Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:26 PM GMT

PDB ID	:	4LGD
Title	:	Structural Basis for Autoactivation of Human Mst2 Kinase and Its Regulation by RASSF5
Authors	:	Luo, X.; Ni, L.; Tomchick, D.R.
Deposited on	:	2013-06-27
Resolution	:	3.05 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:

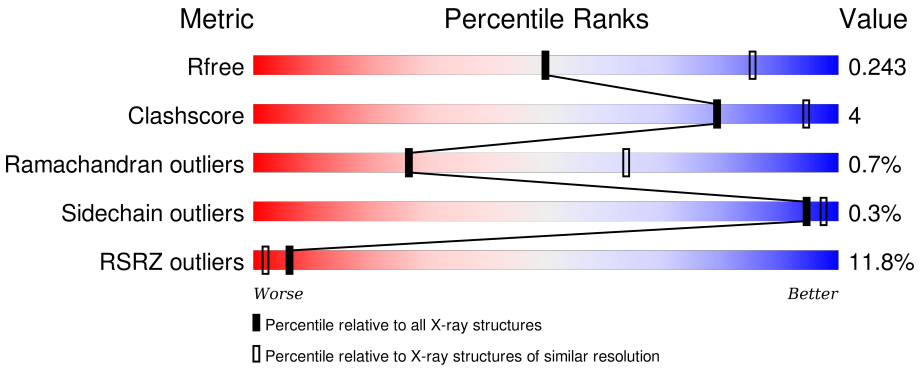
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.05 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.



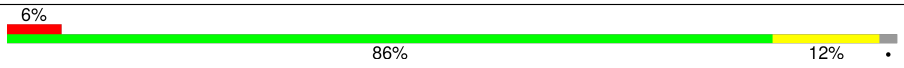
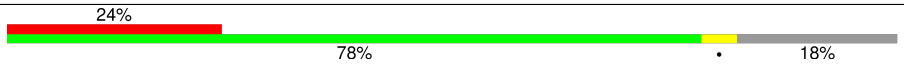
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	378	16% 82% 11% 7%
1	B	378	14% 84% 9% 7%
1	C	378	7% 84% 8% 8%
1	D	378	2% 82% 7% • 11%
2	E	49	10% 84% 12% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	49	
2	G	49	
2	H	49	

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
5	SO4	A	503	-	-	X	-
5	SO4	B	503	-	-	X	-
5	SO4	B	506	-	-	-	X
5	SO4	D	503	-	-	X	-
6	NA	C	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25637 atoms, of which 12852 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 Serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	H	N	O	S	0	0	0
			5690	1799	2865	479	530	17			
1	B	350	Total	C	H	N	O	S	0	0	0
			5698	1794	2879	480	528	17			
1	C	349	Total	C	H	N	O	S	0	0	0
			5706	1800	2879	482	528	17			
1	D	338	Total	C	H	N	O	S	0	0	0
			5486	1731	2765	463	511	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q13188
A	1	HIS	-	EXPRESSION TAG	UNP Q13188
A	2	HIS	-	EXPRESSION TAG	UNP Q13188
A	3	HIS	-	EXPRESSION TAG	UNP Q13188
A	4	HIS	-	EXPRESSION TAG	UNP Q13188
A	5	HIS	-	EXPRESSION TAG	UNP Q13188
A	6	HIS	-	EXPRESSION TAG	UNP Q13188
A	7	GLY	-	EXPRESSION TAG	UNP Q13188
A	8	SER	-	EXPRESSION TAG	UNP Q13188
A	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188
B	0	MET	-	EXPRESSION TAG	UNP Q13188
B	1	HIS	-	EXPRESSION TAG	UNP Q13188
B	2	HIS	-	EXPRESSION TAG	UNP Q13188
B	3	HIS	-	EXPRESSION TAG	UNP Q13188
B	4	HIS	-	EXPRESSION TAG	UNP Q13188
B	5	HIS	-	EXPRESSION TAG	UNP Q13188
B	6	HIS	-	EXPRESSION TAG	UNP Q13188
B	7	GLY	-	EXPRESSION TAG	UNP Q13188
B	8	SER	-	EXPRESSION TAG	UNP Q13188
B	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188
C	0	MET	-	EXPRESSION TAG	UNP Q13188

Continued on next page...

