



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

PDB ID : 3VTH
Title : Crystal structure of full-length HypF in the phosphate- and nucleotide-bound form
Authors : Shomura, Y.; Higuchi, Y.
Deposited on : 2012-05-30
Resolution : 2.00 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 (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

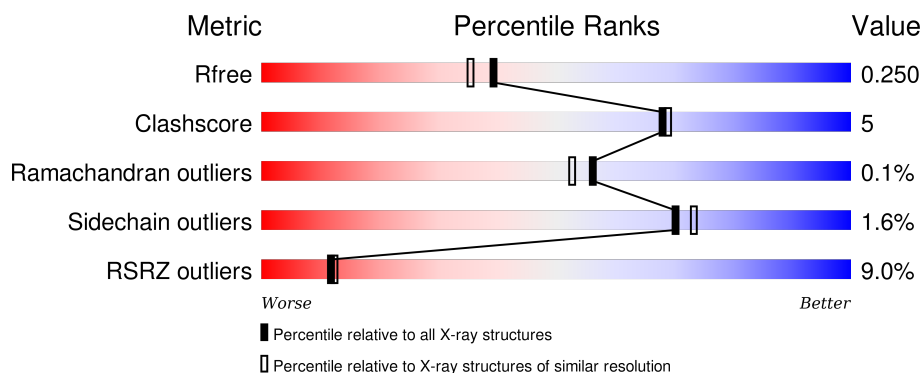
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	761	
1	B	761	

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
3	PO4	A	809	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11800 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 Hydrogenase maturation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	4	0
			6058	3870	1033	1124	31			
1	B	630	Total	C	N	O	S	0	0	0
			5059	3236	867	931	25			

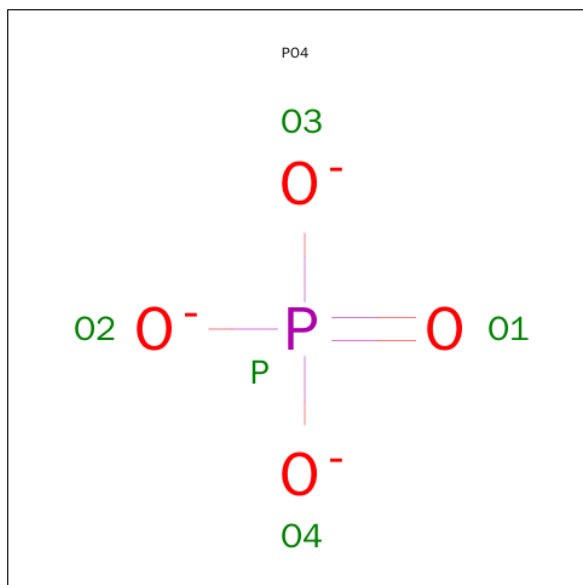
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	SER	-	EXPRESSION TAG	UNP Q8RDB0
A	753	ALA	-	EXPRESSION TAG	UNP Q8RDB0
A	754	TRP	-	EXPRESSION TAG	UNP Q8RDB0
A	755	SER	-	EXPRESSION TAG	UNP Q8RDB0
A	756	HIS	-	EXPRESSION TAG	UNP Q8RDB0
A	757	PRO	-	EXPRESSION TAG	UNP Q8RDB0
A	758	GLN	-	EXPRESSION TAG	UNP Q8RDB0
A	759	PHE	-	EXPRESSION TAG	UNP Q8RDB0
A	760	GLU	-	EXPRESSION TAG	UNP Q8RDB0
A	761	LYS	-	EXPRESSION TAG	UNP Q8RDB0
B	752	SER	-	EXPRESSION TAG	UNP Q8RDB0
B	753	ALA	-	EXPRESSION TAG	UNP Q8RDB0
B	754	TRP	-	EXPRESSION TAG	UNP Q8RDB0
B	755	SER	-	EXPRESSION TAG	UNP Q8RDB0
B	756	HIS	-	EXPRESSION TAG	UNP Q8RDB0
B	757	PRO	-	EXPRESSION TAG	UNP Q8RDB0
B	758	GLN	-	EXPRESSION TAG	UNP Q8RDB0
B	759	PHE	-	EXPRESSION TAG	UNP Q8RDB0
B	760	GLU	-	EXPRESSION TAG	UNP Q8RDB0
B	761	LYS	-	EXPRESSION TAG	UNP Q8RDB0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

