Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2017 – 02:14 PM EST

PDB ID	:	2JD5
Title	:	Sky1p bound to Npl3p-derived substrate peptide
Authors	:	Nolen, B.; Lukasiewicz, R.; Adams, J.A.; Huang, D.; Ghosh, G.
Deposited on	:	2007-01-04
Resolution	:	2.50 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:

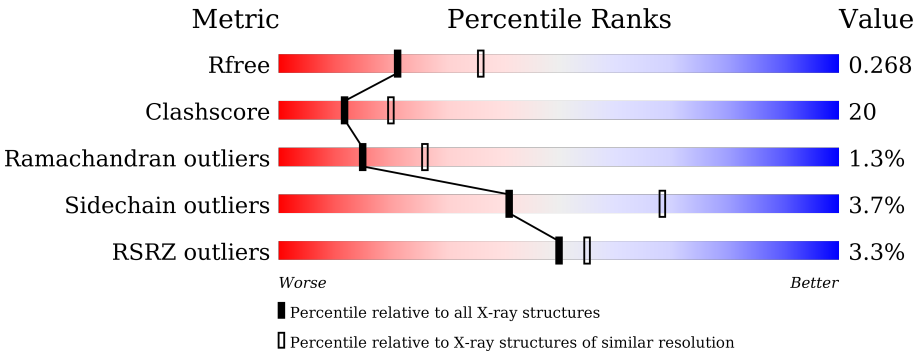
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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% 57% 35% · 5%
1	B	373	% 66% 28% · ·
2	C	7	57% 14% 29%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5920 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 SERINE/THREONINE-PROTEIN KINASE SKY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2841	1824	482	523	12			
1	B	360	Total	C	N	O	S	0	0	0
			2896	1856	491	537	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	PHE	TYR	CONFLICT	UNP Q03656
A	305	VAL	ILE	CONFLICT	UNP Q03656
A	306	ASP	ASN	CONFLICT	UNP Q03656
B	144	PHE	TYR	CONFLICT	UNP Q03656
B	305	VAL	ILE	CONFLICT	UNP Q03656
B	306	ASP	ASN	CONFLICT	UNP Q03656

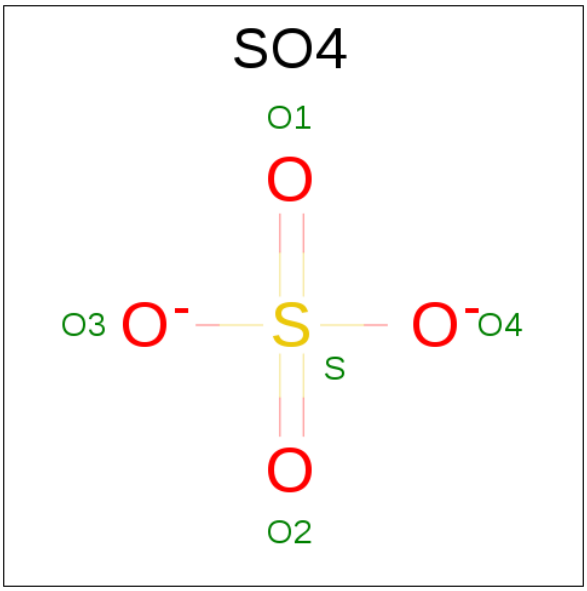
- Molecule 2 is a protein called NUCLEOLAR PROTEIN 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			38	22	8	8			

