Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:07 PM GMT

PDB ID	:	3T0F
Title	:	IspH:HMBPP (substrate) structure of the E126D mutant
Authors	:	Span, I.; Graewert, T.; Bacher, A.; Eisenreich, W.; Groll, M.
Deposited on	:	2011-07-20
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

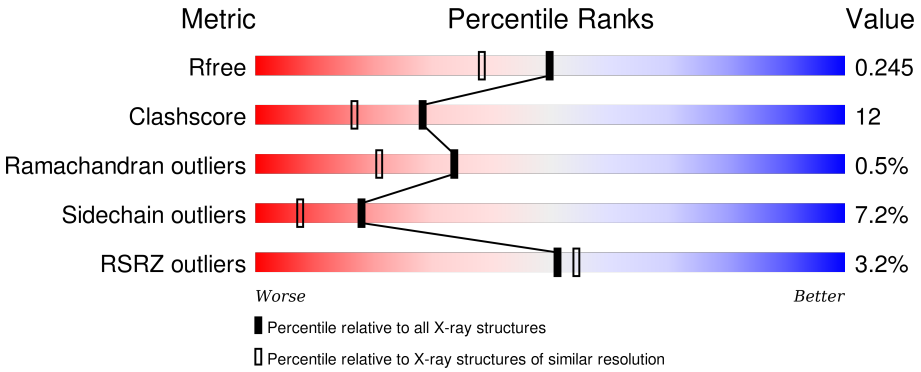
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	328	% 70% 21%
1	B	328	5% 67% 22% 7%

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	H6P	B	998	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4995 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 4-hydroxy-3-methylbut-2-enyl diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2422	1509	438	465	10			
1	B	304	Total	C	N	O	S	0	0	0
			2345	1462	427	446	10			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP P62623
A	-11	ARG	-	EXPRESSION TAG	UNP P62623
A	-10	GLY	-	EXPRESSION TAG	UNP P62623
A	-9	SER	-	EXPRESSION TAG	UNP P62623
A	-8	HIS	-	EXPRESSION TAG	UNP P62623
A	-7	HIS	-	EXPRESSION TAG	UNP P62623
A	-6	HIS	-	EXPRESSION TAG	UNP P62623
A	-5	HIS	-	EXPRESSION TAG	UNP P62623
A	-4	HIS	-	EXPRESSION TAG	UNP P62623
A	-3	HIS	-	EXPRESSION TAG	UNP P62623
A	-2	GLY	-	EXPRESSION TAG	UNP P62623
A	-1	SER	-	EXPRESSION TAG	UNP P62623
A	126	ASP	GLU	ENGINEERED MUTATION	UNP P62623
B	-12	MET	-	EXPRESSION TAG	UNP P62623
B	-11	ARG	-	EXPRESSION TAG	UNP P62623
B	-10	GLY	-	EXPRESSION TAG	UNP P62623
B	-9	SER	-	EXPRESSION TAG	UNP P62623
B	-8	HIS	-	EXPRESSION TAG	UNP P62623
B	-7	HIS	-	EXPRESSION TAG	UNP P62623
B	-6	HIS	-	EXPRESSION TAG	UNP P62623
B	-5	HIS	-	EXPRESSION TAG	UNP P62623
B	-4	HIS	-	EXPRESSION TAG	UNP P62623
B	-3	HIS	-	EXPRESSION TAG	UNP P62623
B	-2	GLY	-	EXPRESSION TAG	UNP P62623
B	-1	SER	-	EXPRESSION TAG	UNP P62623

