Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:51 PM EDT

PDB ID	:	1FXJ
Title	:	CRYSTAL STRUCTURE OF N-ACETYLGLUCOSAMINE 1-PHOSPHATE URIDYLTRANSFERASE
Authors	:	Brown, K.; Pompeo, F.; Dixon, S.; Mengin-Lecreulx, D.; Cambillau, C.; Bourne, Y.
Deposited on	:	2000-09-26
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

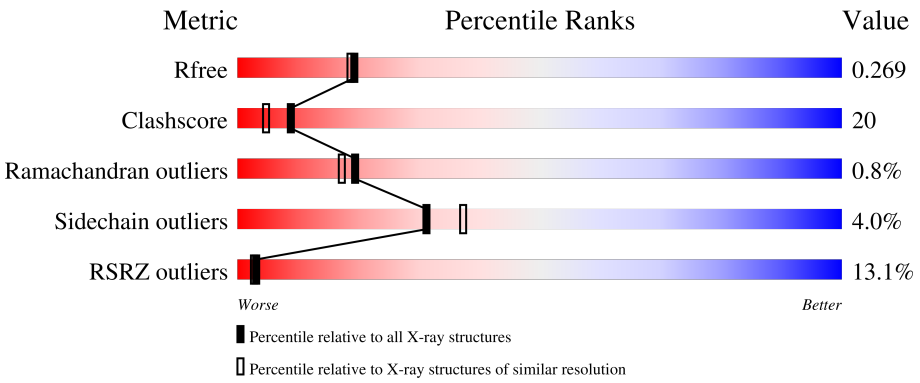
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	331	16% 70% 26%
1	B	331	10% 69% 26%

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	MES	A	333	-	-	X	-

2 Entry composition (i)

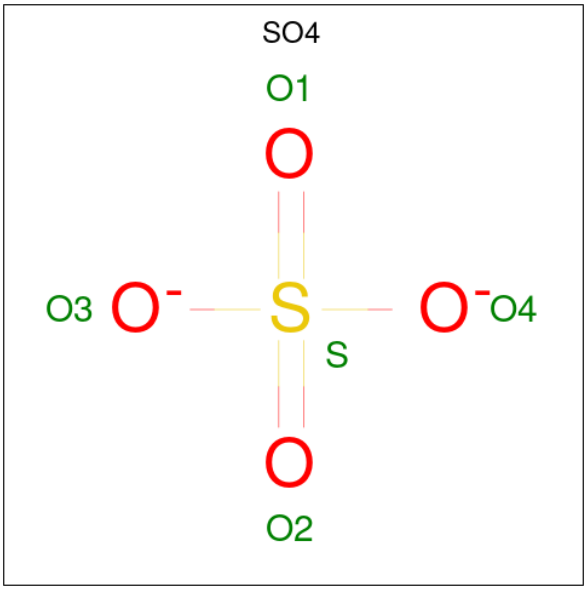
There are 4 unique types of molecules in this entry. The entry contains 5368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE.

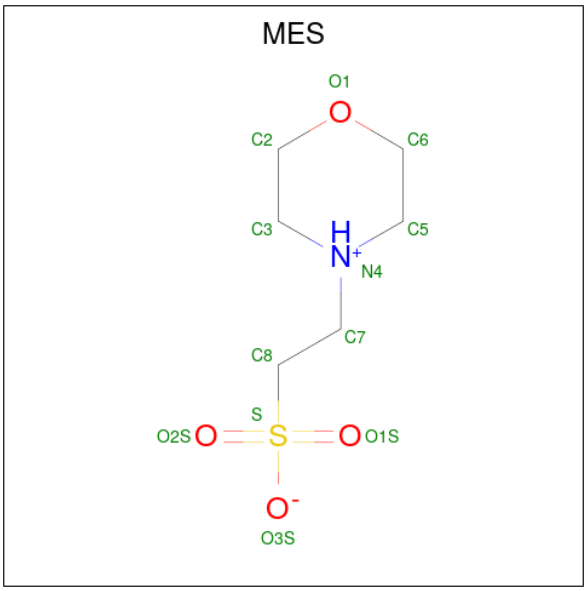
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2504	1563	448	483	10	0	0	0
1	B	324	2482	1547	445	480	10	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0

- Molecule 4 is water.

