Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:42 PM GMT

PDB ID	:	1Q8Y
Title	:	The structure of the yeast SR protein kinase, Sky1p, with bound ADP
Authors	:	Nolen, B.; Ngo, J.; Chakrabarti, S.; Vu, D.; Adams, J.A.; Ghosh, G.
Deposited on	:	2003-08-22
Resolution	:	2.05 Å(reported)

The following versions of software and data (see references (i)) 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 2.05 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.
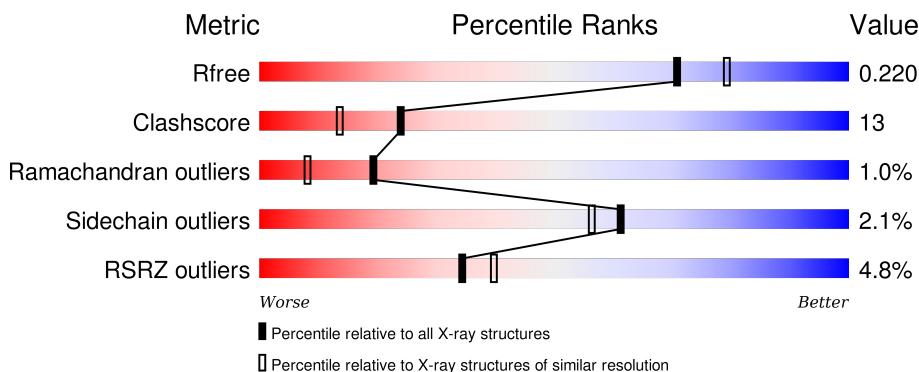
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	373	5% / 69% / 23% / · / 6%
1	B	373	4% / 75% / 19% / · / ·
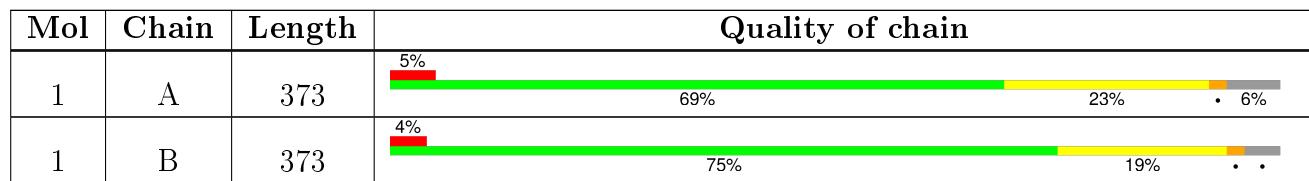
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADE	B	900	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6042 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 SR protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total 2826	C 1816	N 480	O 518	S 12	0	0	0
1	B	357	Total 2876	C 1842	N 488	O 534	S 12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	VAL	-	SEE REMARK 999	UNP Q03656
A	306	ASP	-	SEE REMARK 999	UNP Q03656
B	305	VAL	-	SEE REMARK 999	UNP Q03656
B	306	ASP	-	SEE REMARK 999	UNP Q03656

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
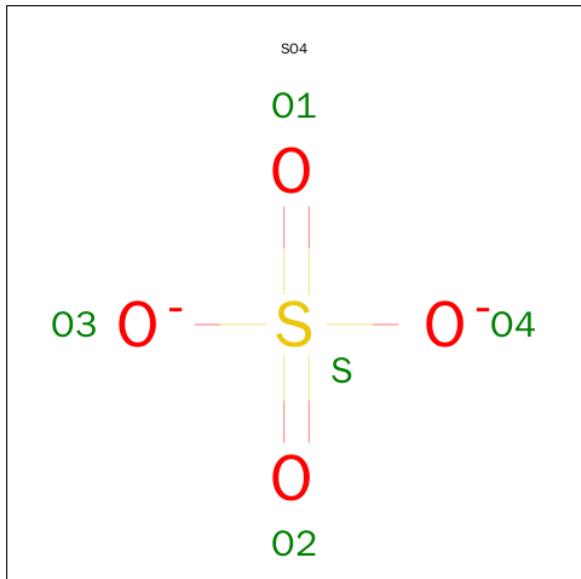
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
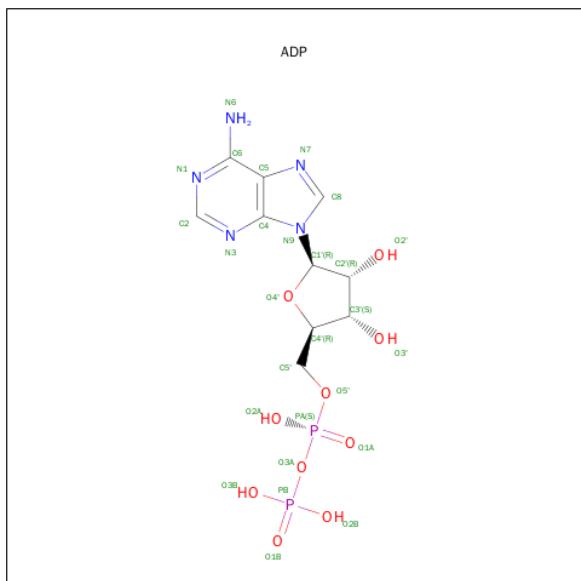
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).