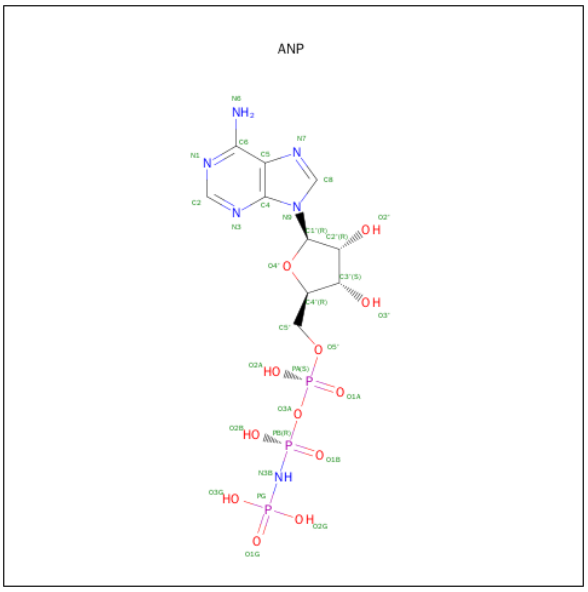
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	HIS	-	EXPRESSION TAG	UNP Q13188
C	2	HIS	-	EXPRESSION TAG	UNP Q13188
C	3	HIS	-	EXPRESSION TAG	UNP Q13188
C	4	HIS	-	EXPRESSION TAG	UNP Q13188
C	5	HIS	-	EXPRESSION TAG	UNP Q13188
C	6	HIS	-	EXPRESSION TAG	UNP Q13188
C	7	GLY	-	EXPRESSION TAG	UNP Q13188
C	8	SER	-	EXPRESSION TAG	UNP Q13188
C	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188
D	0	MET	-	EXPRESSION TAG	UNP Q13188
D	1	HIS	-	EXPRESSION TAG	UNP Q13188
D	2	HIS	-	EXPRESSION TAG	UNP Q13188
D	3	HIS	-	EXPRESSION TAG	UNP Q13188
D	4	HIS	-	EXPRESSION TAG	UNP Q13188
D	5	HIS	-	EXPRESSION TAG	UNP Q13188
D	6	HIS	-	EXPRESSION TAG	UNP Q13188
D	7	GLY	-	EXPRESSION TAG	UNP Q13188
D	8	SER	-	EXPRESSION TAG	UNP Q13188
D	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188

- Molecule 2 is a protein called Ras association domain family member 5, RASSF5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	47	Total	C	H	N	O	0	0	0
			810	260	403	67	80			
2	F	29	Total	C	H	N	O	0	0	0
			489	155	246	39	49			
2	G	48	Total	C	H	N	O	0	0	0
			825	265	409	68	83			
2	H	40	Total	C	H	N	O	0	0	0
			697	226	346	57	68			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

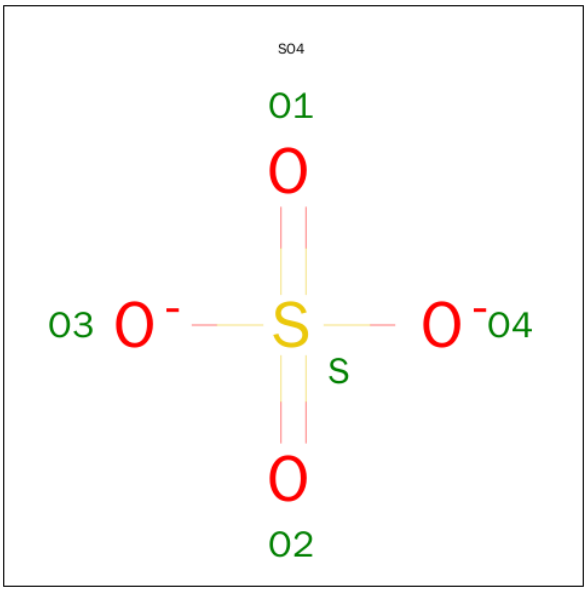


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	C	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	D	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

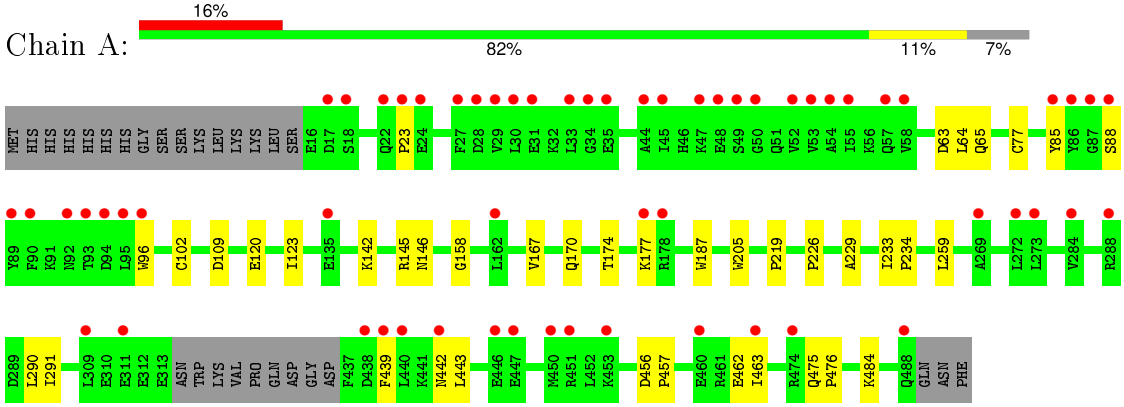
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0
6	C	2	Total Na 2 2	0	0

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.

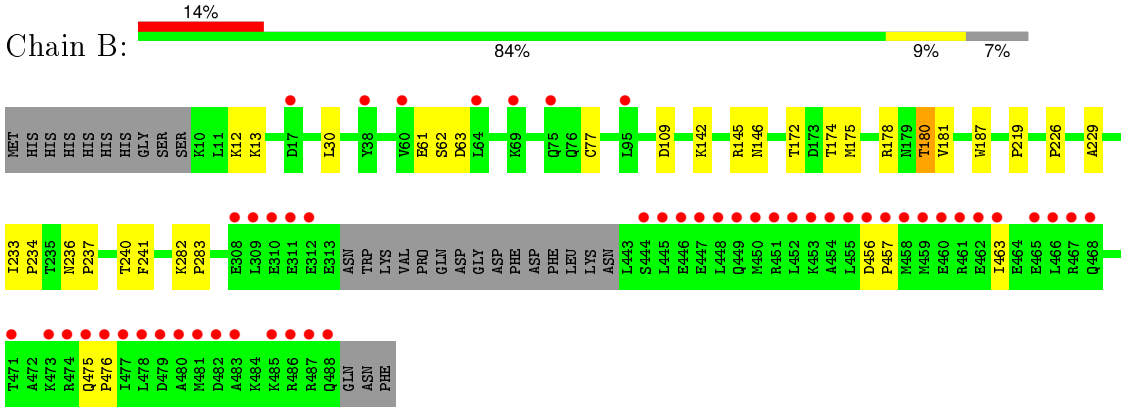
- Molecule 1: Serine/threonine-protein kinase 3

