Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 05:34 PM EDT

PDB ID	:	3IV8
Title	:	N-acetylglucosamine-6-phosphate deacetylase from Vibrio cholerae complexed with fructose 6-phosphate
Authors	:	Osipiuk, J.; Maltseva, N.; Stam, J.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2009-08-31
Resolution	:	2.53 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

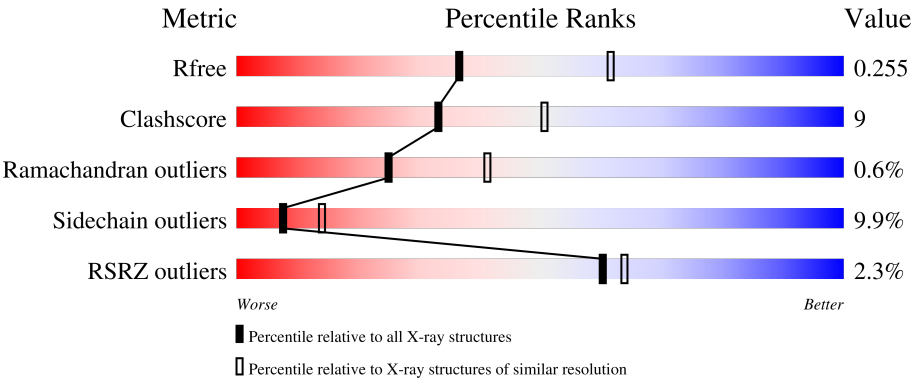
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.53 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	381	80% 17%
1	B	381	71% 26%
1	C	381	78% 18%
1	D	381	4% 74% 17% 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
2	F6P	A	500	X	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11727 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.

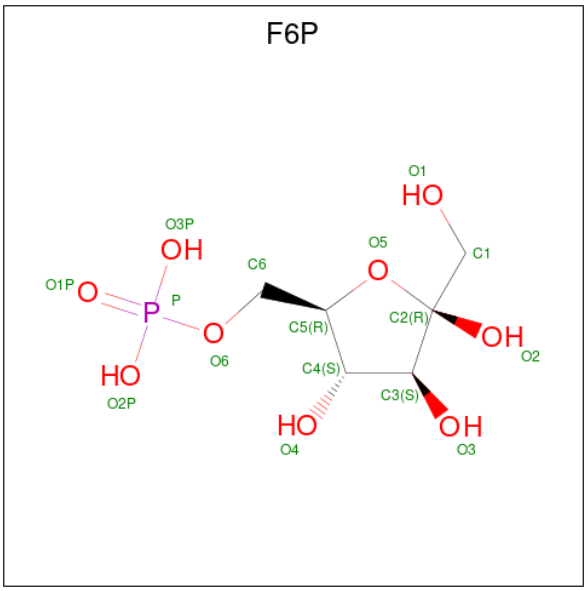
- Molecule 1 is a protein called N-acetylglucosamine-6-phosphate deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	1	0
			2882	1819	484	560	19			
1	B	379	Total	C	N	O	S	0	2	0
			2887	1822	485	561	19			
1	C	379	Total	C	N	O	S	0	3	0
			2894	1828	485	562	19			
1	D	356	Total	C	N	O	S	0	2	0
			2697	1699	454	526	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP O32445
A	-1	ASN	-	expression tag	UNP O32445
A	0	ALA	-	expression tag	UNP O32445
B	-2	SER	-	expression tag	UNP O32445
B	-1	ASN	-	expression tag	UNP O32445
B	0	ALA	-	expression tag	UNP O32445
C	-2	SER	-	expression tag	UNP O32445
C	-1	ASN	-	expression tag	UNP O32445
C	0	ALA	-	expression tag	UNP O32445
D	-2	SER	-	expression tag	UNP O32445
D	-1	ASN	-	expression tag	UNP O32445
D	0	ALA	-	expression tag	UNP O32445

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).

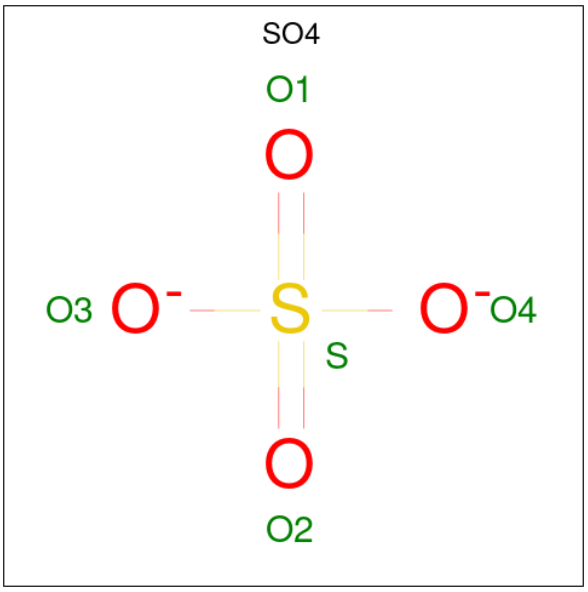


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 16 6 9 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	B	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	D	1	Total Ni 1 1	0	0

- 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
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