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

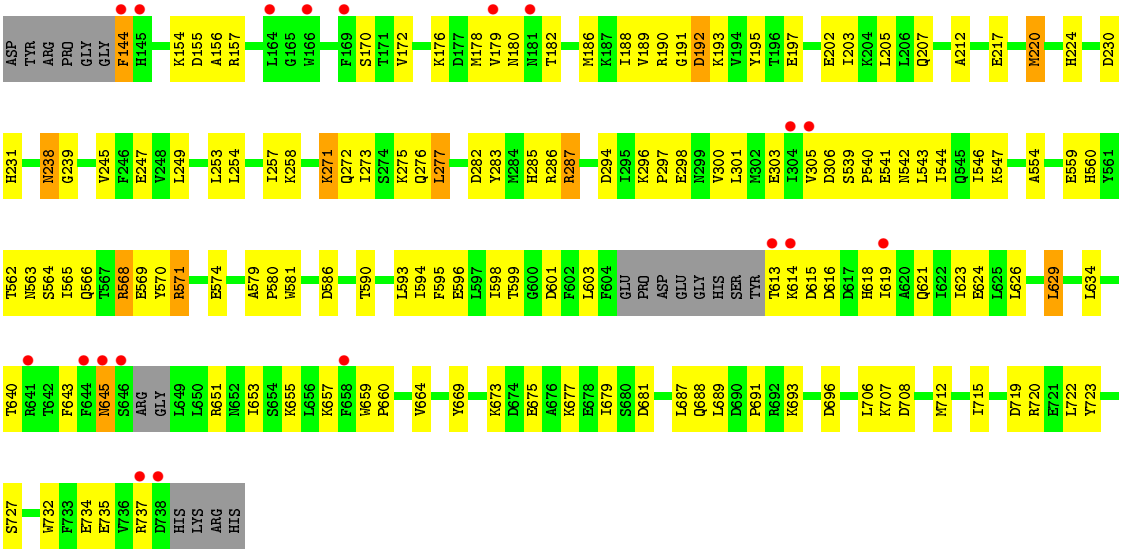
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	78	Total O 78 78	0	0

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.

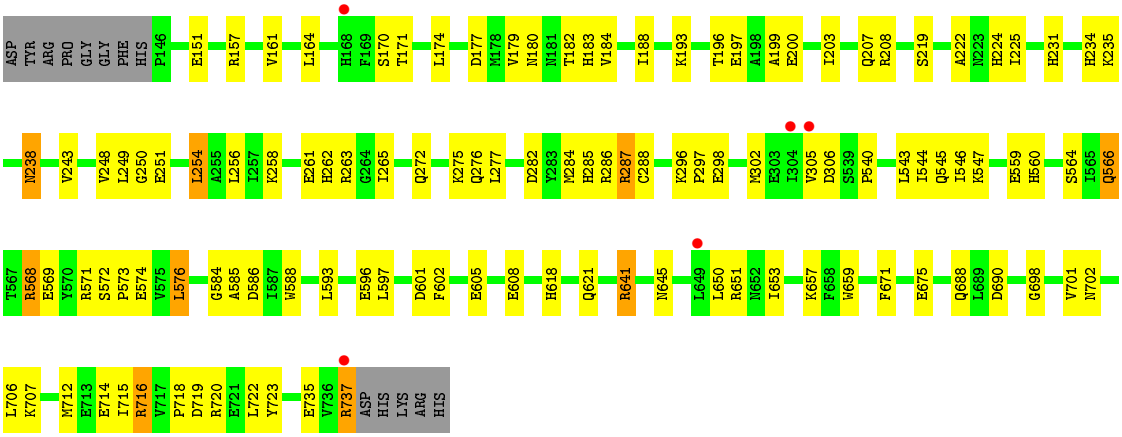
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE SKY1

Chain A:



- Molecule 1: SERINE/THREONINE-PROTEIN KINASE SKY1

Chain B:



- Molecule 2: NUCLEOLAR PROTEIN 3

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.33Å 88.56Å 134.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 44.28 – 2.45	Depositor EDS
% Data completeness (in resolution range)	82.3 (19.99-2.50) 92.5 (44.28-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.255 0.227 , 0.268	Depositor DCC
R_{free} test set	1404 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5920	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 41.06 % 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 2.4963e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.37	0/2905	0.57	0/3928
1	B	0.38	0/2964	0.60	0/4011
2	C	0.42	0/38	0.64	0/50
All	All	0.37	0/5907	0.58	0/7989

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	2841	0	2808	144	0
1	B	2896	0	2868	90	0
2	C	38	0	32	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	55	0	0	3	0
5	B	78	0	0	3	0
All	All	5920	0	5708	232	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 20.