Chain A:



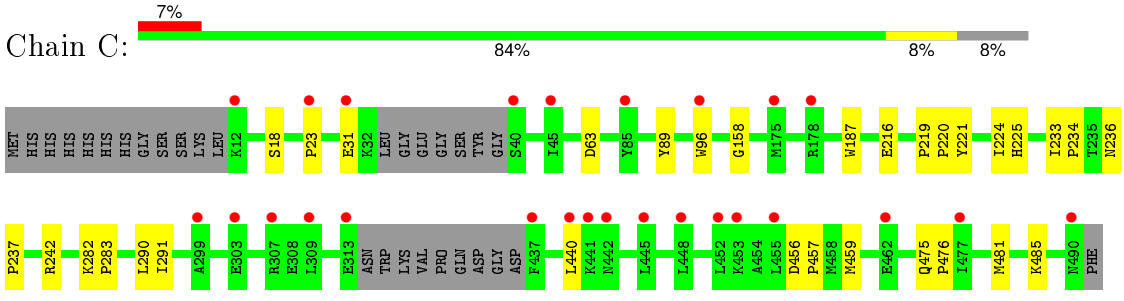
- Molecule 1: Serine/threonine-protein kinase 3

Chain B:



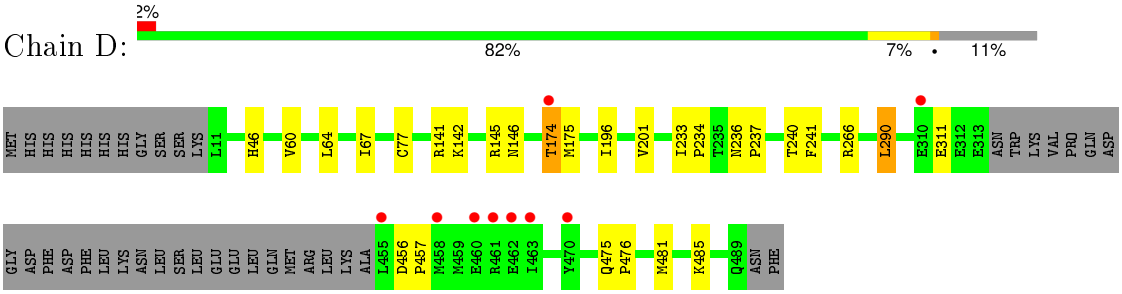
- Molecule 1: Serine/threonine-protein kinase 3

Chain C:



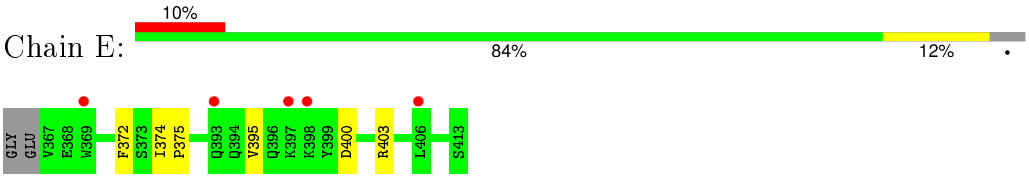
• Molecule 1: Serine/threonine-protein kinase 3

Chain D:



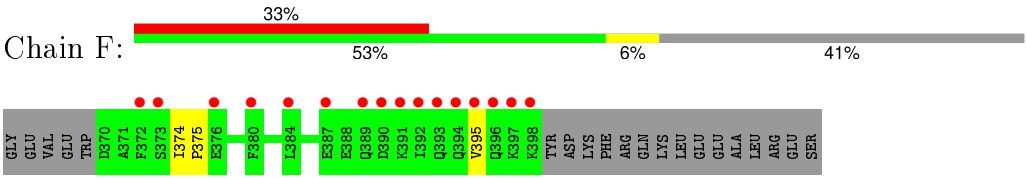
• Molecule 2: Ras association domain family member 5, RASSF5

Chain E:



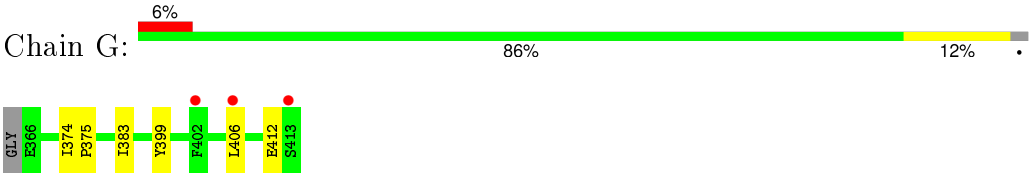
• Molecule 2: Ras association domain family member 5, RASSF5