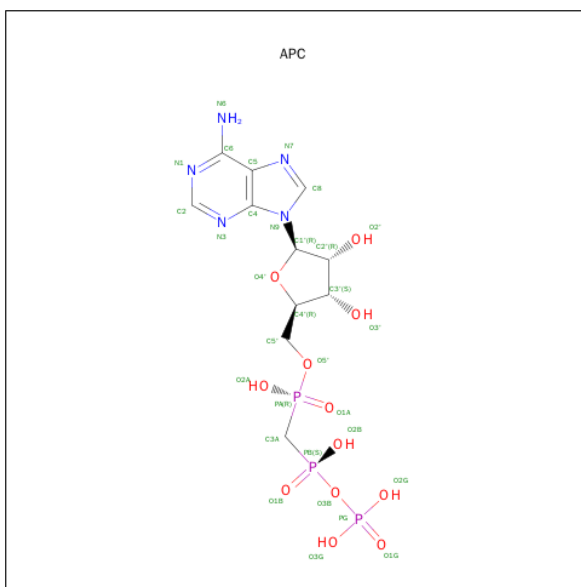
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).

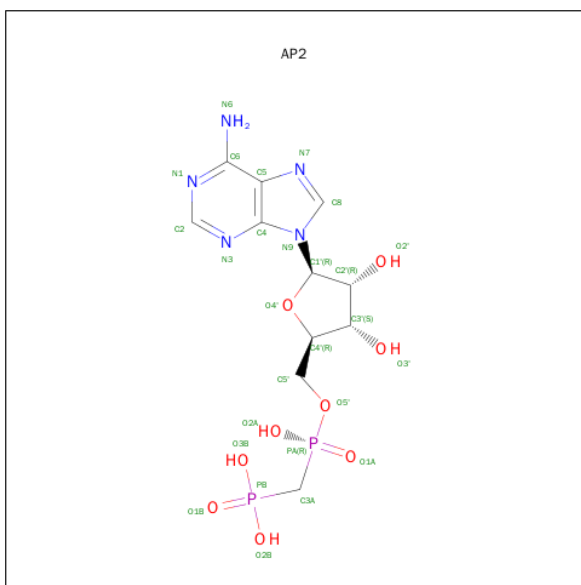


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	B	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: AP2) (formula: $\text{C}_{11}\text{H}_{17}\text{N}_5\text{O}_9\text{P}_2$).

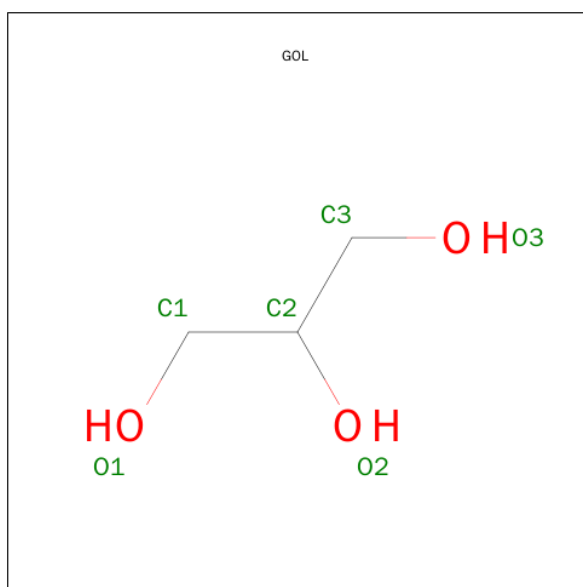


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 27	C 11	N 5	O 9	P 2	0	0
6	B	1	Total 27	C 11	N 5	O 9	P 2	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe 1 1	0	0
7	A	1	Total Fe 1 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