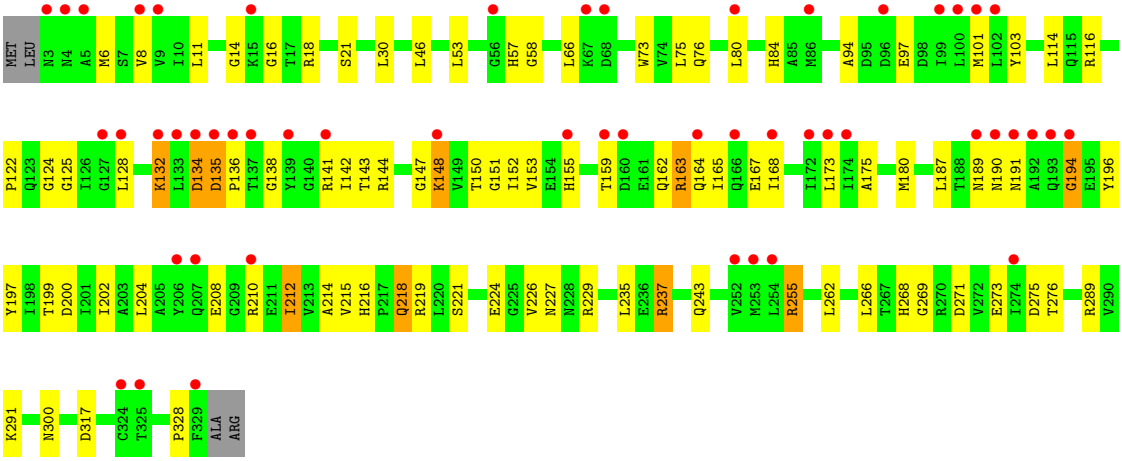
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	183	183	183	0	0
			Total	O		
4	B	177	177	177	0	0

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.

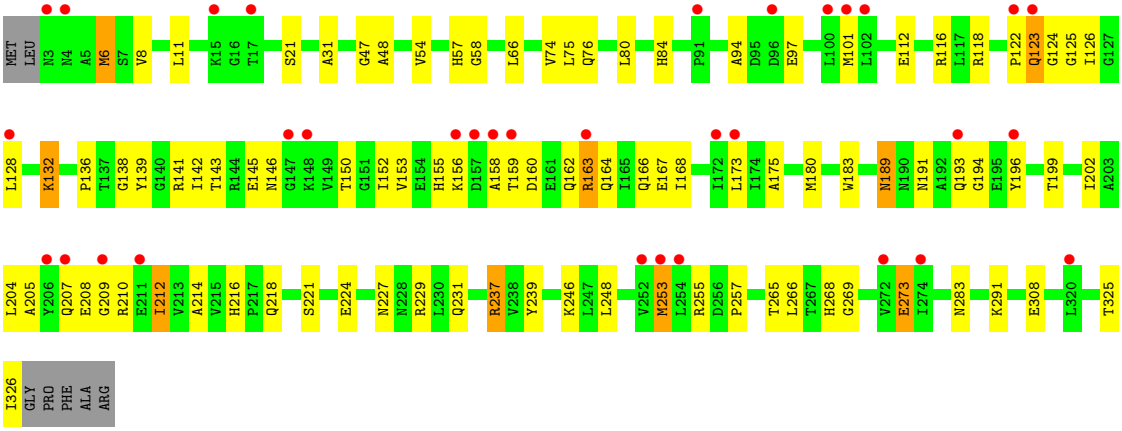
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE

Chain A:



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	142.68Å 142.68Å 248.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.25 23.29 – 2.24	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.25) 96.8 (23.29-2.24)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.274 0.226 , 0.269	Depositor DCC
R_{free} test set	1371 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5368	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MES

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	0.60	0/2539	0.81	1/3442 (0.0%)
1	B	0.62	1/2515 (0.0%)	0.78	0/3409
All	All	0.61	1/5054 (0.0%)	0.80	1/6851 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	MET	CG-SD	5.50	1.95	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	PRO	C-N-CA	5.61	135.72	121.70

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	2504	0	2511	101	0
1	B	2482	0	2492	103	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	13	6	0
4	A	183	0	0	8	0
4	B	177	0	0	4	1
All	All	5368	0	5016	204	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 20.