Chain F:



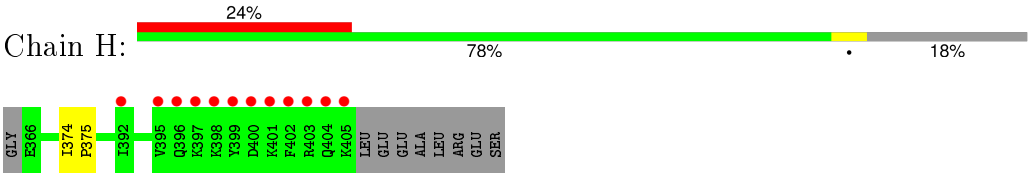
• Molecule 2: Ras association domain family member 5, RASSF5

Chain G:



• Molecule 2: Ras association domain family member 5, RASSF5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.40Å 237.14Å 95.86Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 46.05 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-3.05) 98.6 (46.05-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.06Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.244 0.200 , 0.243	Depositor DCC
R_{free} test set	2523 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 94.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 50494 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25637	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NA, MG, ANP, 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	0.21	0/2879	0.38	0/3882
1	B	0.22	0/2871	0.41	0/3869
1	C	0.21	0/2879	0.38	0/3879
1	D	0.22	0/2773	0.40	0/3740
2	E	0.22	0/413	0.34	0/552
2	F	0.21	0/245	0.32	0/327
2	G	0.22	0/422	0.34	0/564
2	H	0.22	0/357	0.30	0/477
All	All	0.22	0/12839	0.39	0/17290

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2825	2865	2858	25	0
1	B	2819	2879	2872	24	0
1	C	2827	2879	2872	17	0
1	D	2721	2765	2758	19	0
2	E	407	403	403	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	243	246	246	2	0
2	G	416	409	409	7	0
2	H	351	346	346	1	0
3	A	31	15	13	2	0
3	B	31	15	13	1	0
3	C	31	15	13	0	0
3	D	31	15	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	2	0
5	B	20	0	0	3	0
5	C	5	0	0	0	0
5	D	15	0	0	3	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
All	All	12785	12852	12816	90	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 4.