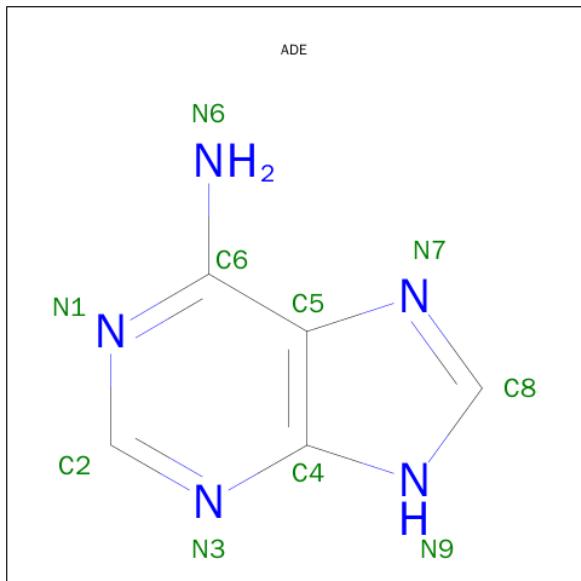
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 10	C 5	N 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	122	Total 122	O 122	0	0
6	B	140	Total 140	O 140	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: SR protein kinase
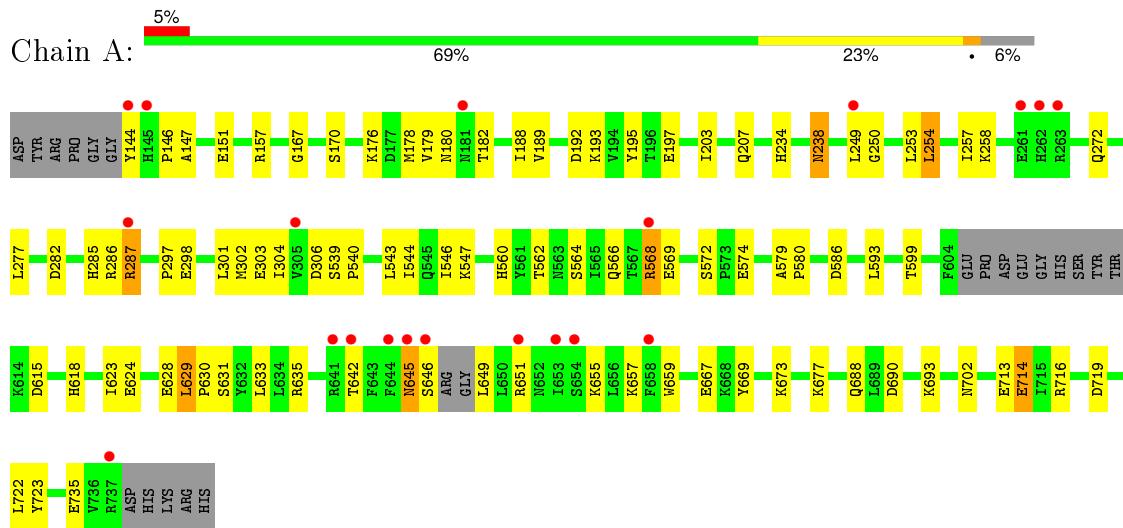
- Molecule 1: SR protein kinase
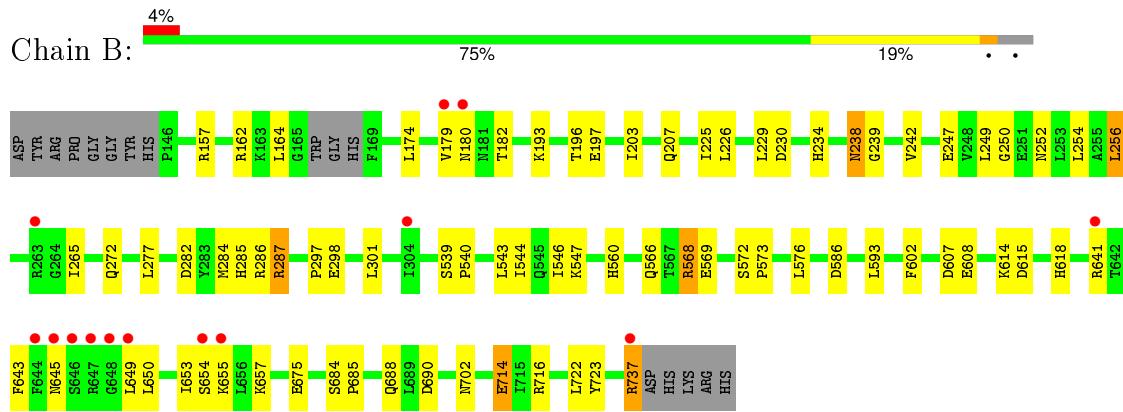
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.58Å 88.65Å 133.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.05 39.84 – 2.05	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.92-2.05) 93.3 (39.84-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.244 0.221 , 0.220	Depositor DCC
R_{free} test set	2533 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.8	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 53244 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 32.64 % 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 9.0931e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADE, SO4, ADP

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	0.31	0/2891	0.56	0/3910
1	B	0.32	0/2942	0.57	0/3980
All	All	0.31	0/5833	0.56	0/7890

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 (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	2826	0	2797	90	1
1	B	2876	0	2853	62	1
2	A	15	0	0	1	0
2	B	25	0	0	1	0
3	A	1	0	0	0	0
4	A	27	0	12	1	0
5	B	10	0	4	1	0
6	A	122	0	0	5	0
6	B	140	0	0	5	0
All	All	6042	0	5666	150	1

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 13.

All (150) 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:B:249:LEU:HD11	1:B:547:LYS:HD2	1.53	0.90
1:A:562:THR:HG22	1:A:564:SER:H	1.38	0.88
1:B:282:ASP:OD1	1:B:286:ARG:HD3	1.76	0.85
1:A:655:LYS:HD3	1:A:657:LYS:NZ	1.93	0.82
1:A:568:ARG:HH22	1:A:615:ASP:HA	1.48	0.77
1:B:737:ARG:NE	1:B:737:ARG:H	1.85	0.74
1:A:254:LEU:HD12	1:A:298:GLU:HG3	1.68	0.73
1:A:631:SER:O	1:A:635:ARG:HB2	1.90	0.72
1:A:623:ILE:CD1	1:A:629:LEU:HD13	2.20	0.72
1:A:282:ASP:OD1	1:A:286:ARG:HD3	1.90	0.72