All (204) 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:132:LYS:HE3	1:B:132:LYS:H	1.22	1.03
1:A:132:LYS:HE3	1:A:132:LYS:H	1.29	0.96
1:A:255:ARG:HG3	1:A:275:ASP:HA	1.46	0.96
1:B:123:GLN:HE21	1:B:123:GLN:H	1.11	0.96
1:B:123:GLN:H	1:B:123:GLN:NE2	1.72	0.88
1:A:124:GLY:O	1:A:210:ARG:HD3	1.75	0.86
1:B:227:ASN:H	1:B:231:GLN:NE2	1.74	0.85
1:A:159:THR:H	1:A:162:GLN:HE21	1.26	0.82
1:A:136:PRO:HB2	1:A:141:ARG:NE	1.95	0.81
1:A:75:LEU:HD23	1:A:76:GLN:N	1.97	0.78
1:A:134:ASP:O	1:A:135:ASP:HB2	1.85	0.76
1:A:202:ILE:HD12	1:A:212:ILE:HD12	1.66	0.76
1:A:175:ALA:HB3	1:A:180:MET:CE	2.17	0.75
1:A:128:LEU:HD22	1:A:212:ILE:HD11	1.68	0.75
1:B:158:ALA:HA	1:B:162:GLN:HE21	1.50	0.75
1:B:75:LEU:HD23	1:B:76:GLN:N	2.03	0.73
1:A:132:LYS:H	1:A:132:LYS:CE	2.02	0.72
1:B:132:LYS:H	1:B:132:LYS:CE	2.00	0.71
1:B:221:SER:HA	1:B:224:GLU:HG3	1.73	0.70
1:B:11:LEU:HD11	1:B:101:MET:HE3	1.74	0.69
1:A:224:GLU:HB2	1:A:235:LEU:HD21	1.74	0.69
1:B:142:ILE:HG13	1:B:167:GLU:HG2	1.75	0.69
1:B:202:ILE:HD12	1:B:212:ILE:HD12	1.75	0.69
1:B:143:THR:HG22	1:B:150:THR:HB	1.75	0.69
1:B:227:ASN:H	1:B:231:GLN:HE21	1.42	0.68
1:A:218:GLN:HE21	1:A:218:GLN:HA	1.60	0.67
1:B:21:SER:HB2	1:B:229:ARG:NH2	2.10	0.66
1:B:273:GLU:HG3	1:B:291:LYS:HG2	1.75	0.66
1:A:189:ASN:O	1:A:191:ASN:N	2.29	0.65
1:A:159:THR:N	1:A:162:GLN:HE21	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:HE21	1:B:123:GLN:N	1.90	0.65
1:A:14:GLY:N	3:A:333:MES:O1S	2.30	0.64
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.63	0.64
1:B:122:PRO:HG2	1:B:125:GLY:HA3	1.80	0.64
1:A:202:ILE:HD12	1:A:212:ILE:CD1	2.28	0.64
1:A:227:ASN:OD1	3:A:333:MES:H22	1.99	0.63
1:A:11:LEU:HD11	1:A:101:MET:HE3	1.79	0.63
1:B:11:LEU:HD11	1:B:101:MET:CE	2.28	0.63
1:B:175:ALA:HB3	1:B:180:MET:CE	2.29	0.63
1:B:204:LEU:O	1:B:208:GLU:HG3	1.97	0.63
1:B:193:GLN:NE2	1:B:193:GLN:HA	2.13	0.62
1:B:132:LYS:HE3	1:B:132:LYS:N	2.06	0.62
1:A:243:GLN:HG2	4:A:419:HOH:O	2.00	0.62
1:B:136:PRO:HG2	1:B:166:GLN:HA	1.81	0.62
1:A:144:ARG:HD3	1:A:147:GLY:O	2.01	0.61
1:B:123:GLN:NE2	1:B:123:GLN:N	2.47	0.61
1:B:141:ARG:HD3	1:B:168:ILE:HD11	1.81	0.61
1:A:197:TYR:HB2	1:A:200:ASP:OD2	2.01	0.61
1:B:202:ILE:HD12	1:B:212:ILE:CD1	2.31	0.61
1:A:148:LYS:HA	1:A:148:LYS:HE3	1.84	0.60