All (90) 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:A:85:TYR:OH	1:A:88:SER:OG	2.08	0.71
1:D:145:ARG:NH1	5:D:503:SO4:S	2.72	0.63
1:B:145:ARG:NH1	5:B:503:SO4:S	2.73	0.61
1:B:145:ARG:NH1	5:B:503:SO4:O2	2.34	0.61
1:B:77:CYS:SG	1:B:142:LYS:NZ	2.73	0.61
1:A:484:LYS:NZ	2:E:372:PHE:O	2.36	0.58
2:E:374:ILE:HB	2:E:375:PRO:HD3	1.86	0.58
1:D:64:LEU:HD11	2:G:383:ILE:HG21	1.86	0.56
1:D:77:CYS:SG	1:D:142:LYS:NZ	2.76	0.55
1:A:77:CYS:SG	1:A:142:LYS:NZ	2.79	0.55
2:F:374:ILE:HB	2:F:375:PRO:HD3	1.90	0.54
1:B:475:GLN:HB3	1:B:476:PRO:HD3	1.91	0.52
1:D:475:GLN:N	1:D:476:PRO:CD	2.73	0.52
2:G:374:ILE:HB	2:G:375:PRO:HD3	1.92	0.51
1:B:236:ASN:HB3	1:B:237:PRO:CD	2.41	0.51
1:A:145:ARG:NH1	5:A:503:SO4:O1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:NH1	5:B:503:SO4:O1	2.44	0.50
1:B:240:THR:OG1	1:B:241:PHE:N	2.44	0.50
1:B:233:ILE:HB	1:B:234:PRO:HD3	1.94	0.50
2:E:400:ASP:OD2	2:E:403:ARG:NH1	2.44	0.50
1:D:233:ILE:HB	1:D:234:PRO:HD3	1.93	0.49
1:B:109:ASP:OD1	3:B:501:ANP:O2'	2.26	0.49
1:D:201:VAL:CG1	1:D:266:ARG:HD2	2.42	0.49
1:D:240:THR:OG1	1:D:241:PHE:N	2.46	0.48
1:C:187:TRP:CZ2	1:C:219:PRO:HG3	2.48	0.48
1:D:145:ARG:NH1	5:D:503:SO4:O4	2.47	0.47
1:A:226:PRO:HG2	1:B:178:ARG:NH1	2.28	0.47
1:B:30:LEU:HD12	1:B:30:LEU:N	2.29	0.47
1:A:23:PRO:HB2	1:A:96:TRP:CZ3	2.49	0.47
1:D:64:LEU:O	1:D:67:ILE:N	2.47	0.47
1:A:158:GLY:HA2	1:A:291:ILE:CD1	2.45	0.47
1:A:109:ASP:OD1	3:A:501:ANP:O2'	2.32	0.47
1:A:187:TRP:CZ2	1:A:219:PRO:HG3	2.50	0.47
1:D:60:VAL:O	1:D:64:LEU:HG	2.14	0.47
1:A:145:ARG:NH1	5:A:503:SO4:S	2.84	0.47
1:C:158:GLY:HA2	1:C:291:ILE:CD1	2.45	0.46
1:D:174:THR:HG22	1:D:175:MET:N	2.30	0.46
1:C:23:PRO:HB2	1:C:96:TRP:CE3	2.50	0.46
1:A:475:GLN:N	1:A:476:PRO:CD	2.78	0.46
1:C:456:ASP:HB2	1:C:457:PRO:HD3	1.98	0.46
1:A:233:ILE:HB	1:A:234:PRO:HD3	1.97	0.46
1:B:174:THR:HG22	1:B:175:MET:N	2.30	0.45
1:B:226:PRO:O	1:B:229:ALA:N	2.50	0.45
1:C:220:PRO:O	1:C:221:TYR:HB2	2.17	0.45
1:C:236:ASN:HB3	1:C:237:PRO:CD	2.47	0.45
1:C:224:ILE:HG22	1:C:225:HIS:N	2.31	0.45
1:C:233:ILE:HB	1:C:234:PRO:HD3	1.98	0.45
1:B:463:ILE:HG22	2:F:395:VAL:HG11	1.98	0.45
1:B:282:LYS:HB3	1:B:283:PRO:HD2	2.00	0.44
1:C:290:LEU:HD12	1:C:290:LEU:C	2.38	0.44
1:A:290:LEU:HD12	1:A:290:LEU:C	2.37	0.44
1:C:459:MET:HB2	2:G:399:TYR:CD1	2.53	0.44
2:H:374:ILE:HB	2:H:375:PRO:HD3	2.00	0.44
1:B:236:ASN:HB3	1:B:237:PRO:HD2	2.00	0.43
1:A:462:GLU:HG2	2:E:395:VAL:HG21	2.00	0.43
1:A:475:GLN:HB3	1:A:476:PRO:HD3	1.99	0.43
1:C:282:LYS:HB3	1:C:283:PRO:HD2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:O	1:A:123:ILE:N	2.51	0.43
1:B:456:ASP:HB2	1:B:457:PRO:HD3	2.01	0.43
1:D:290:LEU:HD12	1:D:290:LEU:C	2.39	0.43
1:B:456:ASP:N	1:B:457:PRO:CD	2.82	0.43
1:D:64:LEU:CD1	2:G:383:ILE:HG21	2.49	0.43
1:C:475:GLN:HB3	1:C:476:PRO:HD3	2.00	0.43
1:C:481:MET:HE3	1:C:485:LYS:HE3	2.02	0.42
1:B:12:LYS:O	1:B:13:LYS:C	2.57	0.42
2:G:412:GLU:OE1	2:G:412:GLU:HA	2.20	0.42