1:A:249:LEU:HD23	1:A:301:LEU:HB2	1.69	0.72
1:B:297:PRO:HD3	1:B:593:LEU:HD13	1.72	0.72
1:B:737:ARG:HE	1:B:737:ARG:H	1.37	0.70
1:B:203:ILE:O	1:B:207:GLN:HG3	1.92	0.69
1:A:297:PRO:HD3	1:A:593:LEU:HD13	1.74	0.69
1:B:688:GLN:HE21	1:B:690:ASP:H	1.39	0.69
1:A:203:ILE:O	1:A:207:GLN:HG3	1.93	0.68
1:B:238:ASN:HD22	1:B:239:GLY:H	1.40	0.68
1:A:623:ILE:HD11	1:A:629:LEU:HD13	1.76	0.68
1:A:170:SER:HB2	1:A:188:ILE:O	1.92	0.68
1:A:655:LYS:HD3	1:A:657:LYS:HZ2	1.58	0.66
1:A:690:ASP:HB3	1:A:693:LYS:HZ3	1.59	0.65
1:B:238:ASN:H	1:B:238:ASN:ND2	1.93	0.65
1:A:667:GLU:HB3	1:B:654:SER:O	1.97	0.64
1:A:569:GLU:CD	1:A:569:GLU:H	2.01	0.64
1:A:659:TRP:CH2	1:B:655:LYS:HG2	2.33	0.64
1:A:645:ASN:HD22	1:A:649:LEU:CB	2.10	0.64
1:B:157:ARG:HG3	1:B:179:VAL:HG23	1.79	0.64
1:A:238:ASN:ND2	1:A:238:ASN:H	1.94	0.64
1:B:272:GLN:HE22	1:B:543:LEU:HA	1.64	0.62
1:A:673:LYS:HE2	1:A:677:LYS:CE	2.29	0.62
1:B:702:ASN:OD1	1:B:716:ARG:HB2	1.99	0.62
1:A:624:GLU:HG3	1:A:657:LYS:O	2.00	0.61
1:A:238:ASN:H	1:A:238:ASN:HD22	1.48	0.61
1:A:302:MET:HG2	1:A:303:GLU:N	2.14	0.61
1:B:650:LEU:HD23	1:B:653:ILE:HG13	1.83	0.60
1:A:642:THR:HA	1:A:651:ARG:NH1	2.15	0.60
1:B:546:ILE:C	1:B:546:ILE:HD12	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLN:HE22	1:A:544:ILE:H	1.50	0.59
1:B:272:GLN:HE22	1:B:544:ILE:H	1.50	0.59
1:A:272:GLN:HE22	1:A:543:LEU:HA	1.68	0.58
1:A:642:THR:HA	1:A:651:ARG:HH11	1.67	0.58
1:B:254:LEU:CD1	1:B:298:GLU:HG3	2.33	0.58
1:A:249:LEU:CD2	1:A:547:LYS:HB2	2.34	0.58
1:A:539:SER:HB3	1:A:540:PRO:HD3	1.86	0.57
1:A:238:ASN:N	1:A:238:ASN:HD22	2.02	0.57
1:A:249:LEU:HD23	1:A:301:LEU:CB	2.35	0.57
1:B:238:ASN:HD22	1:B:239:GLY:N	2.03	0.57
1:A:702:ASN:OD1	1:A:716:ARG:HB2	2.05	0.57
1:B:252:ASN:OD1	1:B:254:LEU:HB2	2.05	0.56
1:A:170:SER:HB3	1:A:189:VAL:HA	1.87	0.56
1:A:623:ILE:HD13	1:A:629:LEU:HD13	1.88	0.56
1:A:304:ILE:HD12	1:A:304:ILE:N	2.21	0.56
1:B:272:GLN:NE2	1:B:544:ILE:H	2.04	0.56
1:A:254:LEU:HD22	1:A:258:LYS:HE2	1.87	0.56
1:A:254:LEU:CD2	1:A:258:LYS:HE2	2.36	0.55