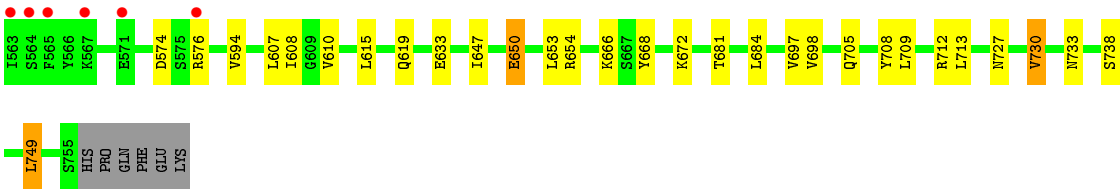
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	400	Total	O	0	0
			400	400		
9	B	107	Total	O	0	0
			107	107		

- Molecule 1: Hydrogenase maturation factor





4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	232.98 Å 232.98 Å 65.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 38.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.00) 96.7 (38.13-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.209 , 0.238 0.222 , 0.250	Depositor DCC
R_{free} test set	6702 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 134095 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11800	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, ZN, AP2, PO4, MG, FE, APC

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	0.56	0/6192	0.61	0/8341
1	B	0.44	0/5161	0.57	0/6952
All	All	0.51	0/11353	0.59	0/15293

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	6058	0	6064	45	0
1	B	5059	0	5084	61	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	0	0
3	B	10	0	0	0	0
4	A	31	0	14	3	0
4	B	31	0	14	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	27	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	12	0	16	0	0
8	B	6	0	8	0	0
9	A	400	0	0	6	0
9	B	107	0	0	2	0
All	All	11800	0	11228	106	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 5.