All (232) 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:613:THR:HG21	1:A:621:GLN:HE22	1.14	1.10
1:A:568:ARG:HB3	1:A:569:GLU:N	1.80	0.96
1:A:688:GLN:HG2	1:A:693:LYS:HB2	1.52	0.91
1:B:254:LEU:HD12	1:B:298:GLU:HG3	1.58	0.85
1:A:673:LYS:HE2	1:A:677:LYS:NZ	1.92	0.84
1:B:249:LEU:HD11	1:B:547:LYS:HD2	1.58	0.84
1:A:568:ARG:O	1:A:569:GLU:N	2.12	0.82
1:A:192:ASP:HB3	1:A:195:TYR:HB2	1.63	0.80
1:A:297:PRO:HD3	1:A:593:LEU:HD13	1.64	0.79
1:A:613:THR:HG21	1:A:621:GLN:NE2	1.96	0.79
1:A:624:GLU:HG3	1:A:657:LYS:O	1.82	0.78
1:A:306:ASP:HB3	1:A:543:LEU:HB2	1.68	0.75
1:A:655:LYS:CE	2:C:659:PRO:HG3	2.17	0.75
1:A:655:LYS:NZ	2:C:659:PRO:HG3	2.02	0.75
1:A:191:GLY:O	1:A:192:ASP:HB2	1.86	0.74
1:A:176:LYS:HE3	1:A:178:MET:SD	2.28	0.73
1:A:688:GLN:CG	1:A:693:LYS:HB2	2.19	0.72
1:A:272:GLN:HE22	1:A:543:LEU:HA	1.52	0.72
1:A:645:ASN:HD22	1:A:651:ARG:NH2	1.87	0.72
1:A:615:ASP:HB3	1:A:643:PHE:HE2	1.55	0.71
1:B:272:GLN:HE22	1:B:544:ILE:H	1.38	0.71
1:B:203:ILE:O	1:B:207:GLN:HG3	1.92	0.70
1:A:562:THR:HG22	1:A:563:ASN:H	1.57	0.69
1:A:180:ASN:O	1:A:182:THR:HG23	1.92	0.69
1:A:655:LYS:HE3	2:C:659:PRO:HG3	1.75	0.69
1:A:629:LEU:HD12	1:A:689:LEU:HD13	1.73	0.69
1:B:305:VAL:CG2	1:B:545:GLN:HB2	2.23	0.69
1:B:272:GLN:NE2	1:B:544:ILE:H	1.91	0.68
1:A:249:LEU:HD23	1:A:301:LEU:HB2	1.75	0.68
1:A:623:ILE:HD13	1:A:629:LEU:HD13	1.75	0.68
1:A:645:ASN:HD22	1:A:651:ARG:HH21	1.39	0.68
1:A:568:ARG:C	1:A:571:ARG:HB2	2.14	0.67
1:A:157:ARG:HG3	1:A:179:VAL:HG23	1.76	0.66
1:A:655:LYS:HE2	1:B:659:TRP:CH2	2.30	0.66
1:B:282:ASP:OD1	1:B:286:ARG:HD3	1.96	0.66
1:B:157:ARG:HG3	1:B:179:VAL:HG23	1.76	0.66
1:B:641:ARG:HE	1:B:641:ARG:HA	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:HE	1:A:568:ARG:HA	1.60	0.65
1:A:568:ARG:HH21	1:A:571:ARG:HH22	1.43	0.65
1:A:645:ASN:HB2	1:A:651:ARG:HE	1.62	0.65
1:A:673:LYS:HE2	1:A:677:LYS:HZ3	1.58	0.65
1:A:170:SER:HB3	1:A:189:VAL:HA	1.79	0.64
1:A:170:SER:HB2	1:A:188:ILE:O	1.97	0.63
1:B:238:ASN:H	1:B:238:ASN:ND2	1.96	0.63
1:A:722:LEU:O	1:A:723:TYR:HB2	1.99	0.62
1:B:722:LEU:O	1:B:723:TYR:HB2	1.98	0.62
1:A:287:ARG:HA	1:A:287:ARG:CZ	2.29	0.62