1:B:238:ASN:N	1:B:238:ASN:HD22	2.04	0.55
1:B:256:LEU:HD13	1:B:265:ILE:HD13	1.88	0.55
1:A:560:HIS:CD2	1:A:735:GLU:HB2	2.42	0.55
1:A:272:GLN:NE2	1:A:544:ILE:H	2.04	0.55
1:A:645:ASN:O	1:A:646:SER:HB2	2.07	0.54
1:B:238:ASN:H	1:B:238:ASN:HD22	1.55	0.54
1:A:546:ILE:C	1:A:546:ILE:HD12	2.28	0.54
1:B:249:LEU:HD12	1:B:301:LEU:HD12	1.90	0.54
1:B:162:ARG:NH1	1:B:174:LEU:HD23	2.24	0.53
1:A:176:LYS:HD3	1:A:178:MET:HE1	1.90	0.53
1:B:722:LEU:O	1:B:723:TYR:HB2	2.09	0.53
1:A:287:ARG:CZ	1:A:287:ARG:HA	2.39	0.53
1:B:254:LEU:HD12	1:B:298:GLU:HG3	1.90	0.53
1:A:287:ARG:NE	1:A:287:ARG:HA	2.24	0.53
1:A:673:LYS:HE2	1:A:677:LYS:HE2	1.90	0.53
1:B:285:HIS:HD2	6:B:902:HOH:O	1.92	0.53
1:A:673:LYS:HG2	1:A:677:LYS:HE2	1.90	0.52
1:A:306:ASP:OD2	1:A:540:PRO:HD2	2.08	0.52
1:A:192:ASP:HB3	1:A:195:TYR:HB2	1.92	0.52
1:B:225:ILE:HD11	1:B:284:MET:HG3	1.92	0.52
1:A:285:HIS:HE1	1:A:586:ASP:OD2	1.92	0.51
1:B:657:LYS:NZ	1:B:657:LYS:HB2	2.26	0.51
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:SER:HB2	1:A:574:GLU:OE2	2.11	0.51
1:B:226:LEU:HD21	5:B:900:ADE:H62	1.75	0.51
1:A:254:LEU:HG	1:A:298:GLU:OE2	2.11	0.51
1:B:249:LEU:HB2	1:B:301:LEU:HD13	1.93	0.50
1:A:623:ILE:HD12	1:A:628:GLU:HA	1.92	0.50
1:A:286:ARG:NH2	1:A:719:ASP:OD2	2.43	0.50
1:B:180:ASN:O	1:B:182:THR:HG23	2.11	0.49
1:B:287:ARG:HG3	1:B:287:ARG:HH11	1.76	0.49
1:A:568:ARG:NH2	1:A:615:ASP:HA	2.24	0.49
1:A:285:HIS:HD2	6:A:825:HOH:O	1.94	0.49
1:B:568:ARG:HH21	1:B:618:HIS:HD2	1.59	0.49
1:A:167:GLY:HA3	4:A:810:ADP:O2B	2.13	0.49
1:A:568:ARG:NH1	1:A:615:ASP:OD1	2.42	0.49
1:A:722:LEU:O	1:A:723:TYR:HB2	2.13	0.48
1:B:247:GLU:HG2	6:B:952:HOH:O	2.13	0.48
1:A:630:PRO:HD2	1:A:633:LEU:HD12	1.96	0.48
1:B:607:ASP:OD1	1:B:608:GLU:N	2.46	0.48
1:A:722:LEU:HD12	6:A:880:HOH:O	2.13	0.48
1:B:234:HIS:HD2	2:B:802:SO4:O1	1.97	0.47
1:B:650:LEU:HD23	1:B:653:ILE:CG1	2.43	0.47
1:B:714:GLU:HG2	6:B:918:HOH:O	2.14	0.47
1:B:657:LYS:HZ2	1:B:657:LYS:HB2	1.78	0.47
1:A:144:TYR:CE1	1:A:146:PRO:HD3	2.49	0.47
1:B:285:HIS:HE1	1:B:586:ASP:OD2	1.98	0.46