All (106) 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:13:GLN:HE21	1:A:15:ASN:HD21	1.20	0.88
1:B:405:VAL:HG22	1:B:439:TYR:OH	1.77	0.84
1:A:636:GLU:H	1:A:655:GLN:HE22	1.28	0.79
1:B:321:ILE:HG13	1:B:322:ASP:H	1.49	0.76
1:A:615:LEU:H	1:A:619:GLN:NE2	1.84	0.76
1:B:321:ILE:HD11	1:B:323:PHE:CZ	2.22	0.74
1:B:615:LEU:H	1:B:619:GLN:HE22	1.35	0.74
1:B:245:LYS:HE3	1:B:331:ASN:O	1.87	0.73
1:B:615:LEU:H	1:B:619:GLN:NE2	1.87	0.71
1:A:615:LEU:H	1:A:619:GLN:HE22	1.40	0.69
1:B:247:ARG:HE	1:B:250:LYS:HB2	1.59	0.67
1:A:247:ARG:HE	4:A:804:APC:H3A2	1.61	0.66
1:B:247:ARG:NH2	1:B:251:PRO:O	2.30	0.65
1:B:371:THR:HG23	1:B:380:ILE:HA	1.79	0.64
1:A:311:ALA:H	1:A:314:HIS:HD2	1.46	0.63
1:B:321:ILE:HG13	1:B:322:ASP:N	2.15	0.62
1:A:636:GLU:N	1:A:655:GLN:HE22	1.98	0.61
1:B:221:LYS:HD3	1:B:358:ASN:CB	2.30	0.61
1:A:462:HIS:HD2	1:A:464:GLY:H	1.46	0.61
1:A:247:ARG:HH21	4:A:804:APC:H3A1	1.67	0.60
1:B:221:LYS:HD3	1:B:358:ASN:HB2	1.84	0.59
1:B:371:THR:HG21	1:B:378:GLU:OE2	2.01	0.59
1:B:727:ASN:HB3	1:B:730:VAL:O	2.03	0.58
1:A:247:ARG:HE	4:A:804:APC:C3A	2.16	0.58
1:B:402:ILE:HD11	1:B:749:LEU:HD13	1.85	0.58
1:B:341:ASN:HD21	1:B:357:LEU:HD13	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLN:NE2	1:A:733:ASN:HD22	2.02	0.57
1:A:311:ALA:H	1:A:314:HIS:CD2	2.22	0.57
1:B:371:THR:HG22	1:B:372:SER:H	1.68	0.57
1:B:256:MET:HG2	1:B:324:PRO:HB3	1.86	0.56
1:A:314:HIS:CE1	9:A:1300:HOH:O	2.59	0.56
1:A:712:ARG:HD2	9:A:1023:HOH:O	2.06	0.55
1:B:705:GLN:NE2	1:B:733:ASN:HD22	2.05	0.55
1:B:339:LYS:HB3	1:B:365:ARG:HB3	1.88	0.55
1:B:412:THR:HG22	1:B:738:SER:OG	2.08	0.54
1:A:256:MET:HG2	1:A:324:PRO:HB3	1.90	0.54
1:B:364:ASN:HB3	1:B:445:ARG:NH1	2.23	0.54
1:A:310:TYR:H	1:A:314:HIS:HD2	1.54	0.54
1:B:562:ASN:HD22	1:B:654:ARG:HD3	1.73	0.54
1:B:220:ILE:HD11	1:B:313:ILE:HD12	1.89	0.54
1:A:426:HIS:HD2	9:A:902:HOH:O	1.91	0.53
1:A:22:GLY:HA2	1:A:151:TYR:CE1	2.42	0.53
1:B:405:VAL:HG13	1:B:467:SER:HB2	1.90	0.53
1:B:545:GLU:O	1:B:548:ILE:HG13	2.09	0.53
1:A:178:ARG:HD3	1:A:184:VAL:HG23	1.91	0.52
1:B:214:GLU:HG3	1:B:216:LYS:HG3	1.90	0.52
1:A:504:ILE:HG12	1:A:522:ILE:HD12	1.91	0.51
1:B:574:ASP:OD1	1:B:576:ARG:HG2	2.11	0.51
1:B:459:HIS:HD2	1:B:460:ASP:O	1.92	0.51
1:A:681:THR:HG21	1:A:713:LEU:HD21	1.92	0.51
1:B:328:THR:HG23	4:B:804:APC:O1A	2.11	0.51
1:A:712:ARG:HD3	9:A:1118:HOH:O	2.11	0.51
1:A:400:ALA:HB1	1:A:455:GLU:OE1	2.11	0.51
1:A:462:HIS:CD2	1:A:464:GLY:H	2.27	0.50
1:A:50:TYR:CE1	1:A:52:GLU:HG3	2.47	0.49