1:A:623:ILE:CD1	1:A:629:LEU:HD13	2.30	0.62
1:B:200:GLU:OE1	1:B:203:ILE:HD12	2.00	0.62
1:A:655:LYS:NZ	1:A:657:LYS:HE3	2.14	0.62
1:B:712:MET:HB3	1:B:715:ILE:HD12	1.82	0.62
1:A:613:THR:HA	5:A:2026:HOH:O	1.98	0.61
1:A:660:PRO:O	1:A:664:VAL:HG23	2.00	0.61
1:B:208:ARG:HG3	1:B:208:ARG:HH11	1.65	0.61
1:B:302:MET:HB3	1:B:546:ILE:HG22	1.82	0.61
1:B:605:GLU:H	1:B:621:GLN:HE22	1.48	0.61
1:A:193:LYS:HE2	1:A:197:GLU:OE1	1.99	0.61
1:A:282:ASP:OD1	1:A:286:ARG:HD3	2.00	0.61
1:A:562:THR:HG22	1:A:564:SER:H	1.65	0.61
1:A:249:LEU:HD21	1:A:547:LYS:HD2	1.82	0.60
1:A:217:GLU:O	1:A:220:MET:HB2	2.01	0.60
1:B:559:GLU:HA	1:B:735:GLU:OE2	2.00	0.60
1:A:253:LEU:HD13	1:A:300:VAL:HB	1.83	0.60
1:A:249:LEU:HD21	1:A:547:LYS:HB2	1.82	0.60
1:A:615:ASP:O	1:A:619:ILE:HG13	2.02	0.60
1:A:253:LEU:O	1:A:257:ILE:HG13	2.02	0.59
1:A:254:LEU:CD2	1:A:258:LYS:HE2	2.31	0.59
1:A:594:ILE:O	1:A:598:ILE:HG13	2.03	0.58
1:B:296:LYS:HB2	1:B:297:PRO:HD2	1.85	0.58
1:B:737:ARG:HD3	1:B:737:ARG:N	2.18	0.58
1:A:238:ASN:ND2	1:A:238:ASN:H	2.01	0.58
1:B:297:PRO:HG2	1:B:298:GLU:OE1	2.03	0.58
1:B:272:GLN:HE22	1:B:543:LEU:HA	1.68	0.58
1:A:562:THR:HG22	1:A:563:ASN:N	2.18	0.58
1:B:164:LEU:HD21	1:B:174:LEU:HB2	1.86	0.58
1:B:297:PRO:HD3	1:B:593:LEU:HD13	1.85	0.58
1:A:655:LYS:HE3	2:C:659:PRO:CB	2.34	0.57
1:B:225:ILE:HD11	1:B:284:MET:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:HD22	1:B:265:ILE:HG12	1.86	0.57
1:B:256:LEU:HD22	1:B:265:ILE:CD1	2.35	0.57
1:A:655:LYS:HE3	2:C:659:PRO:HB3	1.87	0.57
1:B:196:THR:O	1:B:200:GLU:HG2	2.04	0.57
1:A:657:LYS:HE2	1:B:659:TRP:CE3	2.40	0.56
1:A:615:ASP:HB3	1:A:643:PHE:CE2	2.39	0.56
1:A:655:LYS:HZ1	2:C:659:PRO:HG3	1.70	0.56
1:A:249:LEU:HD23	1:A:301:LEU:CB	2.36	0.56
1:B:716:ARG:CZ	1:B:718:PRO:HG3	2.37	0.55
1:A:655:LYS:HE3	2:C:659:PRO:CG	2.36	0.55
1:A:655:LYS:HD3	1:A:657:LYS:HE3	1.89	0.54
1:A:254:LEU:HD21	1:A:258:LYS:HE2	1.88	0.54
1:A:202:GLU:HA	1:A:205:LEU:HD12	1.89	0.54
1:A:546:ILE:C	1:A:546:ILE:HD12	2.28	0.54
1:B:650:LEU:HD23	1:B:653:ILE:HB	1.89	0.53
1:B:671:PHE:HD2	1:B:675:GLU:HG2	1.74	0.53
1:A:645:ASN:HB2	1:A:651:ARG:HH21	1.74	0.53
