Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2016 – 08:57 AM EDT

PDB ID	:	5HPH
Title	:	Structure of TRAP1 fragment
Authors	:	Sung, N.; Chang, C.; Lee, S.; Tsai, F.T.F.
Deposited on	:	2016-01-20
Resolution	:	2.43 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 ⓘ symbol.

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

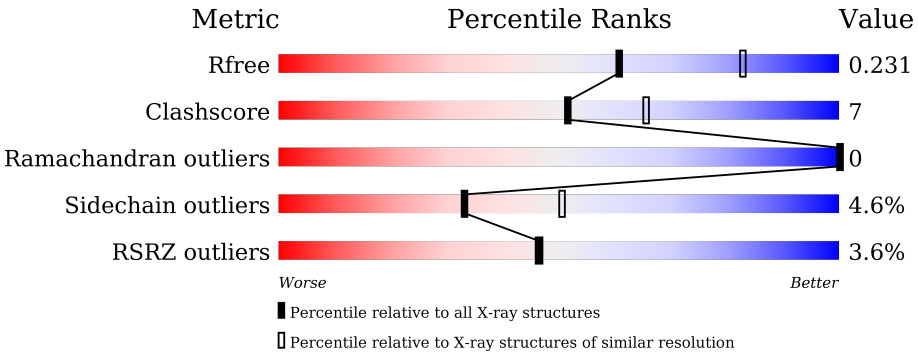
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.43 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	500	5% 76% 19%
1	B	500	2% 82% 13%

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
4	MG	B	805	-	-	-	X
5	GOL	B	806	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7891 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.

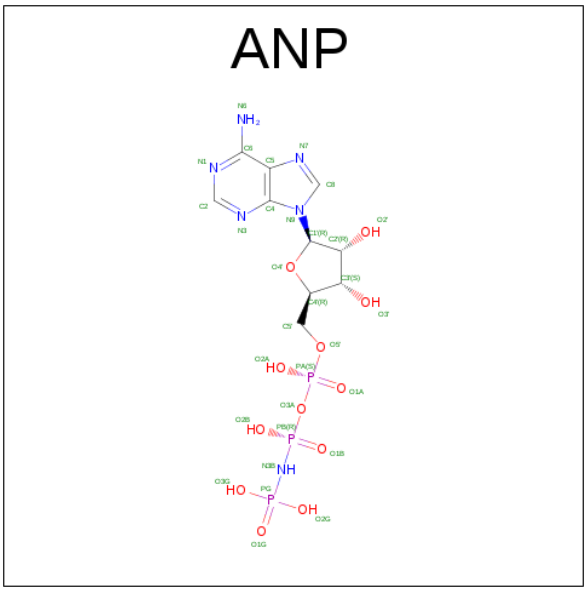
- Molecule 1 is a protein called Heat shock protein 75 kDa, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3825	2429	654	728	14			
1	B	483	Total	C	N	O	S	0	1	0
			3823	2432	648	729	14			

There are 10 discrepancies between the modelled and reference sequences:

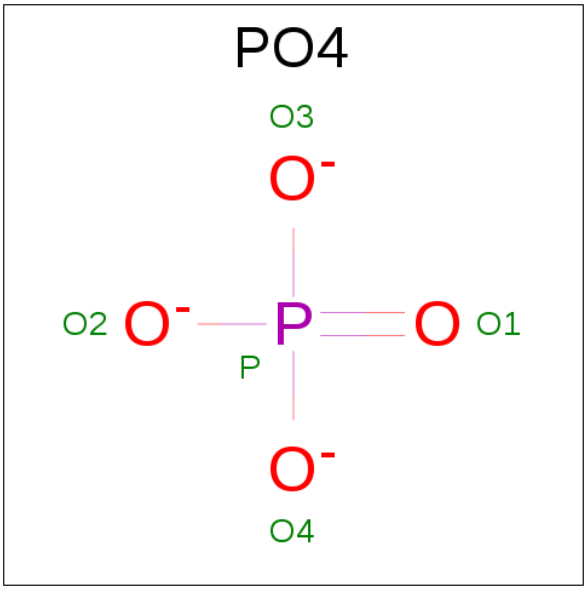
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLY	-	expression tag	UNP Q12931
A	56	ALA	-	expression tag	UNP Q12931
A	57	MET	-	expression tag	UNP Q12931
A	58	GLY	-	expression tag	UNP Q12931
A	59	SER	-	expression tag	UNP Q12931
B	55	GLY	-	expression tag	UNP Q12931
B	56	ALA	-	expression tag	UNP Q12931
B	57	MET	-	expression tag	UNP Q12931
B	58	GLY	-	expression tag	UNP Q12931
B	59	SER	-	expression tag	UNP Q12931