1:B:535:HIS:HD2	1:B:536:LEU:O	1.96	0.49
1:A:212:LEU:HD21	1:A:218:VAL:HG22	1.94	0.49
1:B:331:ASN:HD22	1:B:337:ILE:HA	1.77	0.49
1:A:148:ASP:HB3	1:A:155:LYS:HD3	1.94	0.48
1:B:412:THR:HG21	1:B:423:ILE:HD11	1.96	0.48
1:B:668:TYR:CZ	1:B:672:LYS:HD2	2.48	0.48
1:A:524:VAL:HG23	1:A:533:ILE:HG13	1.95	0.48
1:B:382:ARG:HD3	9:B:930:HOH:O	2.11	0.48
1:B:382:ARG:HD2	1:B:426:HIS:CG	2.48	0.47
1:B:633:GLU:OE2	1:B:668:TYR:OH	2.31	0.47
1:B:364:ASN:HB3	1:B:445:ARG:HH11	1.78	0.47
1:A:363:VAL:O	1:A:445:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TYR:H	1:A:314:HIS:CD2	2.32	0.46
1:B:517:VAL:HB	1:B:594:VAL:HG12	1.97	0.46
1:B:238:VAL:HG11	1:B:297:ILE:HD11	1.96	0.46
1:A:364:ASN:HD22	1:A:445:ARG:HH11	1.63	0.46
1:B:415:MET:HE3	1:B:452:VAL:HG21	1.97	0.45
1:B:647:ILE:CD1	1:B:684:LEU:HD11	2.46	0.45
1:B:218:VAL:HG12	1:B:354:VAL:HG23	1.97	0.45
1:B:210:LYS:HA	1:B:213:LYS:HG2	1.97	0.45
1:A:314:HIS:HE1	9:A:1300:HOH:O	1.97	0.45
1:A:426:HIS:HE1	9:A:940:HOH:O	1.99	0.45
1:B:607:LEU:HD12	1:B:653:LEU:HD22	1.99	0.45
1:A:164:CYS:HB3	1:A:189:CYS:HB3	1.98	0.44
1:A:462:HIS:HD2	1:A:464:GLY:N	2.13	0.44
1:B:488:ILE:HG23	1:B:698:VAL:HG22	1.99	0.44
1:B:466:LEU:HD23	1:B:469:GLN:NE2	2.32	0.44
1:B:412:THR:CG2	1:B:738:SER:OG	2.66	0.43
1:B:457:VAL:CG1	1:B:478:LYS:HD3	2.47	0.43
1:A:50:TYR:HE1	1:A:52:GLU:HG3	1.82	0.43
1:B:247:ARG:NH1	4:B:804:APC:O1A	2.52	0.43
1:A:432:ASN:ND2	1:A:435:ALA:H	2.16	0.43
1:A:517:VAL:HB	1:A:594:VAL:HG12	2.00	0.43
1:B:337:ILE:O	1:B:365:ARG:HD3	2.20	0.42
1:B:221:LYS:HD3	1:B:358:ASN:HB3	2.02	0.42
1:B:650:GLU:HG2	9:B:951:HOH:O	2.19	0.42
1:B:708:TYR:CZ	1:B:712:ARG:HD3	2.55	0.42
1:A:706:ASN:HB2	6:A:806:AP2:N1	2.34	0.42
1:B:681:THR:HG21	1:B:713:LEU:HD21	2.00	0.42
1:B:130:ARG:HG3	1:B:316:LEU:HD22	2.02	0.41
1:A:131:TYR:HA	1:A:132:PRO:HD3	1.82	0.41
1:A:548:ILE:HG23	1:A:617:GLU:OE1	2.21	0.41
1:B:562:ASN:ND2	1:B:654:ARG:HD3	2.34	0.41
1:A:206:LYS:HB2	1:A:206:LYS:HE3	1.79	0.41
1:B:382:ARG:HD2	1:B:426:HIS:CE1	2.56	0.41
1:B:245:LYS:CE	1:B:331:ASN:O	2.63	0.41
1:A:668:TYR:CE2	1:A:672:LYS:HD2	2.56	0.41
1:B:608:ILE:HG13	1:B:610:VAL:HG23	2.03	0.41
1:B:608:ILE:O	1:B:666:LYS:HE3	2.21	0.41
1:A:16:ILE:HG22	1:A:20:VAL:HG11	2.03	0.40
1:A:12:ARG:HG3	1:A:60:ILE:HG21	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	755/761 (99%)	729 (97%)	25 (3%)	1 (0%)	56	53
1	B	624/761 (82%)	598 (96%)	25 (4%)	1 (0%)	52	48
All	All	1379/1522 (91%)	1327 (96%)	50 (4%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ALA
1	B	519	GLY