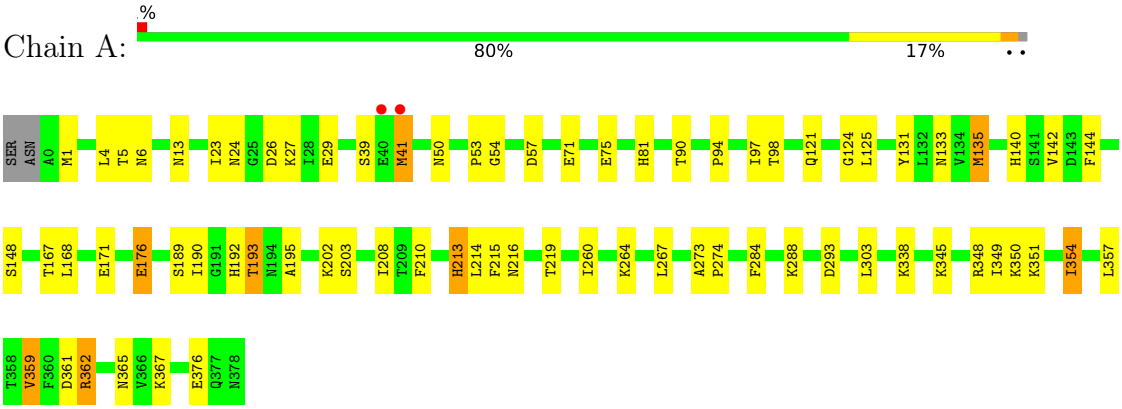
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	100	Total O 100 100	0	0
5	B	78	Total O 78 78	0	0
5	C	77	Total O 77 77	0	0
5	D	77	Total O 77 77	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

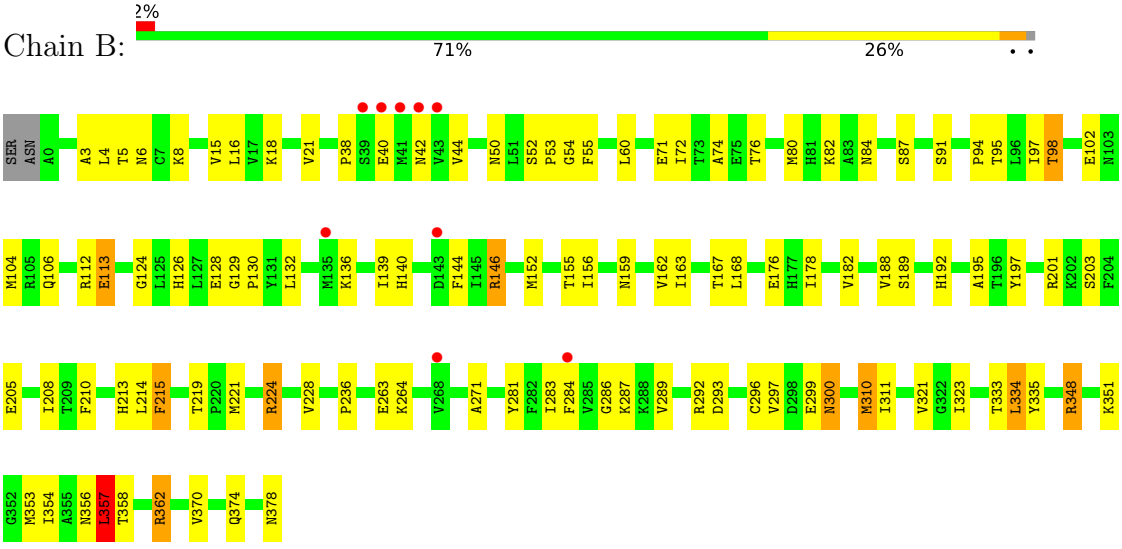
• Molecule 1: N-acetylglucosamine-6-phosphate deacetylase

Chain A:



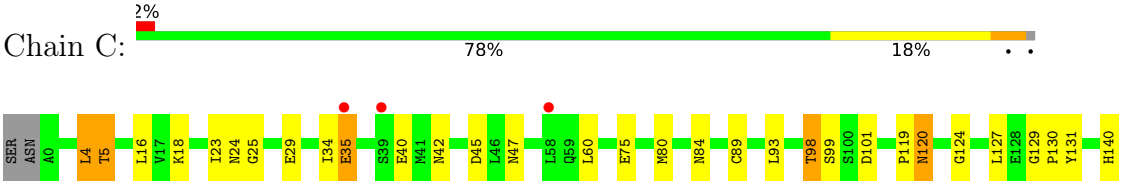
• Molecule 1: N-acetylglucosamine-6-phosphate deacetylase

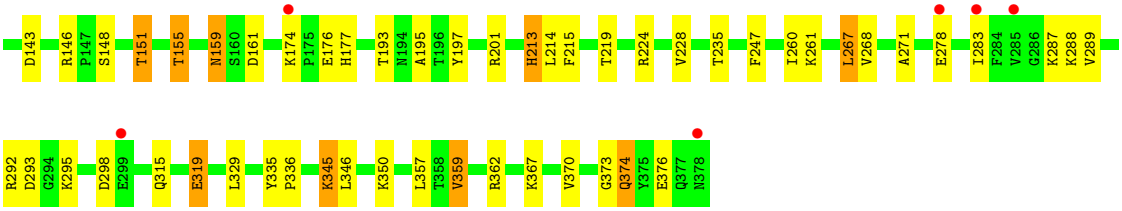
Chain B:



• Molecule 1: N-acetylglucosamine-6-phosphate deacetylase

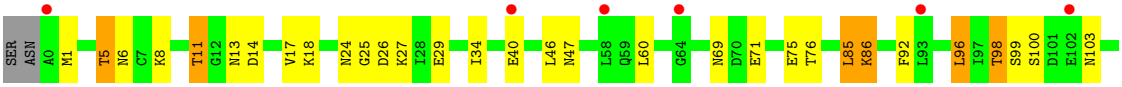
Chain C:

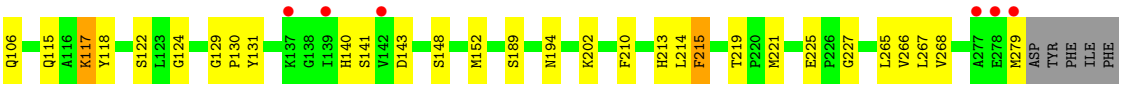


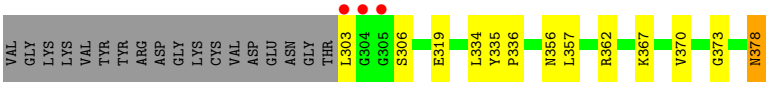


• Molecule 1: N-acetylglucosamine-6-phosphate deacetylase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.18Å 123.05Å 156.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.18 – 2.53 35.18 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.18-2.53) 99.6 (35.18-2.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.183 , 0.253 0.186 , 0.255	Depositor DCC
R_{free} test set	2752 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11727	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: SO4, F6P, NI

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	0.79	0/2934	0.80	1/3976 (0.0%)
1	B	0.74	1/2942 (0.0%)	0.76	2/3987 (0.1%)
1	C	0.75	0/2952	0.77	1/4000 (0.0%)
1	D	0.75	0/2746	0.80	0/3723
All	All	0.76	1/11574 (0.0%)	0.78	4/15686 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	CYS	CB-SG	-6.67	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	357	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	267	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	224	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	2882	0	2882	44	0
1	B	2887	0	2888	72	0
1	C	2894	0	2901	47	0
1	D	2697	0	2707	39	0
2	A	16	0	11	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	1	0
5	A	100	0	0	2	0
5	B	78	0	0	3	0
5	C	77	0	0	4	0
5	D	77	0	0	1	0
All	All	11727	0	11389	196	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 9.