1:A:722:LEU:HD12	1:A:723:TYR:N	2.24	0.53
1:A:616:ASP:HB3	1:A:653:ILE:HD13	1.90	0.53
1:A:297:PRO:CD	1:A:593:LEU:HD13	2.36	0.52
1:B:645:ASN:HB3	1:B:651:ARG:NH1	2.24	0.52
1:B:208:ARG:NH1	1:B:288:CYS:HA	2.25	0.52
1:B:254:LEU:HD12	1:B:298:GLU:CG	2.36	0.52
1:B:571:ARG:HG2	1:B:576:LEU:HD13	1.91	0.52
1:A:230:ASP:HB3	1:A:245:VAL:HG21	1.92	0.52
1:B:170:SER:HB2	1:B:188:ILE:O	2.10	0.52
1:A:179:VAL:O	1:A:179:VAL:HG12	2.09	0.52
1:A:144:PHE:CZ	1:A:238:ASN:HB3	2.45	0.52
1:B:306:ASP:OD1	1:B:540:PRO:HD2	2.09	0.52
1:B:569:GLU:HG2	1:B:602:PHE:CD2	2.45	0.52
1:B:584:GLY:HA3	5:B:2063:HOH:O	2.10	0.52
1:A:297:PRO:HD3	1:A:593:LEU:CD1	2.37	0.51
1:A:306:ASP:OD2	1:A:540:PRO:HD2	2.09	0.51
1:A:275:LYS:HD2	1:A:706:LEU:HB3	1.91	0.51
1:B:224:HIS:NE2	1:B:276:GLN:HG2	2.25	0.51
1:B:572:SER:HB2	1:B:574:GLU:OE2	2.11	0.51
1:B:712:MET:CB	1:B:715:ILE:HD12	2.41	0.51
1:A:569:GLU:CD	1:A:569:GLU:N	2.64	0.51
1:A:253:LEU:HD13	1:A:300:VAL:O	2.10	0.50
1:A:191:GLY:O	1:A:192:ASP:CB	2.59	0.50
1:A:570:TYR:N	1:A:570:TYR:CD1	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:ARG:HG2	1:B:737:ARG:O	2.11	0.50
1:B:231:HIS:HA	1:B:243:VAL:O	2.11	0.50
1:A:541:GLU:O	1:A:542:ASN:HB2	2.12	0.50
1:A:224:HIS:CD2	1:A:276:GLN:HB3	2.47	0.49
1:B:180:ASN:O	1:B:182:THR:HG23	2.13	0.49
1:B:657:LYS:HZ2	1:B:657:LYS:HB2	1.77	0.49
1:A:271:LYS:HE3	1:A:708:ASP:OD1	2.13	0.49
1:B:272:GLN:HE22	1:B:544:ILE:N	2.09	0.48
1:A:249:LEU:CD2	1:A:547:LYS:HB2	2.43	0.48
1:B:238:ASN:N	1:B:238:ASN:HD22	2.11	0.48
1:A:673:LYS:HE2	1:A:677:LYS:CE	2.43	0.48
1:B:183:HIS:O	1:B:184:VAL:HG13	2.14	0.48
1:B:702:ASN:OD1	1:B:716:ARG:HB2	2.12	0.48
1:B:566:GLN:NE2	1:B:585:ALA:HB1	2.29	0.48
1:A:230:ASP:HB3	1:A:245:VAL:CG2	2.43	0.48
1:B:287:ARG:HA	1:B:287:ARG:CZ	2.44	0.47
1:A:277:LEU:HD11	1:A:593:LEU:HD23	1.96	0.47
1:A:277:LEU:HD13	1:A:590:THR:HG23	1.96	0.47
1:A:719:ASP:O	1:A:720:ARG:HD2	2.14	0.47
1:A:722:LEU:HG	1:A:723:TYR:CD1	2.48	0.47
1:A:568:ARG:NH2	1:A:571:ARG:HH22	2.12	0.47
1:A:539:SER:N	1:A:540:PRO:CD	2.77	0.47
1:B:151:GLU:OE2	1:B:234:HIS:CE1	2.68	0.47
1:A:579:ALA:HB1	1:A:580:PRO:HD2	1.96	0.47