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	657/661 (99%)	652 (99%)	5 (1%)	86	89
1	B	545/661 (82%)	531 (97%)	14 (3%)	54	54
All	All	1202/1322 (91%)	1183 (98%)	19 (2%)	70	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	203	ASP
1	A	357	LEU
1	A	600	PHE

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Mol	Chain	Res	Type
1	A	680	PHE
1	B	277	LEU
1	B	326	VAL
1	B	340	ASP
1	B	341	ASN
1	B	371	THR
1	B	382	ARG
1	B	405	VAL
1	B	412	THR
1	B	478	LYS
1	B	650	GLU
1	B	697	VAL
1	B	709	LEU
1	B	730	VAL
1	B	749	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	34	GLN
1	A	44	ASN
1	A	70	ASN
1	A	314	HIS
1	A	364	ASN
1	A	411	ASN
1	A	426	HIS
1	A	432	ASN
1	A	437	ASN
1	A	462	HIS
1	A	562	ASN
1	A	619	GLN
1	A	655	GLN
1	A	705	GLN
1	A	727	ASN
1	B	331	ASN
1	B	341	ASN
1	B	364	ASN
1	B	459	HIS
1	B	516	ASN
1	B	535	HIS
1	B	562	ASN

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Mol	Chain	Res	Type
1	B	619	GLN
1	B	675	ASN
1	B	705	GLN
1	B	727	ASN