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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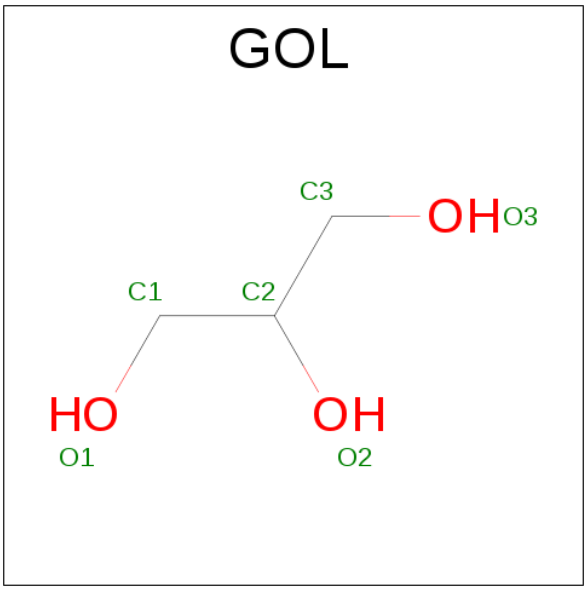
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0

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

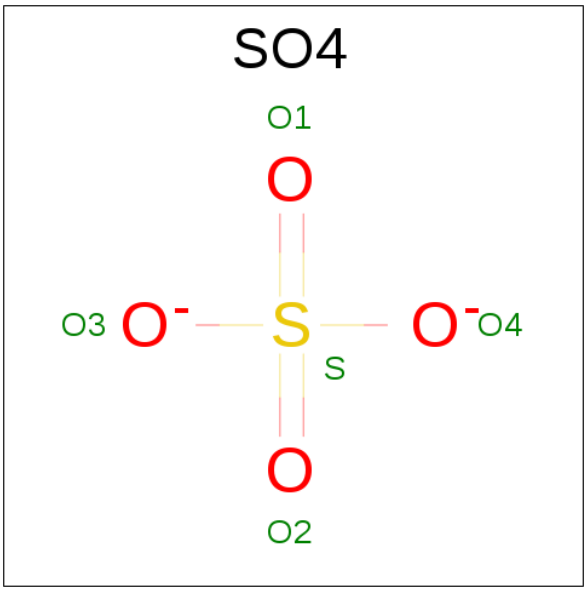
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	1	Total O S 4 3 1	0	0

- Molecule 7 is water.