1:D:46:HIS:NE2	5:D:504:SO4:O2	2.53	0.42
1:C:440:LEU:HD22	2:G:406:LEU:CD2	2.50	0.42
1:D:141:ARG:O	1:D:141:ARG:HG2	2.20	0.42
1:D:456:ASP:N	1:D:457:PRO:CD	2.82	0.42
1:B:237:PRO:HG3	1:D:237:PRO:HG3	2.02	0.42
1:A:463:ILE:HG22	2:E:395:VAL:HG11	2.02	0.42
1:B:180:THR:CG2	1:B:181:VAL:N	2.82	0.42
1:D:481:MET:O	1:D:485:LYS:HG2	2.19	0.42
1:B:172:THR:HG22	1:B:172:THR:O	2.20	0.42
1:A:226:PRO:O	1:A:229:ALA:N	2.53	0.41
1:A:64:LEU:HD12	1:A:65:GLN:N	2.34	0.41
2:G:374:ILE:N	2:G:375:PRO:CD	2.83	0.41
1:A:102:CYS:O	3:A:501:ANP:C2	2.68	0.41
1:A:439:PHE:O	1:A:443:LEU:HB2	2.20	0.41
1:C:224:ILE:CG2	1:C:225:HIS:N	2.84	0.41
1:A:456:ASP:HB2	1:A:457:PRO:HD3	2.02	0.41
1:A:456:ASP:N	1:A:457:PRO:CD	2.83	0.41
1:B:61:GLU:HG3	1:B:62:SER:N	2.35	0.41
1:C:18:SER:O	1:C:89:TYR:OH	2.28	0.41
1:C:216:GLU:OE1	1:C:242:ARG:NH2	2.53	0.41
1:D:236:ASN:HB3	1:D:237:PRO:CD	2.50	0.40
1:B:187:TRP:CZ2	1:B:219:PRO:HG3	2.56	0.40
1:A:205:TRP:CE3	1:A:259:LEU:HA	2.56	0.40
1:A:170:GLN:HB2	1:A:177:LYS:HE2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/378 (92%)	319 (92%)	24 (7%)	3 (1%)	21	58
1	B	346/378 (92%)	328 (95%)	16 (5%)	2 (1%)	30	66
1	C	343/378 (91%)	325 (95%)	16 (5%)	2 (1%)	30	66
1	D	334/378 (88%)	314 (94%)	16 (5%)	4 (1%)	16	50
2	E	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
2	F	27/49 (55%)	26 (96%)	1 (4%)	0	100	100
2	G	46/49 (94%)	46 (100%)	0	0	100	100
2	H	38/49 (78%)	38 (100%)	0	0	100	100
All	All	1525/1708 (89%)	1440 (94%)	74 (5%)	11 (1%)	26	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	GLU
1	A	174	THR
1	C	31	GLU
1	D	174	THR
1	A	63	ASP
1	B	146	ASN
1	A	146	ASN
1	B	63	ASP
1	C	63	ASP
1	D	146	ASN
1	D	196	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	311/337 (92%)	309 (99%)	2 (1%)	90 96
1	B	311/337 (92%)	310 (100%)	1 (0%)	94 97
1	C	313/337 (93%)	313 (100%)	0	100 100
1	D	300/337 (89%)	299 (100%)	1 (0%)	94 97
2	E	45/46 (98%)	45 (100%)	0	100 100
2	F	28/46 (61%)	28 (100%)	0	100 100
2	G	46/46 (100%)	46 (100%)	0	100 100
2	H	39/46 (85%)	39 (100%)	0	100 100
All	All	1393/1532 (91%)	1389 (100%)	4 (0%)	94 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	VAL
1	A	442	ASN
1	B	180	THR
1	D	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	A	501	4	27,33,33	1.61	8 (29%)	30,52,52	2.55	7 (23%)
5	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.08	0
3	ANP	B	501	4	27,33,33	1.56	7 (25%)	30,52,52	2.54	7 (23%)
5	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	505	-	4,4,4	0.19	0	6,6,6	0.11	0
5	SO4	B	506	-	4,4,4	0.20	0	6,6,6	0.08	0
3	ANP	C	501	4	27,33,33	1.54	7 (25%)	30,52,52	2.55	6 (20%)
5	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.07	0
3	ANP	D	501	4	27,33,33	1.53	7 (25%)	30,52,52	2.54	7 (23%)
5	SO4	D	503	-	4,4,4	0.20	0	6,6,6	0.09	0
5	SO4	D	504	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	D	505	-	4,4,4	0.21	0	6,6,6	0.07	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