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 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	PO4	A	803	-	4,4,4	0.54	0	6,6,6	0.27	0
4	APC	A	804	5	25,33,33	1.49	4 (16%)	30,52,52	2.01	5 (16%)
6	AP2	A	806	7	22,29,29	1.56	4 (18%)	27,45,45	2.45	10 (37%)
3	PO4	A	808	-	4,4,4	0.55	0	6,6,6	0.26	0
3	PO4	A	809	-	4,4,4	0.39	0	6,6,6	0.28	0
3	PO4	A	810	-	4,4,4	0.35	0	6,6,6	0.27	0
3	PO4	A	811	-	4,4,4	0.40	0	6,6,6	0.28	0
8	GOL	A	812	-	5,5,5	0.32	0	5,5,5	0.53	0
8	GOL	A	813	-	5,5,5	0.30	0	5,5,5	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	B	801	-	5,5,5	0.34	0	5,5,5	0.49	0
3	PO4	B	803	-	4,4,4	0.38	0	6,6,6	0.27	0
4	APC	B	804	5	25,33,33	1.49	5 (20%)	30,52,52	2.02	8 (26%)
6	AP2	B	806	7	22,29,29	1.59	4 (18%)	27,45,45	2.25	7 (25%)
3	PO4	B	808	-	4,4,4	0.56	0	6,6,6	0.27	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	PO4	A	803	-	-	0/0/0/0	0/0/0/0
4	APC	A	804	5	-	0/15/38/38	0/3/3/3
6	AP2	A	806	7	-	0/12/32/32	0/3/3/3
3	PO4	A	808	-	-	0/0/0/0	0/0/0/0
3	PO4	A	809	-	-	0/0/0/0	0/0/0/0
3	PO4	A	810	-	-	0/0/0/0	0/0/0/0
3	PO4	A	811	-	-	0/0/0/0	0/0/0/0
8	GOL	A	812	-	-	0/4/4/4	0/0/0/0
8	GOL	A	813	-	-	0/4/4/4	0/0/0/0
8	GOL	B	801	-	-	0/4/4/4	0/0/0/0
3	PO4	B	803	-	-	0/0/0/0	0/0/0/0
4	APC	B	804	5	-	0/15/38/38	0/3/3/3
6	AP2	B	806	7	-	0/12/32/32	0/3/3/3
3	PO4	B	808	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	APC	PA-O2A	-3.01	1.49	1.56
4	B	804	APC	PA-O2A	-2.22	1.50	1.56
4	B	804	APC	PB-O2B	-2.10	1.51	1.56
6	B	806	AP2	PA-O2A	-2.08	1.51	1.56
6	A	806	AP2	PA-O2A	-2.03	1.51	1.56
6	A	806	AP2	O4'-C1'	2.07	1.43	1.41
6	B	806	AP2	O4'-C1'	2.13	1.43	1.41
4	A	804	APC	PB-O3B	2.59	1.61	1.58
4	A	804	APC	C5-C4	3.10	1.47	1.40
6	A	806	AP2	C5-C4	3.25	1.47	1.40
4	B	804	APC	C5-C4	3.27	1.47	1.40
4	B	804	APC	PB-O3B	3.46	1.62	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	806	AP2	C5-C4	3.47	1.48	1.40
4	B	804	APC	PA-O5'	3.48	1.61	1.57
4	A	804	APC	PA-O5'	3.82	1.61	1.57
6	A	806	AP2	PA-O5'	4.38	1.62	1.57
6	B	806	AP2	PA-O5'	4.76	1.62	1.57