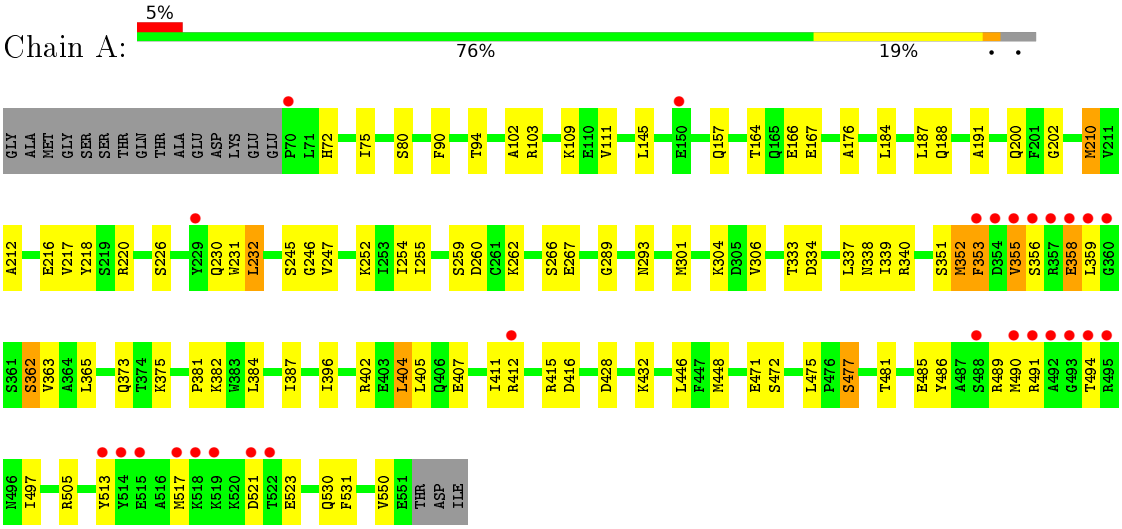
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	73	Total O 73 73	0	0

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.

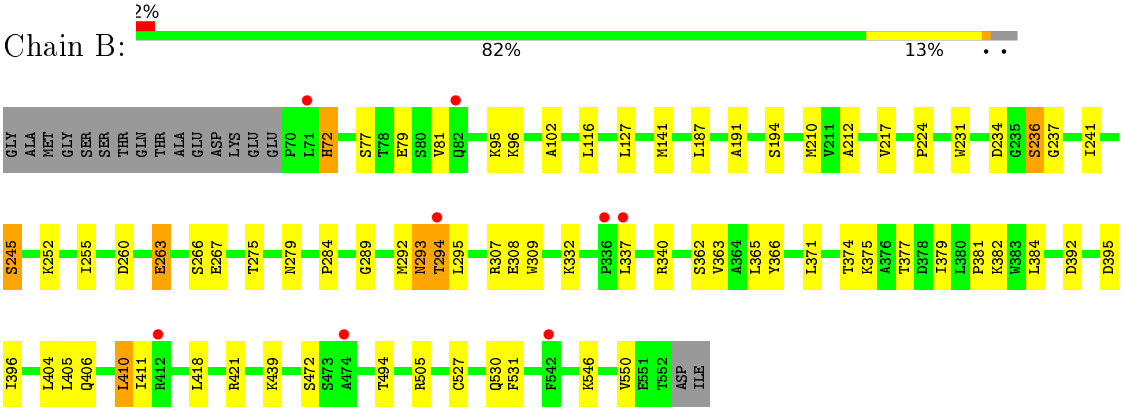
- Molecule 1: Heat shock protein 75 kDa, mitochondrial

Chain A:



- Molecule 1: Heat shock protein 75 kDa, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.44Å 104.95Å 156.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.43 49.76 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.76-2.43) 90.9 (49.76-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.238 0.189 , 0.231	Depositor DCC
R_{free} test set	1828 reflections (3.41%)	DCC
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.2	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	0.95	EDS
Total number of atoms	7891	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, 0.333 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: GOL, MG, ANP, PO4, 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	0.40	0/3903	0.61	0/5266
1	B	0.42	0/3901	0.59	0/5264
All	All	0.41	0/7804	0.60	0/10530

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	A	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	LYS	Peptide
1	A	351	SER	Peptide
1	A	352	MET	Peptide
1	A	358	GLU	Peptide

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	3825	0	3790	62	0
1	B	3823	0	3793	51	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	8	2	0
5	B	18	0	24	2	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
7	A	62	0	0	3	1
7	B	73	0	0	1	1
All	All	7891	0	7641	105	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 7.