1:A:138:GLY:H	1:A:155:HIS:CD2	2.19	0.60
1:B:94:ALA:HB3	1:B:97:GLU:HG2	1.84	0.60
1:B:237:ARG:HD2	4:B:395:HOH:O	2.01	0.60
1:B:158:ALA:HA	1:B:162:GLN:NE2	2.15	0.60
1:B:141:ARG:HH12	1:B:155:HIS:HD2	1.49	0.59
1:B:202:ILE:HG23	1:B:212:ILE:HD13	1.84	0.59
1:A:204:LEU:O	1:A:208:GLU:HG3	2.03	0.58
1:A:151:GLY:HA2	1:A:202:ILE:CG2	2.33	0.58
1:A:221:SER:HA	1:A:224:GLU:HG3	1.85	0.58
1:B:75:LEU:HD23	1:B:76:GLN:H	1.69	0.58
1:B:136:PRO:HB2	1:B:141:ARG:NH2	2.19	0.58
1:A:116:ARG:NH2	1:A:216:HIS:O	2.37	0.58
1:B:152:ILE:HB	1:B:199:THR:HB	1.84	0.57
1:B:159:THR:H	1:B:162:GLN:CG	2.17	0.57
1:A:21:SER:HB2	1:A:229:ARG:NH2	2.19	0.57
1:A:53:LEU:HD23	1:A:73:TRP:CZ3	2.40	0.57
1:B:159:THR:OG1	1:B:162:GLN:HG2	2.04	0.57
1:B:124:GLY:HA3	1:B:210:ARG:NH1	2.20	0.56
1:B:138:GLY:H	1:B:155:HIS:CD2	2.24	0.56
1:B:159:THR:H	1:B:162:GLN:HG3	1.69	0.56
1:A:202:ILE:HG23	1:A:212:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:NH2	1:B:216:HIS:O	2.39	0.55
1:B:189:ASN:N	1:B:189:ASN:OD1	2.40	0.55
1:A:75:LEU:HD23	1:A:76:GLN:H	1.71	0.55
1:B:325:THR:HG22	1:B:325:THR:O	2.05	0.55
1:A:141:ARG:HH22	1:A:155:HIS:CD2	2.25	0.54
1:B:173:LEU:HD12	1:B:173:LEU:C	2.27	0.54
1:B:128:LEU:HD22	1:B:212:ILE:HD11	1.90	0.54
1:A:159:THR:HG23	1:A:162:GLN:NE2	2.22	0.54
1:B:142:ILE:HG12	1:B:167:GLU:O	2.08	0.54
1:B:6:MET:HG2	1:B:118:ARG:NH2	2.22	0.54
1:A:122:PRO:HG2	1:A:125:GLY:HA3	1.90	0.54
1:A:189:ASN:O	1:A:194:GLY:HA2	2.08	0.53
1:A:163:ARG:O	1:A:163:ARG:HG2	2.08	0.53
1:A:255:ARG:NH1	1:A:273:GLU:CG	2.71	0.53
1:A:159:THR:H	1:A:162:GLN:NE2	2.01	0.53
1:A:173:LEU:C	1:A:173:LEU:HD12	2.29	0.52
1:A:141:ARG:HH12	1:A:155:HIS:CD2	2.26	0.52
1:B:112:GLU:HB2	4:B:403:HOH:O	2.09	0.52
1:A:255:ARG:NH1	1:A:273:GLU:HG2	2.24	0.52
1:B:136:PRO:CG	1:B:166:GLN:HA	2.39	0.52
1:A:268:HIS:HE1	4:A:455:HOH:O	1.92	0.51
1:B:139:TYR:CB	1:B:168:ILE:HD12	2.41	0.51
1:B:6:MET:HE1	1:B:8:VAL:CG2	2.41	0.51
1:A:57:HIS:CD2	1:A:58:GLY:H	2.29	0.50
1:A:151:GLY:HA2	1:A:202:ILE:HG22	1.93	0.50
1:B:164:GLN:NE2	1:B:164:GLN:HA	2.26	0.50
1:B:196:TYR:CD1	1:B:196:TYR:N	2.80	0.50
1:A:103:TYR:HD2	3:A:333:MES:H72	1.77	0.50
1:A:30:LEU:C	1:A:30:LEU:HD23	2.30	0.50
1:A:57:HIS:CG	1:A:58:GLY:H	2.29	0.50
1:B:6:MET:CE	1:B:8:VAL:HG23	2.42	0.49