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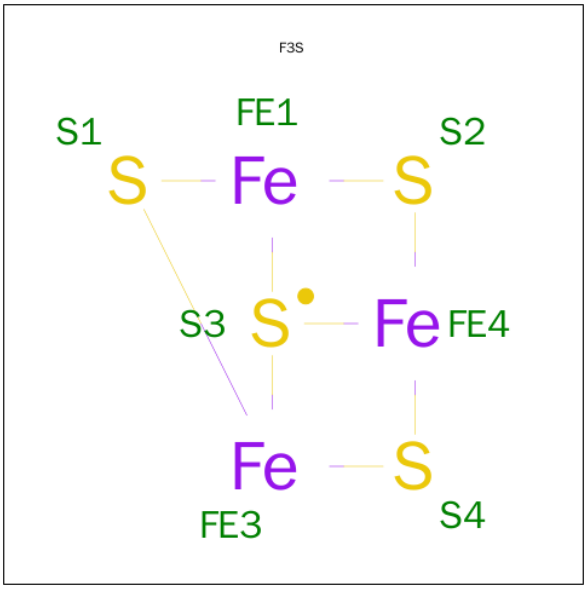
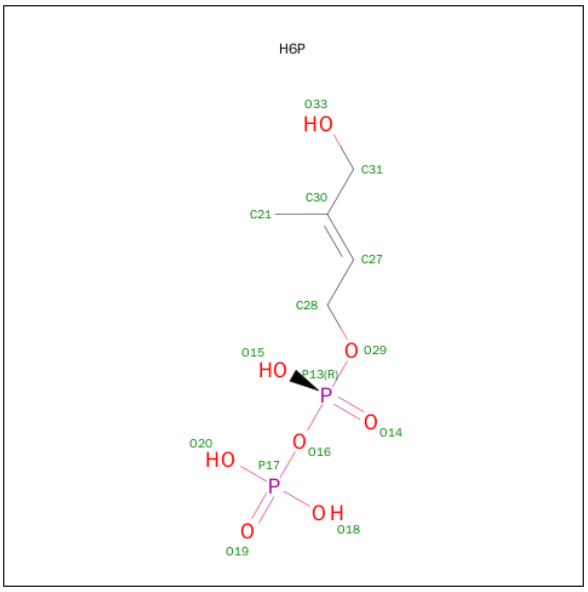
Chain	Residue	Modelled	Actual	Comment	Reference
B	126	ASP	GLU	ENGINEERED MUTATION	UNP P62623

- Molecule 2 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 7 3 4	0	0
2	B	1	Total Fe S 7 3 4	0	0

- Molecule 3 is (2E)-4-HYDROXY-3-METHYLBUT-2-EN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: H6P) (formula: $C_5H_{12}O_8P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 15 5 8 2	0	0
3	B	1	Total C O P 15 5 8 2	0	0

- Molecule 4 is water.

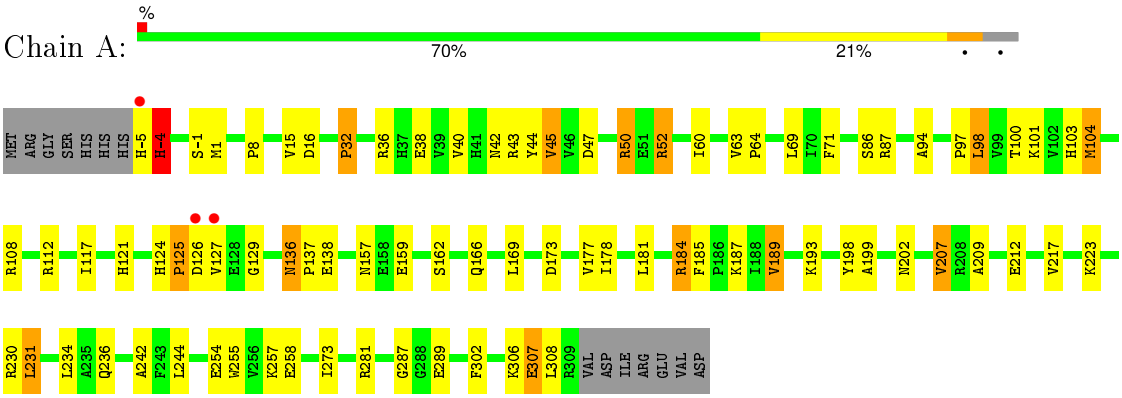
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	73	Total O 73 73	0	0

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.