All (105) 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:234:ASP:OD1	1:B:236:SER:OG	1.99	0.81
1:B:307:ARG:HG3	1:B:309:TRP:H	1.52	0.74
1:A:382:LYS:NZ	7:A:901:HOH:O	2.22	0.72
1:A:352:MET:HB2	1:A:353:PHE:HA	1.72	0.70
1:A:301:MET:HE2	1:A:306:VAL:HG22	1.77	0.66
1:B:405:LEU:HB2	1:B:411:ILE:HD11	1.80	0.63
1:B:191:ALA:O	1:B:194:SER:OG	2.17	0.62
1:B:332:LYS:HE2	1:B:340:ARG:HD2	1.82	0.61
1:B:212:ALA:HB2	1:B:255:ILE:HG23	1.84	0.60
1:B:307:ARG:HG3	1:B:309:TRP:N	2.17	0.59
1:B:217:VAL:HB	1:B:231:TRP:HB3	1.83	0.59
1:A:289:GLY:HA2	1:B:72:HIS:O	2.03	0.59
1:A:334:ASP:HB3	1:A:338:ASN:OD1	2.03	0.58
1:A:477:SER:HB2	1:A:505:ARG:HD2	1.83	0.58
1:B:472:SER:O	1:B:505:ARG:NH2	2.36	0.57
1:A:407:GLU:HA	1:A:411:ILE:HD12	1.85	0.57
1:B:381:PRO:HG2	1:B:384:LEU:HD12	1.86	0.57
1:B:292:MET:O	1:B:294:THR:OG1	2.23	0.56
1:A:334:ASP:HA	1:A:337:LEU:O	2.05	0.56
1:B:396:ILE:HG22	1:B:410:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:OD1	1:A:334:ASP:N	2.38	0.56
1:B:267:GLU:HB3	5:B:807:GOL:H12	1.87	0.55
1:A:216:GLU:HG3	1:A:254:ILE:HB	1.87	0.55
1:A:212:ALA:HB2	1:A:255:ILE:HG23	1.89	0.55
1:B:307:ARG:HD3	1:B:308:GLU:H	1.71	0.55
1:A:218:TYR:CG	1:B:79:GLU:HG2	2.42	0.54
1:A:513:TYR:HB3	1:A:550:VAL:HG12	1.89	0.54
1:A:176:ALA:HB1	1:B:96:LYS:HG2	1.90	0.54
1:A:353:PHE:HZ	1:A:356:SER:HB3	1.73	0.53
1:A:489:ARG:NH2	7:A:903:HOH:O	2.42	0.53
1:B:102:ALA:O	1:B:210:MET:HG2	2.08	0.52
1:A:260:ASP:OD1	1:A:260:ASP:N	2.39	0.52
1:B:371:LEU:HD21	1:B:374:THR:HG23	1.92	0.52
1:A:80:SER:N	1:B:245:SER:O	2.38	0.52
1:A:217:VAL:HB	1:A:231:TRP:HB3	1.92	0.51
1:A:355:VAL:HG22	1:A:358:GLU:HB2	1.91	0.51
1:B:421:ARG:NH2	3:B:802:PO4:O3	2.42	0.50
1:A:333:THR:HG22	1:A:339:ILE:HD12	1.94	0.50
1:B:365:LEU:HD21	1:B:405:LEU:HD11	1.94	0.50
1:A:415:ARG:NH2	7:A:901:HOH:O	2.29	0.50
1:A:102:ALA:O	1:A:210:MET:HG3	2.13	0.49
1:A:202:GLY:H	2:A:801:ANP:HNB1	1.57	0.49
1:A:216:GLU:HB3	1:A:232:LEU:HD13	1.94	0.49
1:A:384:LEU:HD22	1:A:387:ILE:HD12	1.95	0.49
1:A:491:ARG:O	1:A:494:THR:HG22	2.12	0.49
1:A:491:ARG:NH1	1:A:521:ASP:HB3	2.28	0.48
1:A:373:GLN:HE21	1:A:404:LEU:HA	1.77	0.48
1:A:187:LEU:HD13	1:A:191:ALA:HB3	1.96	0.48
1:A:381:PRO:HG2	1:A:384:LEU:HD12	1.96	0.48
1:A:471:GLU:OE1	1:A:505:ARG:NH1	2.47	0.48
1:A:266:SER:OG	5:A:804:GOL:H31	2.14	0.48
1:B:546:LYS:HE2	1:B:546:LYS:HB3	1.61	0.47
1:B:396:ILE:HD12	1:B:405:LEU:HD13	1.95	0.47