1:A:255:ARG:NH1	1:A:273:GLU:OE1	2.45	0.49
1:A:255:ARG:HH11	1:A:273:GLU:CG	2.25	0.49
1:A:80:LEU:HB2	1:A:84:HIS:CG	2.47	0.49
1:A:152:ILE:HB	1:A:199:THR:HB	1.93	0.49
1:B:6:MET:HG2	1:B:118:ARG:CZ	2.42	0.49
1:B:139:TYR:HB2	1:B:168:ILE:CD1	2.42	0.49
1:B:202:ILE:HG23	1:B:212:ILE:CD1	2.42	0.49
1:B:128:LEU:O	1:B:214:ALA:HA	2.12	0.49
1:B:139:TYR:HB2	1:B:168:ILE:HD12	1.95	0.48
1:B:141:ARG:HB2	1:B:153:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB3	1:A:180:MET:HE1	1.92	0.48
1:A:14:GLY:CA	3:A:333:MES:O1S	2.62	0.48
1:A:103:TYR:CD2	3:A:333:MES:H72	2.48	0.48
1:A:150:THR:HG23	4:A:503:HOH:O	2.14	0.48
1:B:6:MET:HA	1:B:97:GLU:HB2	1.96	0.48
1:B:132:LYS:CE	1:B:132:LYS:N	2.73	0.48
1:B:291:LYS:HB2	1:B:308:GLU:HG3	1.96	0.48
1:B:57:HIS:CG	1:B:58:GLY:H	2.31	0.48
1:B:136:PRO:HB2	1:B:141:ARG:HH21	1.79	0.48
1:A:46:LEU:HD11	1:A:114:LEU:CB	2.44	0.48
1:A:132:LYS:CE	1:A:132:LYS:N	2.75	0.47
1:A:11:LEU:HD11	1:A:101:MET:CE	2.42	0.47
1:A:135:ASP:H	1:A:136:PRO:CD	2.28	0.47
1:B:142:ILE:CG1	1:B:167:GLU:HG2	2.42	0.47
1:A:80:LEU:HD12	1:A:84:HIS:CE1	2.50	0.47
1:B:141:ARG:HB2	1:B:153:VAL:HG13	1.97	0.47
1:B:163:ARG:O	1:B:163:ARG:HG2	2.13	0.47
1:B:80:LEU:HB2	1:B:84:HIS:CG	2.50	0.47
1:B:141:ARG:HH12	1:B:155:HIS:CD2	2.30	0.46
1:A:202:ILE:HG23	1:A:212:ILE:CD1	2.44	0.46
1:B:136:PRO:HB2	1:B:141:ARG:CZ	2.45	0.46
1:A:136:PRO:HB2	1:A:141:ARG:HE	1.79	0.46
1:A:271:ASP:O	1:A:289:ARG:HA	2.16	0.46
1:B:123:GLN:C	1:B:125:GLY:H	2.19	0.46
1:B:142:ILE:HG21	1:B:167:GLU:OE1	2.15	0.46
1:A:219:ARG:NH2	4:A:443:HOH:O	2.49	0.46
1:A:18:ARG:HD2	4:A:363:HOH:O	2.16	0.46
1:A:14:GLY:HA3	3:A:333:MES:O1S	2.16	0.45
1:A:136:PRO:HB2	1:A:141:ARG:CD	2.46	0.45
1:A:237:ARG:NE	1:A:237:ARG:HA	2.32	0.45
1:A:6:MET:HE3	1:A:8:VAL:HG23	1.98	0.45
1:A:255:ARG:NH1	1:A:273:GLU:CD	2.70	0.45
1:A:94:ALA:HB3	1:A:97:GLU:HG2	1.99	0.45
1:A:142:ILE:HG21	1:A:167:GLU:OE1	2.16	0.45
1:A:163:ARG:O	1:A:163:ARG:CG	2.65	0.45
1:B:57:HIS:CD2	1:B:58:GLY:H	2.35	0.44
1:B:253:MET:SD	1:B:273:GLU:HB3	2.57	0.44
1:A:275:ASP:OD1	1:A:276:THR:N	2.43	0.44
1:B:268:HIS:HE1	4:B:437:HOH:O	1.99	0.44
1:A:136:PRO:CG	1:A:141:ARG:HE	2.31	0.44
1:B:189:ASN:O	1:B:194:GLY:HA2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HD3	1:B:168:ILE:CD1	2.46	0.44