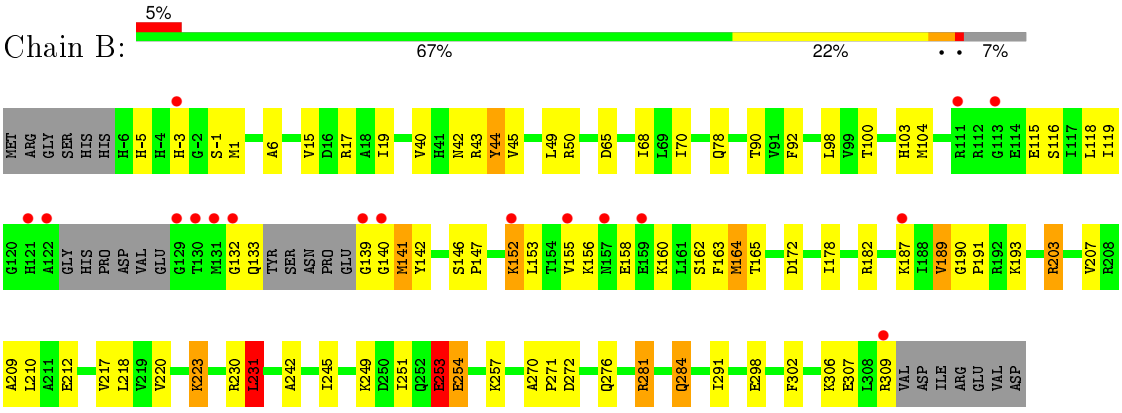
- Molecule 1: 4-hydroxy-3-methylbut-2-enyl diphosphate reductase

Chain A:



- Molecule 1: 4-hydroxy-3-methylbut-2-enyl diphosphate reductase

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	64.85Å 80.18Å 114.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 56.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-1.90) 99.2 (56.43-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.201 , 0.242 0.212 , 0.245	Depositor DCC
R_{free} test set	2352 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.879	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 47419 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H6P, F3S

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	1.29	5/2460 (0.2%)	1.20	15/3330 (0.5%)
1	B	1.28	6/2378 (0.3%)	1.13	9/3213 (0.3%)
All	All	1.28	11/4838 (0.2%)	1.16	24/6543 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	VAL	CB-CG1	8.20	1.70	1.52
1	A	38	GLU	CD-OE1	-8.04	1.16	1.25
1	B	220	VAL	CB-CG2	6.89	1.67	1.52
1	B	298	GLU	CD-OE1	-6.74	1.18	1.25
1	A	189	VAL	CB-CG1	6.60	1.66	1.52
1	A	177	VAL	CB-CG1	6.32	1.66	1.52
1	B	253	GLU	CG-CD	5.70	1.60	1.51
1	B	253	GLU	CB-CG	5.53	1.62	1.52
1	A	255	TRP	CE3-CZ3	5.40	1.47	1.38
1	B	44	TYR	CD2-CE2	5.27	1.47	1.39
1	B	44	TYR	CG-CD1	5.17	1.45	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	87	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	A	281	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	98	LEU	CB-CG-CD1	9.06	126.41	111.00
1	A	173	ASP	CB-CG-OD2	7.97	125.48	118.30
1	A	-4	HIS	N-CA-C	7.61	131.56	111.00
1	A	50	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	A	231	LEU	CB-CG-CD1	6.93	122.78	111.00
1	A	169	LEU	CB-CG-CD2	-6.89	99.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	LEU	CB-CG-CD2	6.44	121.95	111.00
1	B	43	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	B	43	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	B	1	MET	CA-CB-CG	6.12	123.70	113.30
1	B	231	LEU	CB-CG-CD1	6.08	121.34	111.00
1	B	203	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	87	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	38	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	A	104	MET	CG-SD-CE	5.45	108.91	100.20
1	A	281	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	50	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	172	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	284	GLN	CA-CB-CG	5.20	124.83	113.40
1	A	43	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	47	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	184	ARG	NE-CZ-NH1	-5.13	117.73	120.30

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	2422	0	2422	51	1
1	B	2345	0	2358	59	0
2	A	7	0	0	0	0
2	B	7	0	0	1	0
3	A	15	0	9	0	0
3	B	15	0	9	1	0
4	A	111	0	0	16	0
4	B	73	0	0	14	0
All	All	4995	0	4798	111	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 12.