3	ANP	A	501	4	-	0/12/38/38	0/3/3/3
5	SO4	A	503	-	-	0/0/0/0	0/0/0/0
3	ANP	B	501	4	-	0/12/38/38	0/3/3/3
5	SO4	B	503	-	-	0/0/0/0	0/0/0/0
5	SO4	B	504	-	-	0/0/0/0	0/0/0/0
5	SO4	B	505	-	-	0/0/0/0	0/0/0/0
5	SO4	B	506	-	-	0/0/0/0	0/0/0/0
3	ANP	C	501	4	-	0/12/38/38	0/3/3/3
5	SO4	C	503	-	-	0/0/0/0	0/0/0/0
3	ANP	D	501	4	-	1/12/38/38	0/3/3/3
5	SO4	D	503	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	504	-	-	0/0/0/0	0/0/0/0
5	SO4	D	505	-	-	0/0/0/0	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ANP	C2'-C3'	-2.28	1.47	1.53
3	A	501	ANP	O4'-C4'	-2.24	1.39	1.45
3	A	501	ANP	O2'-C2'	-2.18	1.37	1.43
3	C	501	ANP	O4'-C4'	-2.17	1.40	1.45
3	D	501	ANP	O4'-C4'	-2.17	1.40	1.45
3	B	501	ANP	O2'-C2'	-2.14	1.37	1.43
3	B	501	ANP	C2'-C3'	-2.14	1.47	1.53
3	D	501	ANP	C2'-C3'	-2.13	1.47	1.53
3	C	501	ANP	C2'-C3'	-2.12	1.47	1.53
3	D	501	ANP	O2'-C2'	-2.11	1.37	1.43
3	C	501	ANP	O2'-C2'	-2.08	1.38	1.43
3	B	501	ANP	O4'-C4'	-2.06	1.40	1.45
3	A	501	ANP	O3'-C3'	-2.03	1.38	1.43
3	A	501	ANP	C2-N3	2.05	1.35	1.32
3	D	501	ANP	C2-N3	2.08	1.35	1.32
3	C	501	ANP	C2-N3	2.08	1.35	1.32
3	B	501	ANP	C2-N3	2.10	1.35	1.32
3	D	501	ANP	PG-O1G	2.92	1.49	1.46
3	D	501	ANP	PB-O1B	2.98	1.49	1.46
3	B	501	ANP	PG-O1G	3.00	1.49	1.46
3	C	501	ANP	PG-O1G	3.05	1.49	1.46
3	C	501	ANP	PB-O1B	3.15	1.49	1.46
3	C	501	ANP	C6-N6	3.24	1.44	1.34
3	A	501	ANP	C6-N6	3.26	1.45	1.34
3	B	501	ANP	PB-O1B	3.31	1.49	1.46
3	A	501	ANP	PG-O1G	3.32	1.49	1.46
3	B	501	ANP	C6-N6	3.35	1.45	1.34
3	D	501	ANP	C6-N6	3.36	1.45	1.34
3	A	501	ANP	PB-O1B	3.38	1.50	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ANP	N3-C2-N1	-11.59	120.02	128.89
3	C	501	ANP	N3-C2-N1	-11.36	120.19	128.89
3	B	501	ANP	N3-C2-N1	-11.12	120.38	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	ANP	N3-C2-N1	-11.05	120.43	128.89
3	B	501	ANP	PA-O3A-PB	-4.66	117.04	132.67
3	D	501	ANP	PA-O3A-PB	-4.15	118.75	132.67
3	C	501	ANP	PA-O3A-PB	-3.79	119.95	132.67
3	A	501	ANP	PA-O3A-PB	-3.74	120.14	132.67
3	D	501	ANP	O1G-PG-N3B	-3.16	107.05	111.90
3	A	501	ANP	C2'-C1'-N9	-3.10	109.56	114.29
3	C	501	ANP	C2'-C1'-N9	-2.69	110.18	114.29
3	B	501	ANP	C4-C5-N7	-2.55	107.14	109.48
3	B	501	ANP	C2'-C1'-N9	-2.52	110.45	114.29
3	D	501	ANP	C4-C5-N7	-2.38	107.29	109.48
3	C	501	ANP	C4-C5-N7	-2.35	107.32	109.48
3	C	501	ANP	O1G-PG-N3B	-2.23	108.47	111.90
3	A	501	ANP	O1B-PB-N3B	-2.23	108.48	111.90
3	C	501	ANP	O1B-PB-N3B	-2.18	108.56	111.90
3	A	501	ANP	C4-C5-N7	-2.13	107.52	109.48
3	D	501	ANP	C2'-C1'-N9	-2.10	111.09	114.29
3	B	501	ANP	O1G-PG-N3B	-2.08	108.70	111.90
3	A	501	ANP	O2G-PG-O1G	-2.00	108.17	113.49
3	A	501	ANP	O3A-PB-N3B	2.06	112.10	106.44
3	D	501	ANP	O3A-PA-O5'	2.38	109.26	102.94
3	D	501	ANP	O3A-PB-N3B	2.45	113.18	106.44
3	B	501	ANP	O3A-PB-N3B	2.45	113.18	106.44
3	B	501	ANP	O3A-PA-O5'	3.05	111.03	102.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	ANP	O1B-PB-N3B-PG