1:A:655:LYS:CD	1:A:657:LYS:HE3	2.44	0.47
1:A:675:GLU:HG3	1:A:679:ILE:HD12	1.95	0.47
1:B:199:ALA:O	1:B:203:ILE:HG13	2.15	0.47
1:A:189:VAL:HG12	1:A:190:ARG:N	2.31	0.46
1:A:301:LEU:O	1:A:546:ILE:HA	2.15	0.46
1:B:235:LYS:HG2	4:B:1738:SO4:O2	2.15	0.46
1:B:716:ARG:HH11	1:B:716:ARG:HG3	1.79	0.46
1:A:565:ILE:HD13	1:A:581:TRP:CZ2	2.50	0.46
1:A:559:GLU:HA	1:A:735:GLU:OE2	2.15	0.46
1:B:238:ASN:N	1:B:238:ASN:ND2	2.58	0.46
1:B:546:ILE:C	1:B:546:ILE:HD12	2.35	0.46
1:A:305:VAL:HG13	1:A:306:ASP:N	2.31	0.46
1:B:258:LYS:HG2	1:B:262:HIS:HE1	1.81	0.46
1:A:287:ARG:HA	1:A:287:ARG:NE	2.31	0.46
1:B:256:LEU:HD22	1:B:265:ILE:CG1	2.45	0.46
1:A:737:ARG:HG2	1:A:737:ARG:HH11	1.81	0.46
1:A:144:PHE:CE1	1:A:238:ASN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:HIS:HE1	1:A:586:ASP:OD2	2.00	0.45
1:A:298:GLU:H	1:A:298:GLU:CD	2.19	0.45
1:B:200:GLU:OE1	1:B:200:GLU:HA	2.15	0.45
1:A:172:VAL:HA	1:A:186:MET:O	2.16	0.45
1:A:619:ILE:O	1:A:623:ILE:HG12	2.17	0.45
1:B:596:GLU:HA	1:B:601:ASP:O	2.16	0.45
1:A:144:PHE:C	1:A:144:PHE:CD2	2.88	0.45
1:A:238:ASN:N	1:A:238:ASN:ND2	2.63	0.45
1:A:696:ASP:HA	1:A:732:TRP:CH2	2.52	0.45
1:A:273:ILE:O	1:A:277:LEU:HB2	2.17	0.45
1:A:249:LEU:CD2	1:A:547:LYS:HD2	2.46	0.45
1:B:219:SER:HA	1:B:222:ALA:HB3	1.98	0.45
1:A:539:SER:HB3	1:A:540:PRO:HD3	1.98	0.45
1:B:698:GLY:O	1:B:701:VAL:HB	2.16	0.45
1:A:626:LEU:HD11	1:A:687:LEU:HB3	1.99	0.44
1:A:596:GLU:HG3	1:A:601:ASP:O	2.17	0.44
1:A:581:TRP:O	1:A:734:GLU:HA	2.17	0.44
1:B:688:GLN:HE21	1:B:690:ASP:H	1.65	0.44
1:B:177:ASP:OD1	1:B:179:VAL:HB	2.18	0.44
1:A:294:ASP:OD2	1:A:296:LYS:HE2	2.18	0.44
1:B:568:ARG:HH21	1:B:618:HIS:HD2	1.65	0.44
1:B:282:ASP:O	1:B:286:ARG:HB2	2.18	0.44
1:A:203:ILE:O	1:A:207:GLN:HG3	2.18	0.43
1:B:573:PRO:HD3	1:B:588:TRP:CZ2	2.54	0.43
1:A:205:LEU:HD13	1:A:554:ALA:HB3	2.00	0.43
1:B:261:GLU:O	1:B:263:ARG:HG3	2.18	0.43
1:B:593:LEU:O	1:B:597:LEU:HG	2.18	0.43
1:A:202:GLU:O	1:A:203:ILE:C	2.56	0.43
1:A:574:GLU:HG2	1:A:691:PRO:HG3	2.00	0.43
1:A:212:ALA:HB3	1:A:283:TYR:OH	2.19	0.43
1:B:258:LYS:HG2	1:B:262:HIS:CE1	2.54	0.43
1:B:707:LYS:HA	1:B:707:LYS:HD2	1.85	0.43
1:B:737:ARG:CD	1:B:737:ARG:N	2.80	0.43