All (111) 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:254:GLU:HA	1:B:257:LYS:HD2	1.43	1.00
1:A:166:GLN:HG2	4:A:401:HOH:O	1.61	0.99
1:B:139:GLY:HA3	4:B:385:HOH:O	1.65	0.96
1:A:52:ARG:HD2	4:A:355:HOH:O	1.66	0.94
1:B:153:LEU:HB3	4:B:349:HOH:O	1.68	0.92
1:A:258:GLU:HG2	4:A:388:HOH:O	1.70	0.91
1:B:223:LYS:HD2	4:B:325:HOH:O	1.72	0.88
1:B:254:GLU:HA	1:B:257:LYS:CD	2.04	0.87
1:B:253:GLU:H	1:B:253:GLU:CD	1.79	0.85
1:A:125:PRO:HB3	4:A:417:HOH:O	1.81	0.81
1:A:-4:HIS:HB2	1:A:289:GLU:OE2	1.82	0.79
1:A:126:ASP:HB3	1:A:166:GLN:HE21	1.53	0.73
1:A:42:ASN:HD22	1:A:45:VAL:H	1.35	0.72
1:B:65:ASP:CB	4:B:360:HOH:O	2.38	0.71
1:B:68:ILE:HD12	1:B:90:THR:HB	1.73	0.68
1:B:162:SER:HA	1:B:189:VAL:O	1.92	0.68
1:B:119:ILE:HD12	1:B:165:THR:HG22	1.76	0.68
1:A:-4:HIS:CE1	4:A:424:HOH:O	2.45	0.68
1:B:245:ILE:HD13	1:B:251:ILE:HD11	1.77	0.67
1:A:212:GLU:CB	4:A:367:HOH:O	2.42	0.67
1:B:118:LEU:HB2	1:B:141:MET:CE	2.25	0.67
1:A:101:LYS:HD3	4:A:346:HOH:O	1.95	0.66
1:B:146:SER:HB2	1:B:147:PRO:HD2	1.76	0.66
1:A:178:ILE:HD13	1:A:193:LYS:O	1.96	0.65
1:B:42:ASN:HD22	1:B:45:VAL:H	1.43	0.65
1:A:212:GLU:HB3	4:A:367:HOH:O	1.95	0.64
1:A:126:ASP:HB3	1:A:166:GLN:NE2	2.12	0.63
1:B:147:PRO:HD2	4:B:359:HOH:O	1.99	0.62
1:B:223:LYS:CD	4:B:325:HOH:O	2.34	0.62
1:B:163:PHE:CZ	1:B:191:PRO:HD2	2.34	0.62
1:A:136:ASN:HD22	1:A:137:PRO:HD2	1.65	0.61
1:B:155:VAL:HG21	1:B:158:GLU:HB3	1.84	0.59
1:A:236:GLN:HG3	1:A:242:ALA:HB3	1.85	0.59
1:A:15:VAL:HG13	1:A:40:VAL:HG11	1.84	0.59
1:B:253:GLU:N	1:B:253:GLU:CD	2.53	0.58
1:B:115:GLU:HA	1:B:140:GLY:O	2.03	0.58
1:A:254:GLU:HA	1:A:257:LYS:HD2	1.86	0.58
1:A:108:ARG:HG3	1:A:112:ARG:NH2	2.19	0.58
2:B:317:F3S:S2	3:B:998:H6P:H21A	2.43	0.57
1:B:291:ILE:HD11	4:B:368:HOH:O	2.04	0.57
1:A:-4:HIS:CB	1:A:289:GLU:OE2	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:CD1	1:B:251:ILE:HD11	2.34	0.56
1:B:152:LYS:O	1:B:152:LYS:HG3	2.04	0.56
1:B:209:ALA:O	1:B:212:GLU:HG2	2.06	0.56
1:A:117:ILE:HG21	1:A:181:LEU:HD21	1.88	0.55
1:B:65:ASP:CG	4:B:360:HOH:O	2.45	0.55
1:A:212:GLU:HB2	4:A:367:HOH:O	2.07	0.54
1:A:32:PRO:HB3	4:A:364:HOH:O	2.08	0.54
1:B:281:ARG:HD3	4:B:347:HOH:O	2.07	0.54
1:B:164:MET:N	1:B:164:MET:SD	2.82	0.53
1:B:17:ARG:HD2	1:B:302:PHE:HB3	1.91	0.53
1:A:209:ALA:O	1:A:212:GLU:HG2	2.08	0.53
1:A:71:PHE:O	1:A:94:ALA:HB3	2.09	0.53
1:A:42:ASN:ND2	1:A:45:VAL:H	2.05	0.52
1:B:92:PHE:HE1	1:B:307:GLU:HG3	1.74	0.52