All (196) 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:C:195:ALA:O	1:C:219:THR:HG21	1.55	1.06
1:C:4:LEU:HD22	1:C:23:ILE:HD11	1.38	1.05
1:B:98:THR:HG23	1:B:140:HIS:ND1	1.73	1.04
1:B:195:ALA:O	1:B:219:THR:HG21	1.58	1.03
1:C:98:THR:HG23	1:C:140:HIS:ND1	1.73	1.03
1:D:11:THR:HG21	5:D:422:HOH:O	1.58	1.02
1:D:11:THR:HG22	1:D:13:ASN:H	1.37	0.89
1:C:219:THR:HG23	1:C:228:VAL:H	1.40	0.87
1:D:98:THR:HB	1:D:130:PRO:HA	1.57	0.87
1:B:98:THR:HG22	1:B:129:GLY:HA3	1.55	0.87
1:A:303:LEU:O	2:A:500:F6P:H3	1.77	0.85
1:D:98:THR:HG23	1:D:140:HIS:ND1	1.93	0.83
1:C:98:THR:HG22	1:C:129:GLY:HA3	1.60	0.83
1:B:178:ILE:O	1:B:182:VAL:HG23	1.78	0.83
1:C:292:ARG:NH2	5:C:422:HOH:O	2.15	0.79
1:B:156:ILE:HG23	1:B:163:ILE:HD13	1.66	0.78
1:D:24:ASN:HB2	1:D:29:GLU:HG2	1.69	0.73
1:C:98:THR:CG2	1:C:140:HIS:ND1	2.51	0.72
1:A:192:HIS:HE1	2:A:500:F6P:H12	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:THR:CG2	1:D:13:ASN:H	2.03	0.70
1:B:219:THR:HG23	1:B:228:VAL:H	1.57	0.70
1:A:97:ILE:HB	1:A:140:HIS:CE1	2.27	0.70
1:B:300:ASN:N	1:B:300:ASN:HD22	1.91	0.69
1:C:214:LEU:O	1:C:215:PHE:HB2	1.93	0.69
1:C:98:THR:HB	1:C:130:PRO:HA	1.74	0.68
1:C:219:THR:CG2	1:C:228:VAL:H	2.06	0.68
1:B:299:GLU:HG3	1:B:300:ASN:ND2	2.09	0.68
1:B:5:THR:HG22	1:B:6:ASN:H	1.59	0.68
1:D:24:ASN:CB	1:D:29:GLU:HG2	2.25	0.66
1:B:74:ALA:HB2	1:B:113:GLU:HG2	1.78	0.66
1:C:219:THR:HG23	1:C:228:VAL:N	2.11	0.66
1:D:11:THR:HG22	1:D:14:ASP:H	1.61	0.65
1:D:26:ASP:OD1	1:D:27:LYS:HG3	1.97	0.65
1:D:24:ASN:HB2	1:D:29:GLU:CG	2.26	0.65
1:B:362:ARG:NH2	5:B:456:HOH:O	2.22	0.65
1:D:11:THR:HG22	1:D:13:ASN:N	2.09	0.64
1:C:151:THR:O	1:C:155:THR:HG23	1.98	0.62
1:A:192:HIS:CE1	2:A:500:F6P:H12	2.34	0.62
1:C:155:THR:O	1:C:159:ASN:ND2	2.31	0.62
1:B:98:THR:CG2	1:B:140:HIS:ND1	2.58	0.62
1:D:115:GLN:HE22	1:D:124:GLY:HA2	1.64	0.62
1:C:4:LEU:HD22	1:C:23:ILE:CD1	2.25	0.61
1:D:98:THR:CG2	1:D:140:HIS:ND1	2.62	0.61
1:D:98:THR:HG22	1:D:129:GLY:HA3	1.83	0.61
1:C:5:THR:HG22	1:C:45:ASP:HA	1.82	0.60
1:B:144:PHE:O	1:B:146:ARG:HD3	2.01	0.60
1:B:236:PRO:O	1:B:264:LYS:HE2	2.02	0.60
1:B:76:THR:HG22	1:B:80:MET:CE	2.32	0.60
1:B:197:TYR:CZ	1:B:201:ARG:HD2	2.36	0.59
1:B:104:MET:HE1	1:B:130:PRO:HG3	1.84	0.58
1:B:188:VAL:O	1:B:208:ILE:HG23	2.02	0.58
1:B:263:GLU:HA	1:B:335:TYR:CE2	2.38	0.58
1:C:261:LYS:HE2	5:C:432:HOH:O	2.04	0.58
1:B:156:ILE:HG23	1:B:163:ILE:CD1	2.33	0.58
1:A:260:ILE:HD11	1:C:260:ILE:HD11	1.85	0.58
1:A:362:ARG:NH1	1:B:362:ARG:HD3	2.19	0.58
1:B:5:THR:HG22	1:B:6:ASN:N	2.19	0.57
1:D:98:THR:HB	1:D:130:PRO:CA	2.33	0.57
1:D:356:ASN:HA	1:D:370:VAL:O	2.04	0.57
1:A:354:ILE:HD12	5:A:385:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:HB	1:B:130:PRO:HA	1.86	0.57
1:C:197:TYR:CZ	1:C:201:ARG:HD2	2.39	0.57
1:B:214:LEU:O	1:B:215:PHE:HB2	2.05	0.56
1:A:176:GLU:H	1:A:176:GLU:CD	2.08	0.56
1:B:102:GLU:HG3	1:B:106:GLN:HE21	1.69	0.56
1:C:261:LYS:CE	5:C:432:HOH:O	2.53	0.56
1:A:214:LEU:O	1:A:215:PHE:HB2	2.05	0.56
1:B:112:ARG:NH1	1:B:159:ASN:OD1	2.38	0.56
1:A:4:LEU:CD2	1:A:23:ILE:HD13	2.36	0.56
1:A:24:ASN:CB	1:A:29:GLU:HG2	2.36	0.56
1:B:76:THR:O	1:B:80:MET:HG3	2.07	0.54
1:A:362:ARG:HD3	1:B:362:ARG:CZ	2.38	0.53
1:C:219:THR:HG22	1:C:228:VAL:HG23	1.91	0.53
1:D:86:LYS:HA	1:D:378:ASN:HD21	1.73	0.53
1:D:141:SER:OG	1:D:143:ASP:HB2	2.09	0.53
1:B:8:LYS:HB3	1:B:50:ASN:HD22	1.73	0.53
1:B:224:ARG:NH2	4:B:701:SO4:O4	2.42	0.53
1:D:266:VAL:HG13	1:D:336:PRO:HG3	1.91	0.53
1:D:99:SER:HB2	1:D:103:ASN:HD22	1.74	0.52
1:B:176:GLU:H	1:B:176:GLU:CD	2.13	0.52
1:D:5:THR:HG23	1:D:6:ASN:N	2.24	0.52
1:A:216:ASN:HB3	2:A:500:F6P:H5	1.90	0.52
1:B:76:THR:HG22	1:B:80:MET:HE3	1.91	0.52
1:A:26:ASP:OD1	1:A:27:LYS:HG3	2.10	0.51
1:A:303:LEU:HB2	2:A:500:F6P:O4	2.09	0.51
1:B:205:GLU:OE2	1:C:350:LYS:HD2	2.10	0.51
1:D:71:GLU:HB3	1:D:76:THR:OG1	2.09	0.51
1:D:214:LEU:O	1:D:215:PHE:HB2	2.10	0.51
1:C:359:VAL:HG22	1:C:367:LYS:HB2	1.92	0.51
1:A:273:ALA:N	1:A:274:PRO:CD	2.74	0.51
1:B:299:GLU:HG2	5:B:429:HOH:O	2.10	0.50
1:B:357:LEU:HB2	1:B:370:VAL:HB	1.93	0.50
1:B:300:ASN:N	1:B:300:ASN:ND2	2.59	0.50
1:A:361:ASP:OD2	1:A:365:ASN:HB2	2.12	0.49
1:B:189:SER:HB2	1:B:210:PHE:HB3	1.94	0.49
2:A:500:F6P:P	1:C:224:ARG:HH22	2.35	0.49
1:B:60:LEU:CD1	1:B:271:ALA:HB3	2.42	0.49
1:D:5:THR:CG2	1:D:6:ASN:N	2.76	0.49
1:C:247:PHE:CD1	1:C:295:LYS:HE3	2.47	0.49
1:C:131:TYR:CE1	1:C:148:SER:HA	2.48	0.49
1:B:139:ILE:HG22	1:B:139:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:TYR:CE1	1:D:148:SER:HA	2.47	0.49