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ANP	2	0
5	A	503	SO4	2	0
3	B	501	ANP	1	0
5	B	503	SO4	3	0
5	D	503	SO4	2	0
5	D	504	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	350/378 (92%)	1.05	60 (17%) 2 1	98, 160, 251, 332	0
1	B	350/378 (92%)	0.88	52 (14%) 3 1	57, 98, 245, 293	0
1	C	349/378 (92%)	0.70	26 (7%) 17 6	72, 122, 204, 242	0
1	D	338/378 (89%)	0.49	9 (2%) 58 32	57, 92, 175, 232	0
2	E	47/49 (95%)	0.90	5 (10%) 8 3	97, 128, 163, 181	0
2	F	29/49 (59%)	2.66	16 (55%) 0 0	179, 258, 279, 304	0
2	G	48/49 (97%)	0.63	3 (6%) 23 9	62, 119, 154, 180	0
2	H	40/49 (81%)	1.36	12 (30%) 1 0	119, 153, 213, 255	0
All	All	1551/1708 (90%)	0.83	183 (11%) 6 2	57, 122, 238, 332	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	450	MET	9.2
1	C	440	LEU	7.8
1	A	88	SER	7.6
1	B	451	ARG	7.2
2	F	391	LYS	7.0
1	B	452	LEU	6.9
1	B	457	PRO	6.8
1	A	96	TRP	6.7
1	B	463	ILE	6.2
1	A	23	PRO	6.2
1	A	89	TYR	6.0
1	A	85	TYR	6.0
1	A	94	ASP	6.0
1	B	456	ASP	5.9
1	C	437	PHE	5.8
2	F	392	ILE	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	31	GLU	5.5
1	B	477	ILE	5.5
2	F	384	LEU	5.5
1	B	454	ALA	5.5
1	D	460	GLU	5.4
2	F	380	PHE	5.4
1	B	447	GLU	5.3
1	B	460	GLU	5.3
1	B	453	LYS	5.3
1	A	45	ILE	5.2
2	F	389	GLN	4.9
1	B	455	LEU	4.9
1	A	47	LYS	4.9
1	A	27	PHE	4.9
2	F	372	PHE	4.8
1	A	50	GLY	4.7
1	B	478	LEU	4.6
1	B	479	ASP	4.6
1	A	33	LEU	4.6
1	B	449	GLN	4.5
1	A	44	ALA	4.5
1	A	17	ASP	4.4
1	A	87	GLY	4.4
1	C	441	LYS	4.3
2	F	396	GLN	4.2
2	H	404	GLN	4.2
1	A	442	ASN	4.1
1	B	487	ARG	4.0
1	B	38	TYR	4.0
1	A	93	THR	3.9
1	B	474	ARG	3.9
1	B	466	LEU	3.8
1	A	28	ASP	3.8
1	A	460	GLU	3.8
2	F	397	LYS	3.8
1	B	485	LYS	3.8
1	B	312	GLU	3.8
1	A	450	MET	3.7
1	D	455	LEU	3.7
2	F	398	LYS	3.7
2	H	402	PHE	3.7
2	H	397	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	178	ARG	3.6
1	B	311	GLU	3.6
1	B	467	ARG	3.6
1	B	459	MET	3.6
2	H	403	ARG	3.6
2	F	395	VAL	3.5
2	G	413	SER	3.5
2	H	400	ASP	3.5
1	A	22	GLN	3.5
1	B	475	GLN	3.5
2	H	395	VAL	3.5
1	B	476	PRO	3.5
1	C	455	LEU	3.4
1	A	24	GLU	3.4
1	B	482	ASP	3.4
1	A	52	VAL	3.4
1	A	447	GLU	3.4
1	B	310	GLU	3.3
2	G	402	PHE	3.3
1	C	23	PRO	3.3
1	C	85	TYR	3.3
1	B	308	GLU	3.3
1	B	486	ARG	3.2
1	C	96	TRP	3.2
1	A	438	ASP	3.2
1	A	86	TYR	3.2
1	C	445	LEU	3.2
2	H	392	ILE	3.2
2	E	369	TRP	3.1
2	H	396	GLN	3.1
1	B	445	LEU	3.1
2	F	376	GLU	3.1
1	C	442	ASN	3.1
1	B	309	LEU	3.1
1	C	490	ASN	3.1
1	A	309	LEU	3.1
1	D	174	THR	3.0
1	B	481	MET	3.0
2	E	393	GLN	3.0
1	D	310	GLU	3.0
1	A	53	VAL	3.0
2	H	401	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	48	GLU	2.9
1	C	178	ARG	2.9
1	B	473	LYS	2.9
1	A	18	SER	2.9
1	A	49	SER	2.9
2	F	373	SER	2.9
1	A	453	LYS	2.8
2	F	393	GLN	2.8
1	A	284	VAL	2.8
1	A	54	ALA	2.8
1	A	90	PHE	2.8
1	C	313	GLU	2.8
1	B	461	ARG	2.8
1	C	453	LYS	2.8
1	B	446	GLU	2.8
1	D	470	TYR	2.7
2	H	399	TYR	2.7
1	C	40	SER	2.7
1	A	440	LEU	2.7
1	C	307	ARG	2.7
1	A	29	VAL	2.7
2	E	397	LYS	2.6
1	B	444	SER	2.6
1	A	34	GLY	2.6
1	D	463	ILE	2.5
1	D	461	ARG	2.5
1	A	273	LEU	2.5
2	F	387	GLU	2.5
1	B	483	ALA	2.5
1	B	458	MET	2.5
1	B	448	LEU	2.5
1	D	462	GLU	2.4
2	H	405	LYS	2.4
2	F	390	ASP	2.4
2	E	406	LEU	2.4
1	B	60	VAL	2.4
1	C	462	GLU	2.4
1	A	57	GLN	2.4
1	B	64	LEU	2.4
1	C	452	LEU	2.4
1	B	17	ASP	2.3
1	C	12	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	448	LEU	2.3
1	A	451	ARG	2.3
1	A	474	ARG	2.3
2	H	398	LYS	2.3
1	B	480	ALA	2.3
2	F	394	GLN	2.3
1	A	162	LEU	2.3
1	A	439	PHE	2.3
1	B	468	GLN	2.3
1	C	31	GLU	2.2
1	B	471	THR	2.2
1	B	75	GLN	2.2
1	C	303	GLU	2.2
1	A	30	LEU	2.2
1	A	92	ASN	2.2
1	A	463	ILE	2.2
1	B	69	LYS	2.2
1	B	465	GLU	2.2
1	A	311	GLU	2.2
1	C	299	ALA	2.2
1	B	462	GLU	2.1
1	C	175	MET	2.1
1	B	488	GLN	2.1
2	E	398	LYS	2.1
1	C	477	ILE	2.1
1	A	55	ILE	2.1
1	A	135	GLU	2.1
1	A	446	GLU	2.1
1	A	488	GLN	2.1
1	A	95	LEU	2.1
1	A	35	GLU	2.1
2	G	406	LEU	2.1
1	A	269	ALA	2.1
1	D	458	MET	2.1
1	C	309	LEU	2.1
1	A	272	LEU	2.0
1	A	177	LYS	2.0
1	C	45	ILE	2.0
1	A	288	ARG	2.0
1	A	58	VAL	2.0
1	B	95	LEU	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
5	SO4	B	506	5/5	0.84	0.49	2.71	187,190,193,199	0
6	NA	C	504	1/1	0.34	0.37	2.48	103,103,103,103	0
5	SO4	D	505	5/5	0.87	0.34	1.03	128,150,162,168	0
3	ANP	C	501	31/31	0.75	0.34	0.90	140,192,243,292	0
3	ANP	D	501	31/31	0.95	0.28	0.27	57,93,183,229	0
5	SO4	B	503	5/5	0.92	0.24	0.04	108,110,116,132	0
5	SO4	D	504	5/5	0.76	0.28	-0.02	125,138,149,156	0
5	SO4	D	503	5/5	0.93	0.27	-0.09	77,78,105,145	0
3	ANP	B	501	31/31	0.95	0.27	-0.13	57,101,168,247	0
5	SO4	B	505	5/5	0.89	0.24	-0.32	113,128,140,166	0
3	ANP	A	501	31/31	0.74	0.26	-0.41	144,191,249,314	0
6	NA	D	506	1/1	0.89	0.22	-0.68	65,65,65,65	0
5	SO4	A	503	5/5	0.93	0.16	-1.24	133,149,152,155	0
6	NA	C	505	1/1	0.80	0.14	-1.27	189,189,189,189	0
5	SO4	B	504	5/5	0.83	0.18	-1.38	191,191,196,199	0
5	SO4	C	503	5/5	0.96	0.20	-1.57	94,96,107,133	0
4	MG	C	502	1/1	0.64	0.58	-	221,221,221,221	0
4	MG	A	502	1/1	0.88	0.59	-	219,219,219,219	0
4	MG	B	502	1/1	0.84	0.43	-	104,104,104,104	0
4	MG	D	502	1/1	0.92	0.55	-	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.