1:A:52:ARG:CD	4:A:355:HOH:O	2.38	0.52
1:B:218:LEU:HD13	1:B:251:ILE:HD11	1.91	0.51
1:B:-3:HIS:HB2	4:B:344:HOH:O	2.10	0.51
1:A:223:LYS:NZ	1:A:244:LEU:O	2.44	0.50
1:B:78:GLN:OE1	1:B:133:GLN:NE2	2.44	0.50
1:A:223:LYS:HD3	4:A:321:HOH:O	2.12	0.50
1:B:-5:HIS:HD2	4:B:344:HOH:O	1.94	0.50
1:B:203:ARG:HB3	1:B:231:LEU:HD11	1.94	0.49
1:B:218:LEU:HD13	1:B:251:ILE:CD1	2.42	0.49
1:B:42:ASN:ND2	1:B:44:TYR:HB3	2.28	0.49
1:A:36:ARG:HB2	1:A:69:LEU:HD11	1.95	0.49
1:A:8:PRO:HG2	1:A:202:ASN:HB3	1.95	0.48
1:B:42:ASN:HD21	1:B:44:TYR:HB3	1.79	0.47
1:A:306:LYS:HG3	1:A:307:GLU:N	2.28	0.47
1:B:182:ARG:HG2	1:B:182:ARG:HH21	1.80	0.46
1:B:100:THR:O	1:B:104:MET:HG2	2.16	0.46
1:A:217:VAL:O	1:A:242:ALA:HA	2.15	0.46
1:A:121:HIS:O	1:A:127:VAL:HG21	2.16	0.46
1:A:100:THR:O	1:A:104:MET:HG3	2.16	0.46
1:A:236:GLN:NE2	4:A:402:HOH:O	2.49	0.45
1:A:124:HIS:HA	1:A:125:PRO:HD2	1.66	0.45
1:B:163:PHE:CE2	1:B:190:GLY:HA3	2.52	0.45
1:B:15:VAL:HG13	1:B:40:VAL:HG11	1.98	0.45
1:A:157:ASN:OD1	1:A:159:GLU:HB2	2.16	0.45
1:B:178:ILE:HD13	1:B:193:LYS:O	2.17	0.45
1:B:17:ARG:HD2	1:B:302:PHE:CB	2.47	0.45
1:B:15:VAL:O	1:B:19:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:N	4:B:380:HOH:O	2.50	0.44
1:B:254:GLU:HA	1:B:257:LYS:CE	2.46	0.44
1:B:217:VAL:O	1:B:242:ALA:HA	2.16	0.44
1:A:1:MET:O	1:A:287:GLY:HA2	2.17	0.44
1:A:63:VAL:HA	1:A:64:PRO:HD3	1.75	0.43
1:A:50:ARG:HD2	1:A:50:ARG:HH11	1.58	0.43
1:B:118:LEU:HB2	1:B:141:MET:HE1	1.97	0.43
1:A:184:ARG:HG2	1:A:185:PHE:CE1	2.54	0.43
1:A:207:VAL:HG12	1:A:234:LEU:HD13	2.01	0.42
1:A:129:GLY:HA3	4:A:347:HOH:O	2.19	0.42
1:A:97:PRO:HG2	1:A:302:PHE:CG	2.54	0.42
1:B:139:GLY:N	1:B:140:GLY:HA2	2.35	0.42
1:B:163:PHE:CE1	1:B:191:PRO:HD2	2.54	0.42
1:B:249:LYS:HE3	1:B:249:LYS:HB3	1.80	0.42
1:A:125:PRO:CB	4:A:417:HOH:O	2.55	0.42
1:A:42:ASN:HD21	1:A:44:TYR:HB3	1.85	0.42
1:B:146:SER:HB2	1:B:147:PRO:CD	2.46	0.42
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.79	0.42
1:A:198:TYR:CG	1:A:199:ALA:N	2.88	0.41
1:A:162:SER:HA	1:A:189:VAL:O	2.20	0.41
1:B:272:ASP:O	1:B:276:GLN:HG3	2.20	0.41
1:B:6:ALA:HB2	1:B:210:LEU:HD22	2.02	0.41
1:B:153:LEU:HD23	4:B:349:HOH:O	2.20	0.41
1:B:115:GLU:HB3	1:B:142:TYR:HE1	1.84	0.41
1:A:52:ARG:NH2	4:A:355:HOH:O	2.54	0.41
1:B:115:GLU:HB3	1:B:142:TYR:CE1	2.56	0.41
1:B:146:SER:HB2	4:B:359:HOH:O	2.21	0.41
1:A:136:ASN:HD22	1:A:137:PRO:CD	2.33	0.41
1:B:270:ALA:HA	1:B:271:PRO:HD2	1.95	0.41