1:C:60:LEU:HD21	1:C:84:ASN:HD21	1.78	0.48
1:C:287:LYS:NZ	1:C:298:ASP:HB3	2.28	0.48
1:C:376:GLU:O	5:C:455:HOH:O	2.20	0.48
1:A:131:TYR:CE1	1:A:148:SER:HA	2.49	0.48
1:D:46:LEU:HA	1:D:46:LEU:HD23	1.63	0.48
1:A:50:ASN:O	1:A:359:VAL:HA	2.14	0.48
1:B:310:MET:HB2	5:B:396:HOH:O	2.13	0.48
1:B:356:ASN:HA	1:B:370:VAL:O	2.14	0.48
1:A:131:TYR:CD1	1:A:148:SER:HA	2.49	0.47
1:A:133:ASN:OD1	1:A:135:MET:CG	2.62	0.47
1:B:4:LEU:HD23	1:B:44:VAL:HB	1.96	0.47
1:B:76:THR:HG22	1:B:80:MET:HE2	1.96	0.47
1:A:13:ASN:OD1	1:A:348:ARG:NH2	2.47	0.47
1:A:53:PRO:HG3	1:A:349:ILE:HG13	1.97	0.47
1:D:335:TYR:HB2	1:D:336:PRO:HD3	1.97	0.47
1:A:24:ASN:HB3	1:A:29:GLU:HG2	1.97	0.47
1:A:171:GLU:HG3	1:A:195:ALA:HB2	1.95	0.47
1:C:84:ASN:HB3	1:C:89:CYS:O	2.14	0.47
1:A:5:THR:CG2	1:A:6:ASN:N	2.77	0.47
1:C:120:ASN:ND2	1:C:345:LYS:HE2	2.29	0.46
1:A:24:ASN:HB2	1:A:29:GLU:HG2	1.95	0.46
1:A:71:GLU:HG3	5:A:380:HOH:O	2.15	0.46
1:B:281:TYR:HA	1:B:289:VAL:O	2.14	0.46
1:B:54:GLY:HA2	1:B:358:THR:OG1	2.16	0.46
1:C:60:LEU:CD1	1:C:271:ALA:HB3	2.45	0.46
1:C:24:ASN:HB2	1:C:29:GLU:HG2	1.98	0.46
1:A:4:LEU:HD22	1:A:23:ILE:HD13	1.98	0.46
1:A:54:GLY:HA3	1:A:90:THR:OG1	2.15	0.46
1:B:299:GLU:HG3	1:B:300:ASN:HD22	1.78	0.45
1:C:219:THR:CG2	1:C:228:VAL:N	2.74	0.45
1:B:72:ILE:HG22	1:B:72:ILE:O	2.16	0.45
1:B:333:THR:OG1	1:B:334:LEU:N	2.49	0.45
1:B:219:THR:HG23	1:B:228:VAL:N	2.28	0.45
1:D:1:MET:HE2	1:D:29:GLU:HG3	1.97	0.45
1:A:362:ARG:HD3	1:B:362:ARG:NH2	2.31	0.45
1:A:167:THR:HA	1:A:189:SER:O	2.17	0.45
1:C:98:THR:HB	1:C:130:PRO:CA	2.46	0.45
1:D:117:LYS:HE3	1:D:117:LYS:HB2	1.55	0.45
1:B:203:SER:OG	1:B:208:ILE:HD12	2.16	0.45
1:B:283:ILE:HG23	1:B:286:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLN:O	1:C:319:GLU:HB2	2.16	0.45
1:B:94:PRO:HD2	1:B:124:GLY:O	2.17	0.45
1:D:189:SER:HA	1:D:210:PHE:O	2.17	0.45
1:B:128:GLU:HA	1:B:167:THR:HB	1.99	0.44
1:B:95:THR:HA	1:B:126:HIS:O	2.17	0.44
1:A:81:HIS:CE1	1:A:121:GLN:HG2	2.53	0.44
1:A:189:SER:HB2	1:A:210:PHE:HB3	1.99	0.44
1:A:135:MET:H	1:A:135:MET:HG2	1.40	0.43
1:B:53:PRO:HG3	1:B:348:ARG:HA	2.01	0.43
1:B:152:MET:O	1:B:156:ILE:HG13	2.18	0.43
1:C:24:ASN:CB	1:C:29:GLU:HG2	2.48	0.43
1:D:69:ASN:OD1	1:D:96:LEU:HD22	2.19	0.43
1:A:98:THR:HG22	1:A:144:PHE:HB2	1.99	0.43
1:C:35:GLU:H	1:C:35:GLU:HG3	1.53	0.43
1:A:168:LEU:C	1:A:168:LEU:HD12	2.39	0.43
1:C:101:ASP:OD1	1:C:146:ARG:NH2	2.52	0.42
1:D:40:GLU:OE2	1:D:40:GLU:N	2.43	0.42
1:A:133:ASN:OD1	1:A:135:MET:HG2	2.19	0.42
1:C:370:VAL:HA	1:C:374:GLN:O	2.18	0.42
1:C:176:GLU:H	1:C:176:GLU:CD	2.23	0.42
1:B:60:LEU:HD21	1:B:84:ASN:HD21	1.84	0.42
1:A:133:ASN:OD1	1:A:135:MET:HG3	2.19	0.42
1:B:281:TYR:CD2	1:B:281:TYR:C	2.93	0.42
1:A:1:MET:C	1:A:41:MET:HE1	2.40	0.42
1:C:335:TYR:N	1:C:336:PRO:HD2	2.34	0.42
1:B:40:GLU:HA	1:B:40:GLU:OE2	2.18	0.42
1:B:155:THR:O	1:B:159:ASN:ND2	2.42	0.42
1:B:321:VAL:HG12	1:B:323:ILE:HG13	2.01	0.42
1:C:120:ASN:HD21	1:C:345:LYS:HE2	1.85	0.42
1:A:24:ASN:HB2	1:A:29:GLU:CG	2.50	0.42
1:B:132:LEU:HD22	1:B:192:HIS:HB2	2.02	0.42
1:C:174:LYS:O	1:C:177:HIS:HB2	2.19	0.42
1:D:25:GLY:O	1:D:373:GLY:HA3	2.19	0.42
1:B:87:SER:HB2	1:B:311:ILE:HG22	2.02	0.41
1:D:219:THR:HG22	1:D:227:GLY:HA3	2.03	0.41
1:B:168:LEU:HD12	1:B:168:LEU:C	2.40	0.41
1:D:60:LEU:HD23	1:D:92:PHE:CD1	2.55	0.41
1:B:98:THR:HG21	1:B:132:LEU:HD12	2.03	0.41
1:D:11:THR:CG2	1:D:14:ASP:H	2.32	0.41
1:B:3:ALA:HA	1:B:21:VAL:O	2.21	0.41
1:B:55:PHE:HB3	1:B:310:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLU:HB3	1:B:76:THR:HG1	1.86	0.41
1:B:221:MET:CE	1:D:221:MET:HE2	2.51	0.41
1:C:25:GLY:O	1:C:373:GLY:HA3	2.21	0.41
1:C:93:LEU:HD22	1:C:124:GLY:O	2.21	0.41
1:C:159:ASN:ND2	1:C:159:ASN:N	2.69	0.41
1:D:85:LEU:HD12	1:D:85:LEU:HA	1.91	0.41
1:A:94:PRO:HD2	1:A:124:GLY:O	2.20	0.41
1:D:117:LYS:HB3	1:D:118:TYR:CD2	2.56	0.41
1:B:52:SER:HB2	1:B:53:PRO:HD2	2.03	0.40
1:C:120:ASN:HB3	1:C:346:LEU:HD11	2.03	0.40
1:A:190:ILE:HG12	1:A:193:THR:HG21	2.03	0.40
1:A:203:SER:OG	1:A:208:ILE:HD12	2.21	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	378/381 (99%)	357 (94%)	20 (5%)	1 (0%)	41	59
1	B	379/381 (100%)	358 (94%)	18 (5%)	3 (1%)	19	33
1	C	380/381 (100%)	355 (93%)	23 (6%)	2 (0%)	29	47
1	D	354/381 (93%)	333 (94%)	18 (5%)	3 (1%)	19	33
All	All	1491/1524 (98%)	1403 (94%)	79 (5%)	9 (1%)	25	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	213	HIS
1	B	213	HIS
1	C	213	HIS