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	806	AP2	N3-C2-N1	-7.77	122.94	128.89
6	B	806	AP2	N3-C2-N1	-7.55	123.11	128.89
4	B	804	APC	N3-C2-N1	-7.27	123.32	128.89
4	A	804	APC	N3-C2-N1	-6.86	123.64	128.89
4	A	804	APC	C2'-C1'-N9	-5.16	106.41	114.29
6	A	806	AP2	C2'-C1'-N9	-4.72	107.09	114.29
6	A	806	AP2	O1B-PB-C3A	-3.88	102.30	111.13
6	B	806	AP2	C2'-C1'-N9	-3.63	108.74	114.29
4	B	804	APC	C2'-C1'-N9	-3.60	108.80	114.29
6	B	806	AP2	C4-C5-N7	-3.34	106.40	109.48
6	A	806	AP2	O1A-PA-C3A	-3.30	100.71	109.02
6	B	806	AP2	O1B-PB-C3A	-3.15	103.95	111.13
4	A	804	APC	C1'-N9-C4	-3.15	122.19	126.94
6	B	806	AP2	O1A-PA-C3A	-3.05	101.36	109.02
6	A	806	AP2	C4-C5-N7	-2.76	106.94	109.48
4	B	804	APC	C4-C5-N7	-2.74	106.95	109.48
4	B	804	APC	O5'-PA-O1A	-2.73	106.71	113.98
4	B	804	APC	PG-O3B-PB	-2.35	124.77	132.67
4	A	804	APC	C4-C5-N7	-2.22	107.43	109.48
4	B	804	APC	O3G-PG-O2G	2.02	115.07	107.38
4	A	804	APC	C2-N1-C6	2.04	122.41	118.77
4	B	804	APC	O2A-PA-O1A	2.12	116.77	110.12
6	A	806	AP2	O2A-PA-C3A	2.14	116.21	106.88
6	A	806	AP2	C2-N1-C6	2.16	122.63	118.77
6	A	806	AP2	O4'-C1'-N9	2.23	112.78	108.10
6	B	806	AP2	O4'-C1'-N9	2.25	112.81	108.10
6	A	806	AP2	O3B-PB-O2B	2.32	114.92	108.13
4	B	804	APC	O2B-PB-O1B	2.40	117.66	110.12
6	B	806	AP2	O2A-PA-O1A	2.61	118.34	110.12
6	A	806	AP2	O2A-PA-O1A	2.99	119.52	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	APC	3	0
6	A	806	AP2	1	0
4	B	804	APC	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, 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	753/761 (98%)	0.07	13 (1%) 73 73	20, 33, 49, 70	0
1	B	630/761 (82%)	0.84	111 (17%) 2 2	27, 56, 118, 149	0
All	All	1383/1522 (90%)	0.42	124 (8%) 12 12	20, 39, 105, 149	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	TYR	8.6
1	B	319	GLU	7.1
1	B	115	GLU	6.1
1	B	125	LYS	6.1
1	B	322	ASP	5.8
1	B	119	ARG	5.6
1	B	237	ALA	5.2
1	B	175	HIS	5.1
1	B	172	HIS	4.9
1	B	293	LEU	4.8
1	B	399	LYS	4.8
1	B	206	LYS	4.5
1	B	134	ILE	4.4
1	B	171	TYR	4.3
1	B	565	PHE	4.3
1	B	184	VAL	4.3
1	B	124	PRO	4.2
1	B	340	ASP	4.2
1	B	350	ASP	4.1
1	B	277	LEU	4.0
1	B	180	HIS	4.0
1	B	547	ALA	3.9
1	B	349	LYS	3.8
1	B	162	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	345	LEU	3.7
1	B	262	VAL	3.6
1	B	169	ARG	3.6
1	B	185	ALA	3.6
1	B	369	SER	3.6
1	B	384	ALA	3.5
1	B	257	ARG	3.5
1	B	129	TYR	3.5
1	B	238	VAL	3.4
1	B	233	LEU	3.4
1	B	210	LYS	3.4
1	B	179	PHE	3.3
1	B	126	ASP	3.3
1	B	225	GLY	3.3
1	A	322	ASP	3.2
1	B	161	PHE	3.1
1	A	384	ALA	3.1
1	B	122	LYS	3.1
1	B	333	SER	3.1
1	B	366	ILE	3.1
1	B	545	GLU	3.1
1	B	258	ASP	3.1
1	B	239	ALA	3.0
1	B	546	LEU	3.0
1	B	342	GLU	3.0
1	B	343	GLU	3.0
1	B	173	ASP	3.0
1	B	571	GLU	3.0
1	B	564	SER	3.0
1	B	300	ASP	2.9
1	B	311	ALA	2.9
1	B	158	MET	2.9
1	B	183	PRO	2.9
1	A	395	LYS	2.8
1	B	283	ILE	2.8
1	B	216	LYS	2.8
1	B	208	VAL	2.8
1	B	346	GLU	2.7
1	B	226	PHE	2.7
1	A	145	ILE	2.7
1	B	355	PHE	2.7
1	B	236	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	155	LYS	2.7
1	B	130	ARG	2.6
1	B	433	GLU	2.6
1	B	352	ALA	2.6
1	B	260	GLU	2.6
1	B	154	ALA	2.6
1	B	234	ASP	2.6
1	A	311	ALA	2.6
1	B	228	LEU	2.5
1	B	274	ARG	2.5
1	B	110	ASP	2.5
1	B	290	GLY	2.5
1	A	223	ILE	2.5
1	B	223	ILE	2.5
1	B	127	ARG	2.5
1	A	691	GLU	2.4
1	B	295	LYS	2.4
1	B	111	MET	2.4
1	B	320	GLU	2.4
1	B	436	PHE	2.4
1	B	243	ARG	2.4
1	B	576	ARG	2.4
1	B	395	LYS	2.4
1	B	222	GLY	2.4
1	B	220	ILE	2.4
1	B	347	LYS	2.4
1	B	209	ALA	2.3
1	B	426	HIS	2.3
1	B	348	LEU	2.3
1	B	112	GLY	2.3
1	B	326	VAL	2.3
1	B	270	PRO	2.3
1	B	381	ILE	2.3
1	B	235	ASP	2.3
1	B	240	THR	2.2
1	A	453	ASP	2.2
1	B	337	ILE	2.2
1	B	244	ARG	2.2
1	A	399	LYS	2.2
1	B	292	LYS	2.2
1	B	553	ARG	2.2
1	B	123	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	120	GLU	2.2
1	B	567	LYS	2.2
1	B	351	ILE	2.1
1	B	174	PRO	2.1
1	B	563	ILE	2.1
1	B	289	LYS	2.1
1	B	178	ARG	2.1
1	B	291	GLU	2.1
1	B	224	GLY	2.1
1	B	318	MET	2.1
1	A	109	PRO	2.0
1	B	247	ARG	2.0
1	A	735	GLY	2.0
1	A	248	TYR	2.0
1	A	370	VAL	2.0
1	B	321	ILE	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
3	PO4	A	809	5/5	0.80	0.21	2.48	70,71,72,72	0
8	GOL	B	801	6/6	0.96	0.12	-0.01	27,30,31,31	0
3	PO4	A	803	5/5	0.99	0.10	-0.17	23,24,26,27	0
4	APC	B	804	31/31	0.90	0.16	-0.26	55,59,72,74	0
2	ZN	A	801	1/1	1.00	0.10	-0.28	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	APC	A	804	31/31	0.97	0.13	-0.39	28,32,35,37	0
8	GOL	A	812	6/6	0.94	0.11	-0.41	37,39,43,47	0
8	GOL	A	813	6/6	0.96	0.10	-0.59	30,32,33,34	0
3	PO4	B	808	5/5	0.96	0.08	-0.98	58,58,59,59	0
3	PO4	A	808	5/5	0.96	0.08	-0.99	51,51,54,54	0
2	ZN	A	802	1/1	1.00	0.06	-1.24	35,35,35,35	0
6	AP2	B	806	27/27	0.93	0.11	-1.63	45,53,56,57	0
5	MG	A	805	1/1	0.91	0.07	-1.69	45,45,45,45	0
6	AP2	A	806	27/27	0.95	0.11	-1.75	29,37,39,40	0
2	ZN	B	802	1/1	0.91	0.05	-2.00	97,97,97,97	0
7	FE	A	807	1/1	1.00	0.09	-3.56	27,27,27,27	0
7	FE	B	807	1/1	1.00	0.10	-4.13	37,37,37,37	0
5	MG	B	805	1/1	0.93	0.41	-	86,86,86,86	0
3	PO4	B	803	5/5	0.92	0.09	-	60,60,60,61	0
3	PO4	A	810	5/5	0.89	0.18	-	58,58,60,61	0
3	PO4	A	811	5/5	0.89	0.22	-	83,83,84,84	0

6.5 Other polymers

There are no such residues in this entry.