1:A:90:PHE:HD2	1:B:237:GLY:HA2	1.78	0.47
1:A:103:ARG:O	1:B:406:GLN:NE2	2.44	0.46
1:B:260:ASP:OD1	1:B:260:ASP:N	2.46	0.46
1:A:396:ILE:HG12	1:A:405:LEU:HD22	1.97	0.46
1:A:267:GLU:H	5:A:804:GOL:H12	1.81	0.46
1:B:363:VAL:HB	1:B:379:ILE:HD11	1.98	0.46
1:A:109:LYS:HE2	1:A:109:LYS:HB3	1.69	0.45
1:B:362:SER:HB2	1:B:375:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:SER:H	1:A:358:GLU:HG3	1.80	0.45
1:A:472:SER:O	1:A:505:ARG:NH2	2.49	0.44
1:A:481:THR:HG22	1:A:485:GLU:HB2	1.98	0.44
1:B:365:LEU:HD21	1:B:405:LEU:HD21	2.00	0.44
1:A:75:ILE:HG23	1:B:252:LYS:HE3	2.00	0.44
1:A:428:ASP:O	1:A:432:LYS:HG2	2.18	0.44
1:A:72:HIS:O	1:B:289:GLY:HA2	2.17	0.44
1:B:530:GLN:HG2	1:B:531:PHE:CD2	2.53	0.44
1:B:267:GLU:HB3	5:B:807:GOL:H32	1.99	0.44
1:A:220:ARG:HD3	1:A:247:VAL:O	2.17	0.44
1:B:396:ILE:HG22	1:B:410:LEU:CD2	2.48	0.44
1:A:245:SER:HA	1:A:246:GLY:HA2	1.74	0.44
1:A:157:GLN:OE1	1:A:252:LYS:HE3	2.18	0.44
1:B:366:TYR:O	1:B:392:ASP:HA	2.17	0.43
1:A:530:GLN:HG2	1:A:531:PHE:CD2	2.53	0.43
1:A:362:SER:HB2	1:A:375:LYS:HB3	2.00	0.43
1:A:489:ARG:NH1	1:A:523:GLU:OE2	2.52	0.43
1:B:127:LEU:HD23	1:B:141:MET:HE3	2.00	0.42
1:B:127:LEU:HD23	1:B:141:MET:CE	2.49	0.42
1:B:332:LYS:HE2	1:B:340:ARG:CD	2.49	0.42
1:A:164:THR:OG1	1:A:167:GLU:HG3	2.19	0.42
1:A:486:TYR:CE1	1:A:497:ILE:HG23	2.55	0.42
1:B:141:MET:O	1:B:284:PRO:HD2	2.19	0.42
1:B:418:LEU:HA	1:B:418:LEU:HD23	1.86	0.42
1:A:200:GLN:HG2	1:A:402:ARG:NH2	2.35	0.42
1:A:365:LEU:HD21	1:A:405:LEU:HD11	2.02	0.41
1:B:337:LEU:HA	1:B:337:LEU:HD23	1.92	0.41
1:B:263:GLU:HB3	7:B:902:HOH:O	2.19	0.41
1:B:95:LYS:HD2	1:B:236:SER:O	2.20	0.41
1:A:217:VAL:O	1:A:230:GLN:HA	2.21	0.41
1:A:448:MET:HG2	1:A:448:MET:H	1.66	0.41
1:B:275:THR:O	1:B:279:ASN:HB2	2.21	0.41
1:B:382:LYS:HE3	1:B:382:LYS:HB2	1.71	0.41
1:A:412:ARG:NH1	1:A:416:ASP:OD2	2.53	0.41
1:A:490:MET:HB3	1:A:494:THR:CG2	2.51	0.41
1:B:396:ILE:HD12	1:B:405:LEU:HD22	2.01	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.91	0.40
1:B:187:LEU:HD13	1:B:191:ALA:HB3	2.02	0.40
1:A:293:ASN:OD1	1:A:293:ASN:N	2.53	0.40
1:A:475:LEU:HD11	1:A:489:ARG:HH22	1.86	0.40
1:B:116:LEU:HD11	1:B:255:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:C	1:B:295:LEU:H	2.24	0.40
1:A:353:PHE:CZ	1:A:356:SER:HB3	2.56	0.40
1:B:337:LEU:HD22	1:B:395:ASP:HB3	2.04	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)
7:A:961:HOH:O	7:B:940:HOH:O[4_455]	2.17	0.03