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:86:SER:O	1:A:258:GLU:OE1[1_655]	2.11	0.09

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	312/328 (95%)	302 (97%)	9 (3%)	1 (0%)	46 35
1	B	298/328 (91%)	288 (97%)	8 (3%)	2 (1%)	26 14
All	All	610/656 (93%)	590 (97%)	17 (3%)	3 (0%)	34 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	GLY
1	B	152	LYS
1	A	125	PRO

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	261/274 (95%)	244 (94%)	17 (6%)	21 10
1	B	252/274 (92%)	232 (92%)	20 (8%)	15 6
All	All	513/548 (94%)	476 (93%)	37 (7%)	18 7

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	-4	HIS
1	A	-1	SER

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Mol	Chain	Res	Type
1	A	16	ASP
1	A	32	PRO
1	A	52	ARG
1	A	60	ILE
1	A	98	LEU
1	A	103	HIS
1	A	136	ASN
1	A	138	GLU
1	A	187	LYS
1	A	207	VAL
1	A	230	ARG
1	A	231	LEU
1	A	273	ILE
1	A	307	GLU
1	B	-1	SER
1	B	70	ILE
1	B	98	LEU
1	B	103	HIS
1	B	116	SER
1	B	141	MET
1	B	160	LYS
1	B	164	MET
1	B	187	LYS
1	B	189	VAL
1	B	207	VAL
1	B	223	LYS
1	B	230	ARG
1	B	231	LEU
1	B	253	GLU
1	B	254	GLU
1	B	281	ARG
1	B	284	GLN
1	B	306	LYS
1	B	309	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	42	ASN
1	A	78	GLN
1	A	103	HIS

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Mol	Chain	Res	Type
1	A	133	GLN
1	A	136	ASN
1	A	236	GLN
1	A	252	GLN
1	B	-5	HIS
1	B	42	ASN
1	B	78	GLN
1	B	133	GLN
1	B	229	ASN
1	B	283	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

4 ligands are modelled in this entry.

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	F3S	A	317	1	0,9,9	0.00	-	0,15,15	0.00	-
3	H6P	A	998	-	11,14,14	1.37	2 (18%)	16,20,20	1.52	2 (12%)
2	F3S	B	317	1	0,9,9	0.00	-	0,15,15	0.00	-
3	H6P	B	998	-	11,14,14	1.10	0	16,20,20	1.76	2 (12%)

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	F3S	A	317	1	-	0/0/24/24	0/0/3/3
3	H6P	A	998	-	-	0/15/15/15	0/0/0/0
2	F3S	B	317	1	-	0/0/24/24	0/0/3/3
3	H6P	B	998	-	-	0/15/15/15	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	H6P	O29-C28	-2.24	1.40	1.43
3	A	998	H6P	P17-O18	-2.08	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	998	H6P	O33-C31-C30	-3.36	104.69	111.76
3	A	998	H6P	O20-P17-O16	-2.31	94.62	105.09
3	A	998	H6P	O18-P17-O20	3.50	120.71	107.38
3	B	998	H6P	O18-P17-O20	4.57	124.78	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	317	F3S	1	0
3	B	998	H6P	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

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	314/328 (95%)	0.03	3 (0%) 84 86	2, 7, 25, 49	0
1	B	304/328 (92%)	0.25	17 (5%) 28 31	2, 8, 29, 35	0
All	All	618/656 (94%)	0.14	20 (3%) 51 54	2, 8, 27, 49	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-5	HIS	6.2
1	B	139	GLY	5.0
1	B	155	VAL	4.5
1	B	131	MET	4.2
1	B	-3	HIS	3.8
1	B	309	ARG	3.8
1	B	113	GLY	3.5
1	B	159	GLU	3.4
1	B	130	THR	3.2
1	B	187	LYS	2.8
1	A	127	VAL	2.8
1	A	126	ASP	2.8
1	B	157	ASN	2.5
1	B	140	GLY	2.4
1	B	152	LYS	2.3
1	B	129	GLY	2.2
1	B	111	ARG	2.2
1	B	121	HIS	2.2
1	B	132	GLY	2.1
1	B	122	ALA	2.1

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
3	H6P	B	998	15/15	0.98	0.13	2.81	10,13,16,20	0
3	H6P	A	998	15/15	0.98	0.15	0.72	10,13,20,27	0
2	F3S	A	317	7/7	0.99	0.05	-3.98	2,2,2,2	0
2	F3S	B	317	7/7	0.99	0.04	-4.18	2,2,3,3	0

6.5 Other polymers (i)

There are no such residues in this entry.