1:B:615:ASP:HB3	1:B:643:PHE:CE2	2.51	0.46
1:B:164:LEU:HD21	1:B:174:LEU:HB2	1.97	0.46
1:A:193:LYS:HE2	1:A:197:GLU:OE1	2.16	0.46
1:B:568:ARG:HH21	1:B:618:HIS:CD2	2.33	0.46
1:B:568:ARG:HD3	1:B:614:LYS:HD3	1.97	0.46
1:A:249:LEU:HD22	1:A:547:LYS:HB2	1.96	0.46
1:A:569:GLU:N	1:A:569:GLU:CD	2.68	0.46
1:A:599:THR:HB	1:A:669:TYR:CE2	2.51	0.45
1:A:560:HIS:HD2	6:A:877:HOH:O	1.98	0.45
1:B:539:SER:HB3	1:B:540:PRO:HD3	1.97	0.45
1:B:569:GLU:HG2	1:B:602:PHE:CD2	2.52	0.45
1:B:572:SER:HB2	1:B:573:PRO:HD2	1.98	0.45
1:A:714:GLU:HG2	6:A:817:HOH:O	2.16	0.44
1:A:568:ARG:HH21	1:A:618:HIS:CD2	2.34	0.44
1:A:238:ASN:ND2	1:A:238:ASN:N	2.59	0.44
1:B:238:ASN:N	1:B:238:ASN:ND2	2.56	0.44
1:B:675:GLU:HG3	6:B:989:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:THR:HG23	1:B:242:VAL:HG23	1.99	0.44
1:B:641:ARG:HE	1:B:641:ARG:HA	1.83	0.44
1:B:641:ARG:NH1	1:B:645:ASN:C	2.71	0.44
1:A:673:LYS:HE2	1:A:677:LYS:HE3	1.97	0.44
1:A:560:HIS:HE1	6:A:816:HOH:O	1.99	0.44
1:A:673:LYS:O	1:A:677:LYS:HG3	2.17	0.44
1:B:287:ARG:HG3	1:B:287:ARG:NH1	2.33	0.44
1:A:157:ARG:HG3	1:A:179:VAL:HG23	2.00	0.43
1:A:688:GLN:HG2	1:A:693:LYS:HB2	2.01	0.43
1:A:690:ASP:HB3	1:A:693:LYS:NZ	2.33	0.43
1:A:180:ASN:O	1:A:182:THR:HG23	2.18	0.43
1:A:579:ALA:HB1	1:A:580:PRO:HD2	2.01	0.43
1:A:249:LEU:HD22	1:A:547:LYS:HD2	2.00	0.43
1:A:688:GLN:NE2	1:A:693:LYS:NZ	2.66	0.43
1:A:253:LEU:O	1:A:257:ILE:HG13	2.19	0.42
1:A:688:GLN:HE21	1:A:690:ASP:H	1.67	0.42
1:A:302:MET:CG	1:A:303:GLU:N	2.82	0.42
1:A:287:ARG:NH1	1:A:287:ARG:HG3	2.34	0.42
1:A:147:ALA:HA	1:A:151:GLU:OE1	2.20	0.42
1:A:688:GLN:NE2	1:A:693:LYS:HZ3	2.18	0.41
1:B:649:LEU:HD12	1:B:649:LEU:N	2.35	0.41
1:A:176:LYS:HB3	1:A:178:MET:CE	2.51	0.41
1:B:560:HIS:HE1	6:B:916:HOH:O	2.02	0.41
1:B:641:ARG:HH12	1:B:645:ASN:C	2.23	0.41
1:A:234:HIS:HD2	2:A:801:SO4:O2	2.04	0.41
1:A:629:LEU:HA	1:A:630:PRO:HD3	1.91	0.41
1:B:684:SER:HB2	1:B:685:PRO:HD3	2.03	0.40
1:A:176:LYS:HB3	1:A:178:MET:HE1	2.04	0.40
1:B:229:LEU:O	1:B:230:ASP:HB2	2.22	0.40