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	481/500 (96%)	463 (96%)	18 (4%)	0	100	100
1	B	482/500 (96%)	467 (97%)	15 (3%)	0	100	100
All	All	963/1000 (96%)	930 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	413/438 (94%)	393 (95%)	20 (5%)	31	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	413/438 (94%)	394 (95%)	19 (5%)	33 50
All	All	826/876 (94%)	787 (95%)	39 (5%)	33 49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	THR
1	A	111	VAL
1	A	145	LEU
1	A	166	GLU
1	A	188	GLN
1	A	210	MET
1	A	226	SER
1	A	232	LEU
1	A	259	SER
1	A	304	LYS
1	A	340	ARG
1	A	353	PHE
1	A	355	VAL
1	A	359	LEU
1	A	362	SER
1	A	363	VAL
1	A	404	LEU
1	A	446	LEU
1	A	477	SER
1	A	517	MET
1	B	72	HIS
1	B	77	SER
1	B	81	VAL
1	B	224	PRO
1	B	236	SER
1	B	241	ILE
1	B	245	SER
1	B	263	GLU
1	B	266	SER
1	B	293	ASN
1	B	294	THR
1	B	377	THR
1	B	404	LEU
1	B	410	LEU
1	B	439	LYS
1	B	494	THR

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Mol	Chain	Res	Type
1	B	527[A]	CYS
1	B	527[B]	CYS
1	B	550	VAL