1:A:254:LEU:HD12	1:A:298:GLU:HG3	2.01	0.43
1:A:272:GLN:NE2	1:A:544:ILE:H	2.17	0.43
1:A:619:ILE:HD12	1:A:643:PHE:CD2	2.54	0.42
1:B:224:HIS:CD2	1:B:276:GLN:HB3	2.54	0.42
1:A:296:LYS:HB2	1:A:297:PRO:HD2	2.01	0.42
1:A:203:ILE:HD13	1:A:231:HIS:CD2	2.54	0.42
1:A:624:GLU:HG2	5:A:2034:HOH:O	2.19	0.42
1:B:305:VAL:HG21	1:B:545:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:ASP:OD1	1:B:719:ASP:N	2.51	0.42
1:A:712:MET:HB3	1:A:715:ILE:HD12	2.00	0.42
1:A:271:LYS:CE	1:A:708:ASP:OD1	2.68	0.42
1:A:247:GLU:HG2	5:A:2008:HOH:O	2.18	0.42
1:A:722:LEU:HD12	1:A:723:TYR:H	1.85	0.42
1:B:184:VAL:HA	1:B:248:VAL:HG23	2.01	0.42
1:A:659:TRP:CE3	1:A:664:VAL:HG22	2.55	0.42
1:B:251:GLU:HA	5:B:2017:HOH:O	2.20	0.41
1:B:641:ARG:HE	1:B:641:ARG:CA	2.24	0.41
1:A:249:LEU:HD11	1:A:303:GLU:OE1	2.20	0.41
1:A:645:ASN:CB	1:A:651:ARG:HE	2.32	0.41
1:A:675:GLU:HG3	1:A:679:ILE:CD1	2.50	0.41
1:B:164:LEU:HD11	1:B:174:LEU:HB2	2.02	0.41
1:B:224:HIS:HD2	1:B:546:ILE:O	2.03	0.41
1:B:560:HIS:CD2	1:B:735:GLU:HB2	2.56	0.41
1:A:569:GLU:HB2	1:A:570:TYR:CE1	2.55	0.41
1:A:599:THR:HB	1:A:669:TYR:CE2	2.55	0.41
1:B:719:ASP:O	1:B:720:ARG:HD2	2.21	0.41
1:A:189:VAL:CG1	1:A:190:ARG:N	2.83	0.40
1:A:595:PHE:CG	1:A:603:LEU:HD13	2.56	0.40
1:A:677:LYS:O	1:A:681:ASP:OD1	2.39	0.40
1:B:275:LYS:HD2	1:B:706:LEU:HB3	2.01	0.40
1:A:634:LEU:HA	1:A:640:THR:OG1	2.21	0.40
1:B:285:HIS:HE1	1:B:586:ASP:OD2	2.05	0.40
1:A:722:LEU:O	1:A:723:TYR:CB	2.65	0.40
1:B:193:LYS:O	1:B:197:GLU:HG3	2.21	0.40
1:A:224:HIS:NE2	1:A:276:GLN:HG2	2.35	0.40
1:A:155:ASP:O	1:A:156:ALA:HB3	2.22	0.40
1:A:238:ASN:HD22	1:A:239:GLY:N	2.19	0.40
1:B:161:VAL:HA	5:B:2003:HOH:O	2.20	0.40
1:B:170:SER:HB2	1:B:171:THR:H	1.57	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	345/373 (92%)	314 (91%)	25 (7%)	6 (2%)	11 19
1	B	358/373 (96%)	331 (92%)	24 (7%)	3 (1%)	24 41
2	C	3/7 (43%)	3 (100%)	0	0	100 100
All	All	706/753 (94%)	648 (92%)	49 (7%)	9 (1%)	15 26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	LYS
1	B	568	ARG
1	A	192	ASP
1	A	645	ASN
1	B	250	GLY
1	A	566	GLN
1	A	154	LYS
1	B	566	GLN
1	A	727	SER