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Mol	Chain	Res	Type
1	D	47	ASN
1	B	215	PHE
1	A	213	HIS
1	D	215	PHE
1	B	38	PRO
1	C	119	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	311/312 (100%)	284 (91%)	27 (9%)	10 19
1	B	312/312 (100%)	285 (91%)	27 (9%)	10 19
1	C	313/312 (100%)	276 (88%)	37 (12%)	5 9
1	D	292/312 (94%)	260 (89%)	32 (11%)	6 11
All	All	1228/1248 (98%)	1105 (90%)	123 (10%)	8 14

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	41	MET
1	A	75	GLU
1	A	125	LEU
1	A	135	MET
1	A	142	VAL
1	A	176	GLU
1	A	193	THR
1	A	202	LYS
1	A	213	HIS
1	A	219	THR
1	A	264	LYS
1	A	267	LEU
1	A	284	PHE
1	A	288	LYS

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Mol	Chain	Res	Type
1	A	293	ASP
1	A	338	LYS
1	A	345	LYS
1	A	350	LYS
1	A	351	LYS
1	A	354	ILE
1	A	357	LEU
1	A	359	VAL
1	A	362	ARG
1	A	367	LYS
1	A	376[A]	GLU
1	A	376[B]	GLU
1	B	15	VAL
1	B	16	LEU
1	B	18	LYS
1	B	42	ASN
1	B	82	LYS
1	B	91	SER
1	B	97	ILE
1	B	98	THR
1	B	113	GLU
1	B	136	LYS
1	B	146	ARG
1	B	162	VAL
1	B	284	PHE
1	B	287	LYS
1	B	292	ARG
1	B	293	ASP
1	B	297	VAL
1	B	300	ASN
1	B	310	MET
1	B	334	LEU
1	B	348	ARG
1	B	351	LYS
1	B	354	ILE
1	B	357	LEU
1	B	362	ARG
1	B	374	GLN
1	B	378	ASN
1	C	4	LEU
1	C	5	THR
1	C	16	LEU

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Mol	Chain	Res	Type
1	C	18	LYS
1	C	34	ILE
1	C	35	GLU
1	C	40	GLU
1	C	42	ASN
1	C	47	ASN
1	C	75	GLU
1	C	80	MET
1	C	98	THR
1	C	99	SER
1	C	120	ASN
1	C	127	LEU
1	C	143	ASP
1	C	151	THR
1	C	155	THR
1	C	159	ASN
1	C	161	ASP
1	C	193	THR
1	C	213	HIS
1	C	235	THR
1	C	267	LEU
1	C	268	VAL
1	C	278	GLU
1	C	283	ILE
1	C	288	LYS
1	C	289	VAL
1	C	293	ASP
1	C	319	GLU
1	C	329	LEU
1	C	345	LYS
1	C	357	LEU
1	C	359	VAL
1	C	362	ARG
1	C	374	GLN
1	D	5	THR
1	D	8	LYS
1	D	11	THR
1	D	17	VAL
1	D	18	LYS
1	D	34	ILE
1	D	75	GLU
1	D	85	LEU

