLY	2.3
1	K	293	TRP	2.3
1	A	170	LEU	2.3
1	B	258	SER	2.3
1	H	227	LEU	2.3
1	D	350	GLN	2.3
1	D	179	ILE	2.3
1	D	25	ASN	2.3
1	D	410	THR	2.3
1	A	146	ARG	2.3
1	E	96	ARG	2.3
1	B	95	TRP	2.3
1	G	230	LEU	2.3
1	D	250	LYS	2.3
1	E	124	PRO	2.3
1	D	354	ALA	2.3
1	C	24	GLY	2.3
1	I	146	ARG	2.3
1	D	361	LYS	2.3
1	I	206	CYS	2.3
1	I	310	PRO	2.3
1	L	94	ALA	2.3
1	H	41	SER	2.3
1	A	293	TRP	2.3
1	H	293	TRP	2.3
1	B	119	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	120	PRO	2.2
1	D	241	THR	2.2
1	D	297	ALA	2.2
1	C	144	ARG	2.2
1	C	156	LEU	2.2
1	F	367	GLN	2.2
1	I	160	LEU	2.2
1	I	367	GLN	2.2
1	L	300	THR	2.2
1	A	67	ALA	2.2
1	J	360	ALA	2.2
1	D	66	GLU	2.2
1	C	391	TYR	2.2
1	D	146	ARG	2.2
1	B	155	LEU	2.2
1	K	296	ALA	2.2
1	D	26	ARG	2.2
1	D	92	ARG	2.2
1	A	47	GLN	2.2
1	B	352	VAL	2.2
1	L	170	LEU	2.2
1	E	177	ASN	2.2
1	A	61	ILE	2.2
1	D	272	ILE	2.2
1	I	280	VAL	2.2
1	K	7	PHE	2.2
1	D	181	GLY	2.2
1	J	362	GLY	2.2
1	D	65	PRO	2.2
1	D	120	PRO	2.2
1	A	160	LEU	2.2
1	A	394	GLN	2.2
1	F	177	ASN	2.2
1	K	143	ASN	2.2
1	L	207	SER	2.2
1	I	296	ALA	2.2
1	E	272	ILE	2.2
1	B	211	VAL	2.2
1	C	114	VAL	2.2
1	B	197	ASP	2.2
1	C	92	ARG	2.2
1	E	139	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	160	LEU	2.2
1	H	319	ASN	2.2
1	L	143	ASN	2.2
1	A	280	VAL	2.1
1	K	212	GLU	2.1
1	F	217	TYR	2.1
1	I	143	ASN	2.1
1	A	224	LEU	2.1
1	A	361	LYS	2.1
1	K	92	ARG	2.1
1	G	212	GLU	2.1
1	G	229	LEU	2.1
1	E	201	ARG	2.1
1	E	296	ALA	2.1
1	G	47	GLN	2.1
1	I	394	GLN	2.1
1	J	271	GLN	2.1
1	J	315	GLN	2.1
1	H	143	ASN	2.1
1	A	41	SER	2.1
1	B	245	PHE	2.1
1	D	269	ARG	2.1
1	E	146	ARG	2.1
1	F	212	GLU	2.1
1	D	238	GLN	2.1
1	F	209	MET	2.1
1	I	300	THR	2.1
1	K	297	ALA	2.1
1	K	121	PRO	2.1
1	B	172	VAL	2.1
1	I	363	GLN	2.1
1	F	229	LEU	2.1
1	K	155	LEU	2.1
1	A	358	SER	2.1
1	G	256	LEU	2.1
1	L	256	LEU	2.1
1	L	301	ALA	2.1
1	B	5	SER	2.1
1	L	63	SER	2.1
1	D	346	GLU	2.0
1	E	236	VAL	2.1
1	J	273	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	170	LEU	2.0
1	B	227	LEU	2.0
1	D	301	ALA	2.0
1	C	95	TRP	2.0
1	J	146	ARG	2.0
1	H	7	PHE	2.0
1	E	142	ALA	2.0
1	K	426	ALA	2.0
1	D	121	PRO	2.0
1	G	177	ASN	2.0
1	L	4	ILE	2.0
1	A	360	ALA	2.0
1	C	94	ALA	2.0
1	D	304	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	C	1427	5/5	0.95	0.37	2.93	85,85,85,86	0
2	SO4	F	1427	5/5	0.95	0.23	2.48	63,63,66,66	0
2	SO4	D	1427	5/5	0.94	0.26	1.51	63,66,67,68	0
2	SO4	L	1427	5/5	0.99	0.17	0.93	46,47,48,48	0
2	SO4	B	1427	5/5	0.97	0.21	0.86	63,63,64,65	0
2	SO4	J	1427	5/5	0.95	0.24	0.84	74,75,75,76	0
2	SO4	E	1427	5/5	0.99	0.18	0.75	49,50,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	K	1427	5/5	0.98	0.20	0.72	49,49,51,52	0
2	SO4	G	1427	5/5	0.97	0.15	0.60	67,67,68,68	0
2	SO4	A	1427	5/5	0.99	0.15	0.35	48,49,49,50	0
2	SO4	I	1427	5/5	0.97	0.17	0.19	55,56,57,58	0
2	SO4	H	1427	5/5	0.99	0.14	0.05	42,44,45,46	0

6.5 Other polymers

There are no such residues in this entry.