1:B:136:PRO:HB2	1:B:141:ARG:NE	2.32	0.44
1:A:255:ARG:HH11	1:A:273:GLU:HB3	1.83	0.44
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.88	0.44
1:A:215:VAL:HG12	1:A:216:HIS:N	2.32	0.44
1:B:156:LYS:HG3	1:B:156:LYS:O	2.18	0.43
1:B:54:VAL:HA	1:B:74:VAL:O	2.18	0.43
1:B:124:GLY:HA3	1:B:210:ARG:HH11	1.81	0.43
1:B:145:GLU:O	1:B:146:ASN:HB2	2.19	0.43
1:A:142:ILE:HD13	1:A:152:ILE:CD1	2.48	0.43
1:A:243:GLN:OE1	1:A:262:LEU:HD23	2.19	0.43
1:A:128:LEU:O	1:A:214:ALA:HA	2.18	0.43
1:A:162:GLN:O	1:A:165:ILE:HG13	2.19	0.43
1:B:207:GLN:C	1:B:209:GLY:H	2.22	0.43
1:A:168:ILE:HD13	1:A:168:ILE:HA	1.79	0.43
1:B:123:GLN:C	1:B:125:GLY:N	2.72	0.43
1:B:218:GLN:HE21	1:B:218:GLN:HA	1.84	0.43
1:A:224:GLU:CB	1:A:235:LEU:HD21	2.47	0.42
1:A:162:GLN:C	1:A:164:GLN:H	2.21	0.42
1:B:75:LEU:CD2	1:B:76:GLN:N	2.79	0.42
1:A:226:VAL:CG2	1:A:235:LEU:HD12	2.49	0.42
1:B:168:ILE:HD13	1:B:168:ILE:HA	1.85	0.42
1:A:143:THR:HG23	1:A:153:VAL:HG23	2.01	0.42
1:A:268:HIS:HD2	1:A:269:GLY:O	2.02	0.42
1:B:31:ALA:HB2	1:B:239:TYR:CD2	2.55	0.42
1:A:46:LEU:HD11	1:A:114:LEU:HB3	2.01	0.42
1:A:124:GLY:O	1:A:210:ARG:CD	2.59	0.42
1:A:255:ARG:HH11	1:A:273:GLU:CD	2.23	0.42
1:B:248:LEU:HD11	1:B:257:PRO:HB3	2.01	0.41
1:A:218:GLN:HA	1:A:218:GLN:NE2	2.30	0.41
1:B:126:ILE:HD11	1:B:183:TRP:CZ3	2.56	0.41
1:A:143:THR:CG2	1:A:153:VAL:HG23	2.49	0.41
1:A:255:ARG:CG	1:A:275:ASP:HA	2.34	0.41
1:A:136:PRO:CB	1:A:141:ARG:NE	2.75	0.41
1:A:221:SER:HB3	4:A:379:HOH:O	2.19	0.41
1:B:153:VAL:HG21	1:B:162:GLN:NE2	2.36	0.41
1:B:265:THR:HB	1:B:283:ASN:HD22	1.86	0.41
1:A:16:GLY:HA2	4:A:393:HOH:O	2.19	0.41
1:A:300:ASN:O	1:A:317:ASP:HA	2.20	0.41
1:B:253:MET:HE1	1:B:255:ARG:CZ	2.51	0.41
1:A:187:LEU:CB	1:A:196:TYR:HD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:SER:HB2	1:B:229:ARG:HH21	1.84	0.41
1:B:159:THR:O	1:B:160:ASP:C	2.58	0.41
1:B:183:TRP:CZ2	1:B:205:ALA:HB2	2.56	0.41
1:B:268:HIS:HD2	1:B:269:GLY:O	2.04	0.40
1:B:47:GLY:O	1:B:48:ALA:C	2.59	0.40
1:B:162:GLN:O	1:B:164:GLN:N	2.54	0.40
1:B:163:ARG:O	1:B:163:ARG:CG	2.69	0.40
4:A:513:HOH:O	1:B:326:ILE:HG23	2.21	0.40
1:B:136:PRO:CB	1:B:141:ARG:NE	2.85	0.40
1:B:237:ARG:CD	4:B:395:HOH:O	2.67	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)
4:B:370:HOH:O	4:B:478:HOH:O[2_655]	2.18	0.02