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Mol	Chain	Res	Type
1	D	86	LYS
1	D	96	LEU
1	D	98	THR
1	D	100	SER
1	D	106	GLN
1	D	117	LYS
1	D	122	SER
1	D	152	MET
1	D	194	ASN
1	D	202	LYS
1	D	225[A]	GLU
1	D	225[B]	GLU
1	D	265	LEU
1	D	267	LEU
1	D	268	VAL
1	D	279	MET
1	D	303	LEU
1	D	306	SER
1	D	319	GLU
1	D	334	LEU
1	D	357	LEU
1	D	362	ARG
1	D	367	LYS
1	D	378	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	81	HIS
1	A	84	ASN
1	A	103	ASN
1	A	115	GLN
1	A	121	GLN
1	B	42	ASN
1	B	50	ASN
1	B	84	ASN
1	B	106	GLN
1	B	115	GLN
1	B	121	GLN
1	B	172	ASN
1	B	300	ASN

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Mol	Chain	Res	Type
1	B	374	GLN
1	C	24	ASN
1	C	47	ASN
1	C	50	ASN
1	C	84	ASN
1	C	120	ASN
1	C	121	GLN
1	C	365	ASN
1	D	42	ASN
1	D	47	ASN
1	D	84	ASN
1	D	103	ASN
1	D	106	GLN
1	D	115	GLN
1	D	121	GLN
1	D	194	ASN
1	D	378	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	701	-	4,4,4	0.21	0	6,6,6	0.30	0
4	SO4	A	702	-	4,4,4	0.15	0	6,6,6	0.45	0
4	SO4	B	703	-	4,4,4	0.23	0	6,6,6	0.21	0
2	F6P	A	500	-	15,16,16	1.20	1 (6%)	17,25,25	1.61	4 (23%)

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	F6P	A	500	-	1/1/5/5	8/9/28/28	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	F6P	O2-C2	3.97	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	F6P	O5-C5-C6	3.89	118.02	109.45
2	A	500	F6P	O3P-P-O6	2.61	113.67	106.73
2	A	500	F6P	O2P-P-O6	2.27	112.78	106.73
2	A	500	F6P	O3-C3-C4	-2.01	106.37	113.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	500	F6P	C2

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	F6P	O1-C1-C2-O2
2	A	500	F6P	O1-C1-C2-C3
2	A	500	F6P	O1-C1-C2-O5
2	A	500	F6P	C6-O6-P-O2P
2	A	500	F6P	C6-O6-P-O3P
2	A	500	F6P	O5-C5-C6-O6
2	A	500	F6P	C4-C5-C6-O6

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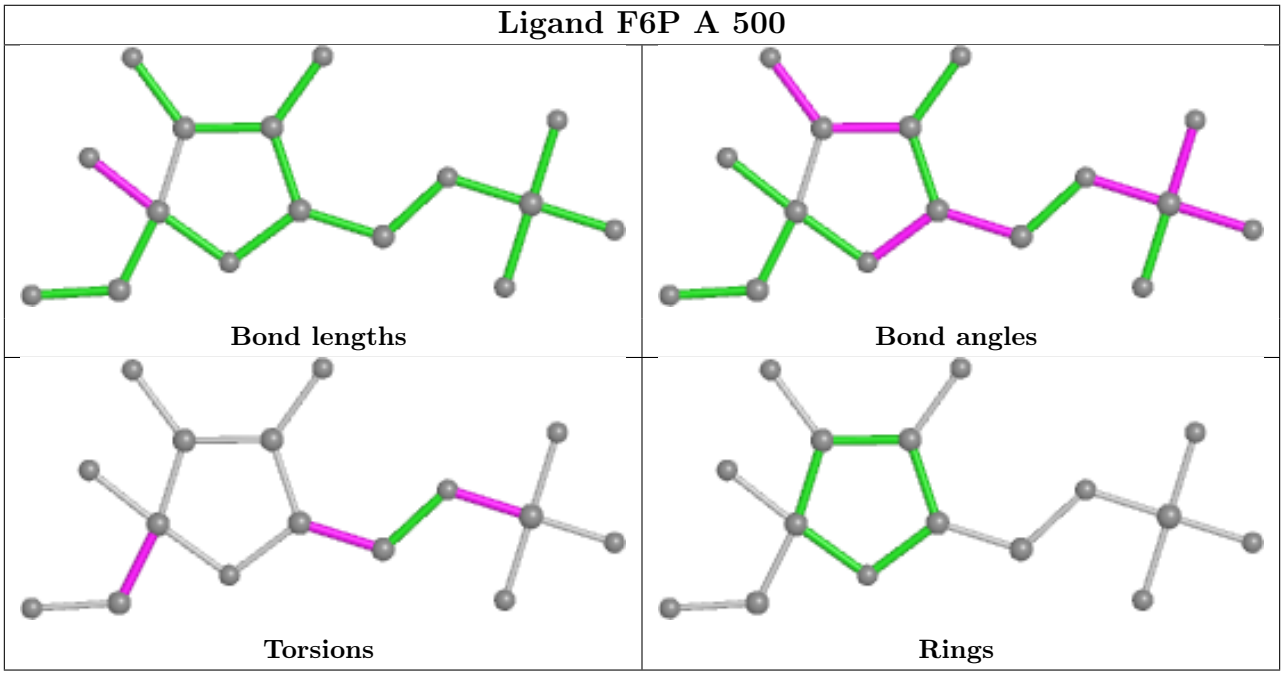
Mol	Chain	Res	Type	Atoms
2	A	500	F6P	C6-O6-P-O1P