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	306/327 (94%)	294 (96%)	12 (4%)	39 66
1	B	313/327 (96%)	302 (96%)	11 (4%)	43 70
2	C	4/7 (57%)	4 (100%)	0	100 100
All	All	623/661 (94%)	600 (96%)	23 (4%)	41 68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	PHE

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Mol	Chain	Res	Type
1	A	220	MET
1	A	238	ASN
1	A	271	LYS
1	A	277	LEU
1	A	287	ARG
1	A	560	HIS
1	A	568	ARG
1	A	571	ARG
1	A	618	HIS
1	A	629	LEU
1	A	707	LYS
1	B	238	ASN
1	B	254	LEU
1	B	277	LEU
1	B	287	ARG
1	B	564	SER
1	B	576	LEU
1	B	608	GLU
1	B	641	ARG
1	B	714	GLU
1	B	716	ARG
1	B	737	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	231	HIS
1	A	234	HIS
1	A	238	ASN
1	A	272	GLN
1	A	285	HIS
1	A	621	GLN
1	A	636	ASN
1	A	645	ASN
1	B	234	HIS
1	B	238	ASN
1	B	262	HIS
1	B	272	GLN
1	B	285	HIS
1	B	618	HIS
1	B	621	GLN

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Mol	Chain	Res	Type
1	B	688	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	SO4	A	1740	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	B	1738	-	4,4,4	0.20	0	6,6,6	0.09	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
4	SO4	A	1740	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1738	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1738	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	353/373 (94%)	0.24	19 (5%) 29 33	18, 34, 59, 81	0
1	B	360/373 (96%)	-0.03	5 (1%) 78 80	15, 29, 50, 64	0
2	C	5/7 (71%)	0.13	0 100 100	31, 38, 41, 43	0
All	All	718/753 (95%)	0.10	24 (3%) 50 55	15, 32, 57, 81	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	THR	8.3
1	A	145	HIS	5.6
1	A	738	ASP	5.6
1	A	646	SER	5.4
1	A	144	PHE	4.2
1	B	737	ARG	4.2
1	A	305	VAL	3.9
1	A	645	ASN	3.9
1	A	644	PHE	3.3
1	A	737	ARG	3.3
1	A	166	TRP	3.2
1	A	181	ASN	3.1
1	A	304	ILE	3.1
1	A	614	LYS	3.0
1	A	641	ARG	2.8
1	A	164	LEU	2.8
1	B	304	ILE	2.6
1	B	649	LEU	2.5
1	A	658	PHE	2.2
1	B	305	VAL	2.2
1	A	169	PHE	2.2
1	A	619	ILE	2.1
1	A	179	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	168	HIS	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
4	SO4	A	1740	5/5	0.97	0.17	1.17	52,52,53,54	0
4	SO4	B	1738	5/5	0.93	0.15	-0.15	83,83,85,85	0
3	MG	B	1739	1/1	0.52	0.17	-	66,66,66,66	0
3	MG	A	1739	1/1	0.89	0.10	-	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.