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	325/331 (98%)	311 (96%)	10 (3%)	4 (1%)	13 9
1	B	322/331 (97%)	302 (94%)	19 (6%)	1 (0%)	41 46
All	All	647/662 (98%)	613 (95%)	29 (4%)	5 (1%)	19 17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
1	A	194	GLY
1	B	163	ARG

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Mol	Chain	Res	Type
1	A	163	ARG
1	A	190	ASN

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	265/268 (99%)	255 (96%)	10 (4%)	33	39
1	B	263/268 (98%)	252 (96%)	11 (4%)	30	34
All	All	528/536 (98%)	507 (96%)	21 (4%)	31	37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	132	LYS
1	A	134	ASP
1	A	148	LYS
1	A	212	ILE
1	A	218	GLN
1	A	237	ARG
1	A	255	ARG
1	A	266	LEU
1	A	291	LYS
1	B	6	MET
1	B	66	LEU
1	B	123	GLN
1	B	132	LYS
1	B	189	ASN
1	B	191	ASN
1	B	212	ILE
1	B	237	ARG
1	B	246	LYS
1	B	266	LEU
1	B	273	GLU

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

Mol	Chain	Res	Type
1	A	57	HIS
1	A	155	HIS
1	A	162	GLN
1	A	164	GLN
1	A	218	GLN
1	A	268	HIS
1	B	57	HIS
1	B	123	GLN
1	B	155	HIS
1	B	162	GLN
1	B	164	GLN
1	B	191	ASN
1	B	193	GLN
1	B	218	GLN
1	B	231	GLN
1	B	268	HIS
1	B	283	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)

3 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	$\#\|Z\| > 2$
3	MES	A	333	-	12,12,12	8.81	8 (66%)	14,16,16	2.57	5 (35%)
2	SO4	A	332	-	4,4,4	0.33	0	6,6,6	0.21	0
2	SO4	B	332	-	4,4,4	0.34	0	6,6,6	0.18	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	MES	A	333	-	-	3/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	333	MES	C8-S	-23.04	1.44	1.77
3	A	333	MES	O2S-S	11.75	1.79	1.45
3	A	333	MES	O1S-S	10.93	1.77	1.45
3	A	333	MES	O3S-S	9.81	1.82	1.47
3	A	333	MES	C7-C8	-4.93	1.39	1.52
3	A	333	MES	C3-C2	-2.37	1.41	1.50
3	A	333	MES	C5-C6	-2.36	1.41	1.50
3	A	333	MES	C7-N4	-2.23	1.42	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	333	MES	O2S-S-C8	5.85	113.96	106.92
3	A	333	MES	O3S-S-C8	5.06	113.95	105.77
3	A	333	MES	O1S-S-C8	3.21	110.78	106.92
3	A	333	MES	O2S-S-O1S	-2.81	104.22	113.95
3	A	333	MES	O3S-S-O1S	-2.22	105.86	111.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	333	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
3	A	333	MES	C7-C8-S-O2S
3	A	333	MES	C7-C8-S-O1S