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 13 ligands modelled in this entry, 1 is modelled with single atom and 2 are 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	ANP	A	801	4	29,33,33	2.03	7 (24%)	26,52,52	2.13	5 (19%)
3	PO4	A	802	-	4,4,4	0.58	0	6,6,6	0.25	0
5	GOL	A	804	-	5,5,5	0.37	0	5,5,5	0.18	0
2	ANP	B	801	4	29,33,33	2.08	6 (20%)	26,52,52	2.23	6 (23%)
3	PO4	B	802	-	4,4,4	0.57	0	6,6,6	0.26	0
3	PO4	B	803	-	4,4,4	0.63	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	B	804	-	1,3,4	0.64	0	0,3,6	0.00	-
5	GOL	B	806	-	5,5,5	0.36	0	5,5,5	0.56	0
5	GOL	B	807	-	5,5,5	0.36	0	5,5,5	0.43	0
5	GOL	B	808	-	5,5,5	0.24	0	5,5,5	0.50	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	ANP	A	801	4	-	1/13/38/38	0/3/3/3
3	PO4	A	802	-	-	0/0/0/0	0/0/0/0
5	GOL	A	804	-	-	0/4/4/4	0/0/0/0
2	ANP	B	801	4	-	0/13/38/38	0/3/3/3
3	PO4	B	802	-	-	0/0/0/0	0/0/0/0
3	PO4	B	803	-	-	0/0/0/0	0/0/0/0
6	SO4	B	804	-	-	0/0/0/0	0/0/0/0
5	GOL	B	806	-	-	0/4/4/4	0/0/0/0
5	GOL	B	807	-	-	0/4/4/4	0/0/0/0
5	GOL	B	808	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PB-O2B	-2.59	1.49	1.56
2	A	801	ANP	PG-O2G	-2.31	1.50	1.56
2	B	801	ANP	PB-O3A	2.04	1.61	1.59
2	B	801	ANP	C5-C4	2.89	1.47	1.40
2	A	801	ANP	PB-O1B	2.90	1.49	1.46
2	A	801	ANP	PB-N3B	3.28	1.72	1.63
2	A	801	ANP	C5-C4	3.44	1.48	1.40
2	B	801	ANP	PG-O1G	3.74	1.50	1.46
2	A	801	ANP	PG-N3B	3.80	1.73	1.63
2	B	801	ANP	PB-N3B	3.85	1.73	1.63
2	B	801	ANP	PG-N3B	4.27	1.75	1.63
2	A	801	ANP	PG-O1G	6.66	1.53	1.46
2	B	801	ANP	PB-O1B	6.93	1.53	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	ANP	N3-C2-N1	-8.28	122.37	128.87
2	A	801	ANP	N3-C2-N1	-6.87	123.47	128.87
2	B	801	ANP	C1'-N9-C4	-2.91	123.56	126.81
2	A	801	ANP	PA-O3A-PB	-2.58	123.33	132.71
2	A	801	ANP	C1'-N9-C4	-2.41	124.12	126.81
2	B	801	ANP	O3G-PG-O2G	2.19	114.03	107.67
2	B	801	ANP	N6-C6-N1	2.25	122.28	118.52
2	B	801	ANP	C2-N1-C6	2.26	122.80	118.77
2	A	801	ANP	O3G-PG-O2G	3.01	116.41	107.67
2	B	801	ANP	O2B-PB-O1B	4.70	119.28	110.02
2	A	801	ANP	O2B-PB-O1B	5.25	120.37	110.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	O1G-PG-N3B-PB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	1	0
5	A	804	GOL	2	0
3	B	802	PO4	1	0
5	B	807	GOL	2	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	482/500 (96%)	0.36	27 (5%) 28 27	51, 76, 135, 246	0
1	B	483/500 (96%)	0.18	8 (1%) 73 72	52, 73, 118, 182	0
All	All	965/1000 (96%)	0.27	35 (3%) 46 46	51, 75, 127, 246	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	VAL	14.7
1	A	356	SER	14.1
1	A	354	ASP	8.1
1	A	492	ALA	5.9
1	A	491	ARG	5.9
1	A	493	GLY	5.3
1	A	522	THR	5.2
1	A	514	TYR	4.8
1	A	517	MET	4.5
1	A	359	LEU	4.4
1	A	494	THR	4.3
1	A	358	GLU	4.1
1	B	71	LEU	3.7
1	A	521	ASP	3.7
1	A	70	PRO	3.3
1	A	490	MET	3.2
1	A	518	LYS	3.1
1	A	353	PHE	3.0
1	B	542	PHE	2.9
1	A	515	GLU	2.9
1	A	519	LYS	2.8
1	B	337	LEU	2.7
1	A	150	GLU	2.6
1	A	229	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	336	PRO	2.4
1	A	357	ARG	2.3
1	A	488	SER	2.2
1	B	294	THR	2.2
1	A	495	ARG	2.2
1	A	412	ARG	2.2
1	B	82	GLN	2.1
1	B	474	ALA	2.1
1	B	412	ARG	2.1
1	A	513	TYR	2.0
1	A	360	GLY	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	MG	B	805	1/1	0.92	0.24	5.54	62,62,62,62	0
5	GOL	B	806	6/6	0.85	0.20	3.60	69,73,80,85	0
5	GOL	B	808	6/6	0.93	0.18	1.90	66,74,79,81	0
3	PO4	B	803	5/5	0.95	0.21	1.33	128,134,138,138	0
4	MG	A	803	1/1	0.98	0.16	1.24	58,58,58,58	0
5	GOL	B	807	6/6	0.92	0.25	0.98	90,93,101,105	0
2	ANP	A	801	31/31	0.99	0.17	0.79	47,54,59,61	0
2	ANP	B	801	31/31	0.99	0.18	0.54	50,56,60,69	0
5	GOL	A	804	6/6	0.84	0.15	-0.06	93,99,105,111	0
6	SO4	B	804	4/5	0.95	0.12	-1.61	128,131,134,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	B	802	5/5	0.84	0.19	-	97,97,115,115	5
6	SO4	A	805	1/5	-0.18	0.87	-	122,122,122,122	0
3	PO4	A	802	5/5	0.95	0.13	-	89,94,100,106	0

6.5 Other polymers (i)

There are no such residues in this entry.