1:B:193:LYS:NZ	1:B:197:GLU:OE1	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:GLU:OE2	1:B:714:GLU:OE1[2_654]	2.18	0.02

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	345/373 (92%)	333 (96%)	8 (2%)	4 (1%)	16	6
1	B	353/373 (95%)	335 (95%)	15 (4%)	3 (1%)	24	12
All	All	698/746 (94%)	668 (96%)	23 (3%)	7 (1%)	19	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	568	ARG
1	A	645	ASN
1	B	568	ARG
1	B	250	GLY
1	A	566	GLN
1	B	566	GLN
1	A	250	GLY

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	304/327 (93%)	298 (98%)	6 (2%)	63	58
1	B	312/327 (95%)	305 (98%)	7 (2%)	60	53
All	All	616/654 (94%)	603 (98%)	13 (2%)	61	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	254	LEU
1	A	277	LEU
1	A	287	ARG
1	A	629	LEU
1	A	714	GLU
1	B	238	ASN
1	B	256	LEU
1	B	277	LEU
1	B	287	ARG
1	B	576	LEU
1	B	714	GLU
1	B	737	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	HIS
1	A	238	ASN
1	A	262	HIS
1	A	272	GLN
1	A	285	HIS
1	A	560	HIS
1	A	636	ASN
1	A	688	GLN
1	B	234	HIS
1	B	238	ASN
1	B	272	GLN
1	B	285	HIS
1	B	560	HIS
1	B	618	HIS
1	B	621	GLN
1	B	688	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)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
2	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	A	805	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	A	806	-	4,4,4	0.24	0	6,6,6	0.10	0
4	ADP	A	810	3	22,29,29	1.62	1 (4%)	27,45,45	2.45	4 (14%)
2	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	B	803	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	B	804	-	4,4,4	0.20	0	6,6,6	0.07	0
2	SO4	B	807	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	B	808	-	4,4,4	0.20	0	6,6,6	0.09	0
5	ADE	B	900	-	8,11,11	1.13	1 (12%)	4,15,15	1.41	1 (25%)

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	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	805	-	-	0/0/0/0	0/0/0/0
2	SO4	A	806	-	-	0/0/0/0	0/0/0/0
4	ADP	A	810	3	-	0/12/32/32	0/3/3/3
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	803	-	-	0/0/0/0	0/0/0/0
2	SO4	B	804	-	-	0/0/0/0	0/0/0/0
2	SO4	B	807	-	-	0/0/0/0	0/0/0/0