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	SO4	1	0
2	A	500	F6P	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	379/381 (99%)	-0.30	2 (0%)	91	92	18, 31, 43, 54	0
1	B	379/381 (99%)	-0.02	9 (2%)	59	62	22, 35, 51, 60	0
1	C	379/381 (99%)	-0.06	9 (2%)	59	62	21, 35, 53, 62	0
1	D	356/381 (93%)	-0.09	15 (4%)	36	40	21, 33, 49, 59	0
All	All	1493/1524 (97%)	-0.12	35 (2%)	60	64	18, 33, 50, 62	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	304	GLY	6.2
1	D	278	GLU	3.9
1	D	279	MET	3.7
1	C	299	GLU	3.6
1	D	303	LEU	3.4
1	D	142	VAL	3.3
1	D	0	ALA	3.3
1	A	41	MET	3.1
1	B	39	SER	3.0
1	B	40	GLU	2.9
1	C	285	VAL	2.8
1	B	143	ASP	2.7
1	C	378	ASN	2.7
1	B	41	MET	2.7
1	D	277	ALA	2.6
1	C	278	GLU	2.6
1	C	35	GLU	2.6
1	B	135	MET	2.6
1	B	284	PHE	2.5
1	D	58	LEU	2.4
1	B	268	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	139	ILE	2.4
1	C	58	LEU	2.3
1	C	283	ILE	2.3
1	D	64	GLY	2.3
1	D	305	GLY	2.3
1	D	102	GLU	2.3
1	B	42	ASN	2.3
1	D	93	LEU	2.3
1	D	137	LYS	2.2
1	A	40	GLU	2.1
1	D	40	GLU	2.1
1	C	39	SER	2.1
1	B	43	VAL	2.0
1	C	174	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

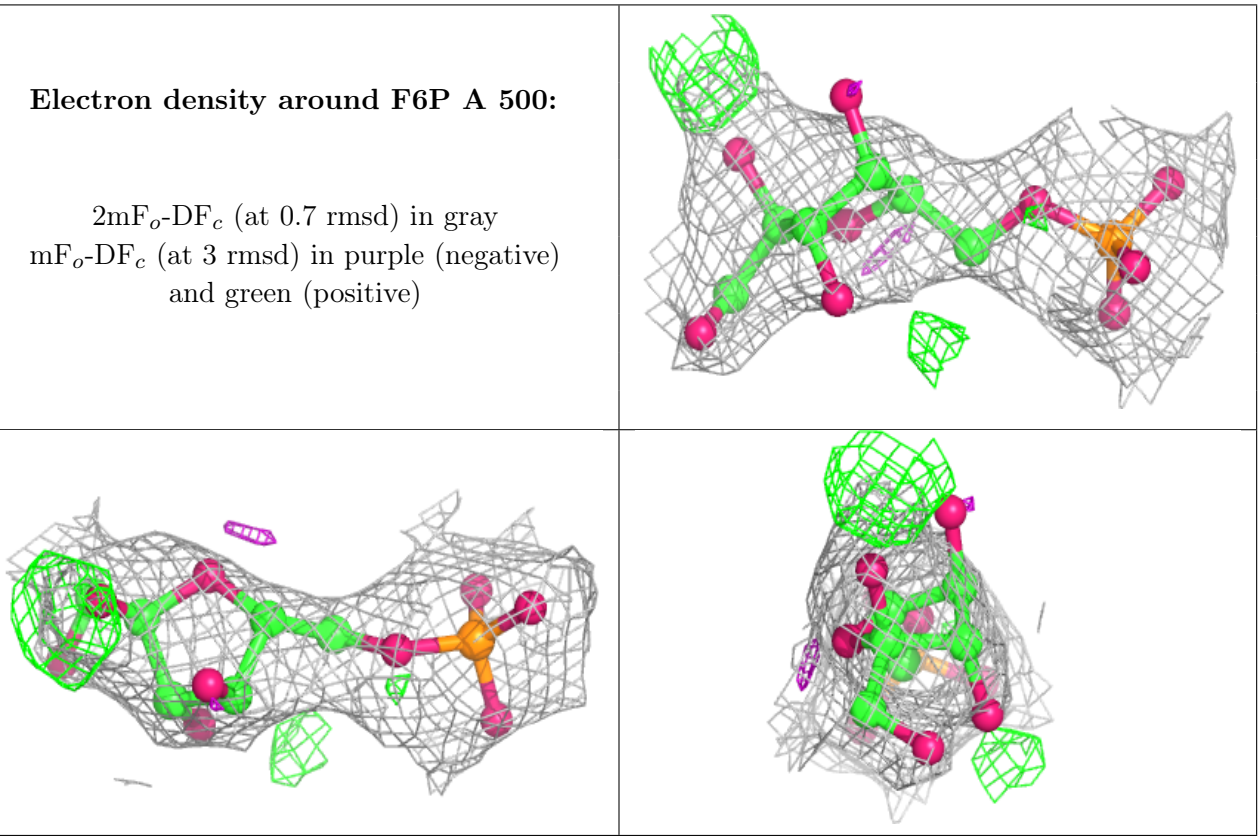
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F6P	A	500	16/16	0.89	0.21	62,70,72,74	0
4	SO4	B	701	5/5	0.89	0.16	58,58,61,62	5
4	SO4	A	702	5/5	0.95	0.19	53,54,56,57	5
3	NI	D	501	1/1	0.95	0.06	76,76,76,76	0
4	SO4	B	703	5/5	0.95	0.28	65,66,66,67	5
3	NI	A	501	1/1	0.96	0.13	65,65,65,65	0
3	NI	C	501	1/1	0.98	0.15	53,53,53,53	0
3	NI	B	501	1/1	0.99	0.16	60,60,60,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F6P A 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.