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	333	MES	6	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	327/331 (98%)	0.67	52 (15%)	1	1	26, 51, 89, 96	0
1	B	324/331 (97%)	0.54	33 (10%)	6	6	28, 53, 85, 95	0
All	All	651/662 (98%)	0.60	85 (13%)	3	3	26, 52, 87, 96	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	8.2
1	A	329	PHE	6.6
1	A	137	THR	5.3
1	B	206	TYR	5.0
1	A	3	ASN	4.9
1	A	164	GLN	4.6
1	B	173	LEU	4.6
1	A	192	ALA	4.6
1	B	123	GLN	4.5
1	A	206	TYR	4.5
1	B	254	LEU	4.3
1	B	207	GLN	4.3
1	A	194	GLY	4.3
1	A	134	ASP	4.3
1	A	207	GLN	4.2
1	A	5	ALA	4.1
1	A	4	ASN	4.1
1	A	193	GLN	4.1
1	B	4	ASN	4.0
1	A	139	TYR	3.8
1	A	101	MET	3.7
1	A	100	LEU	3.6
1	A	166	GLN	3.6
1	A	173	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	135	ASP	3.5
1	A	133	LEU	3.5
1	B	252	VAL	3.4
1	A	191	ASN	3.4
1	A	253	MET	3.4
1	B	253	MET	3.3
1	A	254	LEU	3.3
1	A	141	ARG	3.2
1	B	147	GLY	3.2
1	A	189	ASN	3.2
1	B	15	LYS	3.1
1	A	155	HIS	3.1
1	A	148	LYS	3.0
1	A	102	LEU	3.0
1	B	122	PRO	2.9
1	B	274	ILE	2.9
1	A	160	ASP	2.8
1	A	190	ASN	2.8
1	B	159	THR	2.8
1	B	157	ASP	2.8
1	B	193	GLN	2.8
1	B	196	TYR	2.7
1	B	100	LEU	2.7
1	B	128	LEU	2.6
1	B	102	LEU	2.5
1	A	99	ILE	2.5
1	B	17	THR	2.5
1	A	56	GLY	2.5
1	A	172	ILE	2.5
1	B	172	ILE	2.5
1	A	8	VAL	2.4
1	A	96	ASP	2.4
1	B	101	MET	2.4
1	B	156	LYS	2.4
1	A	174	ILE	2.4
1	A	15	LYS	2.4
1	B	91	PRO	2.4
1	A	274	ILE	2.3
1	B	158	ALA	2.3
1	A	68	ASP	2.3
1	B	272	VAL	2.3
1	B	148	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	80	LEU	2.3
1	B	211	GLU	2.3
1	A	159	THR	2.2
1	A	136	PRO	2.2
1	A	210	ARG	2.2
1	A	67	LYS	2.2
1	B	209	GLY	2.1
1	A	86	MET	2.1
1	A	324	CYS	2.1
1	A	252	VAL	2.1
1	A	127	GLY	2.1
1	B	96	ASP	2.1
1	A	9	VAL	2.1
1	A	132	LYS	2.1
1	A	168	ILE	2.1
1	B	163	ARG	2.1
1	A	128	LEU	2.0
1	B	320	LEU	2.0
1	A	325	THR	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, 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	B-factors(Å^2)	Q<0.9
3	MES	A	333	12/12	0.86	0.17	62,65,73,74	0
2	SO4	A	332	5/5	0.95	0.13	85,86,86,87	0
2	SO4	B	332	5/5	0.97	0.14	76,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.