2	SO4	B	808	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADE	B	900	-	-	0/0/0/0	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	900	ADE	C2-N3	2.45	1.36	1.32
4	A	810	ADP	O4'-C1'	6.28	1.49	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	810	ADP	N3-C2-N1	-10.92	120.53	128.89
4	A	810	ADP	PA-O3A-PB	-3.49	120.95	132.67
4	A	810	ADP	C2'-C1'-N9	-3.38	109.12	114.29
5	B	900	ADE	N3-C2-N1	-2.49	126.99	128.89
4	A	810	ADP	O3B-PB-O1B	2.42	118.38	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SO4	1	0
4	A	810	ADP	1	0
2	B	802	SO4	1	0
5	B	900	ADE	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	351/373 (94%)	0.31	20 (5%)	27	31	12, 25, 45, 60	0
1	B	357/373 (95%)	0.23	14 (3%)	43	48	11, 24, 43, 54	0
All	All	708/746 (94%)	0.27	34 (4%)	34	40	11, 25, 44, 60	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	TYR	5.9
1	A	641	ARG	5.1
1	A	651	ARG	4.7
1	A	645	ASN	4.1
1	B	641	ARG	3.9
1	A	145	HIS	3.7
1	B	646	SER	3.7
1	B	649	LEU	3.4
1	A	305	VAL	3.4
1	A	653	ILE	3.4
1	B	179	VAL	3.1
1	A	654	SER	3.1
1	A	737	ARG	3.0
1	B	655	LYS	3.0
1	B	737	ARG	2.9
1	A	644	PHE	2.8
1	A	181	ASN	2.8
1	A	646	SER	2.8
1	B	304	ILE	2.8
1	A	249	LEU	2.7
1	A	263	ARG	2.6
1	A	262	HIS	2.5
1	B	647	ARG	2.3
1	B	263	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	642	THR	2.3
1	B	648	GLY	2.3
1	A	568	ARG	2.2
1	B	180	ASN	2.2
1	B	644	PHE	2.2
1	A	261	GLU	2.2
1	B	645	ASN	2.2
1	A	658	PHE	2.1
1	A	287	ARG	2.1
1	B	654	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ADE	B	900	10/10	0.79	0.26	2.47	45,47,48,49	0
2	SO4	A	801	5/5	0.99	0.10	0.48	20,21,22,22	0
4	ADP	A	810	27/27	0.95	0.11	-0.68	18,30,37,38	0
2	SO4	B	802	5/5	0.99	0.09	-0.96	24,24,27,27	0
2	SO4	B	807	5/5	0.92	0.20	-	71,71,72,72	0
2	SO4	A	805	5/5	0.90	0.14	-	76,77,77,77	0
2	SO4	A	806	5/5	0.74	0.25	-	82,83,83,84	0
2	SO4	B	803	5/5	0.95	0.12	-	65,65,66,67	0
2	SO4	B	804	5/5	0.93	0.13	-	61,62,62,63	0
3	MG	A	809	1/1	0.88	0.16	-	29,29,29,29	0
2	SO4	B	808	5/5	0.98	0.21	-	63,63,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.