Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:38 PM GMT

PDB ID	:	1Y0E
Title	:	Crystal structure of putative ManNAc-6-P epimerase from Staphylococcus aureus (strain N315)
Authors	:	Chang, C.; Joachimiak, A.; Li, H.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2004-11-15
Resolution	:	1.95 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:

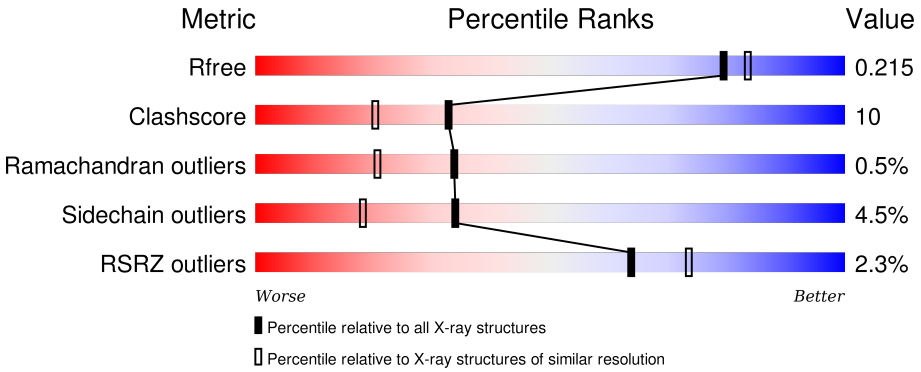
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	223	% 73% 22%
1	B	223	4% 78% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3848 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.

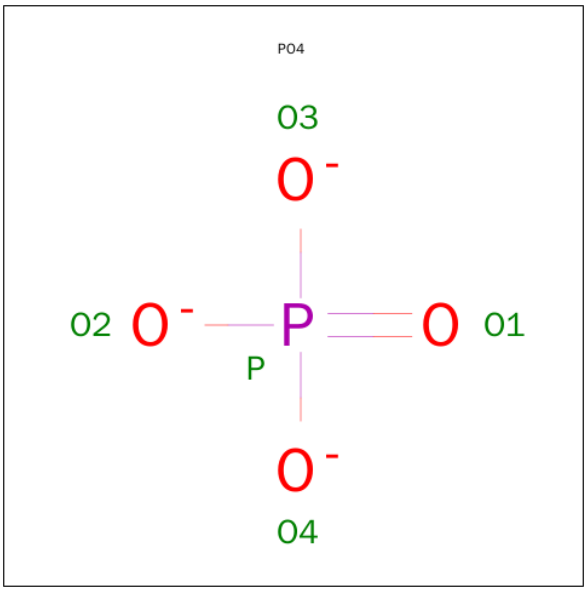
- Molecule 1 is a protein called Putative N-acetylmannosamine-6-phosphate 2-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	Se	0	0	0
			1716	1086	285	335	3	7			
1	B	222	Total	C	N	O	S	Se	0	0	0
			1716	1086	285	335	3	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	CLONING ARTIFACT	UNP P65517
A	1	MSE	MET	MODIFIED RESIDUE	UNP P65517
A	14	PRO	ALA	ENGINEERED	UNP P65517
A	24	MSE	MET	MODIFIED RESIDUE	UNP P65517
A	27	MSE	MET	MODIFIED RESIDUE	UNP P65517
A	122	MSE	MET	MODIFIED RESIDUE	UNP P65517
A	188	MSE	MET	MODIFIED RESIDUE	UNP P65517
A	193	MSE	MET	MODIFIED RESIDUE	UNP P65517
A	220	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	0	ALA	-	CLONING ARTIFACT	UNP P65517
B	1	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	14	PRO	ALA	ENGINEERED	UNP P65517
B	24	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	27	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	122	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	188	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	193	MSE	MET	MODIFIED RESIDUE	UNP P65517
B	220	MSE	MET	MODIFIED RESIDUE	UNP P65517

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

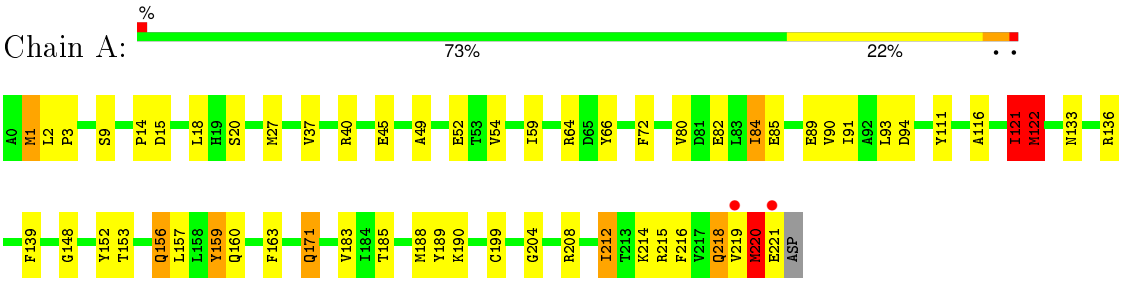
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	227	Total O 227 227	0	0
3	B	174	Total O 174 174	0	0

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.

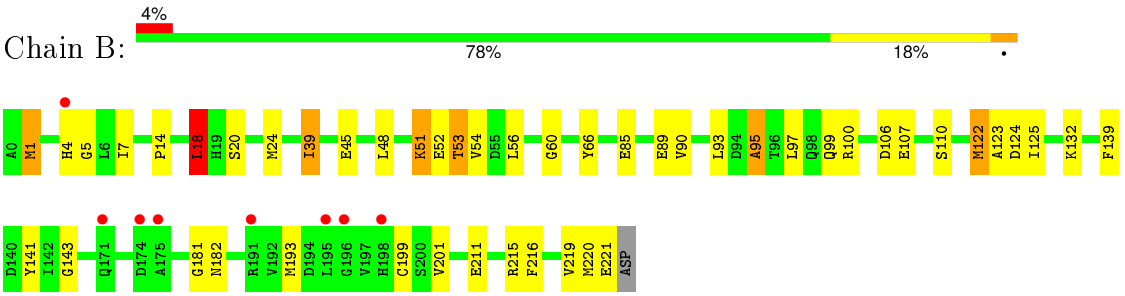
- Molecule 1: Putative N-acetylmannosamine-6-phosphate 2-epimerase

Chain A:



- Molecule 1: Putative N-acetylmannosamine-6-phosphate 2-epimerase

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	52.96Å 76.28Å 183.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 1.95 45.92 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.7 (91.67-1.95) 97.7 (45.92-1.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.177 , 0.216 0.179 , 0.215	Depositor DCC
R_{free} test set	2762 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 54689 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3848	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: PO4

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	1.52	19/1736 (1.1%)	1.15	8/2343 (0.3%)
1	B	1.52	18/1736 (1.0%)	1.26	11/2343 (0.5%)
All	All	1.52	37/3472 (1.1%)	1.21	19/4686 (0.4%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CD-OE1	10.50	1.37	1.25
1	B	1	MSE	SE-CE	9.44	2.51	1.95
1	B	221	GLU	CG-CD	8.64	1.65	1.51
1	A	1	MSE	SE-CE	8.23	2.44	1.95
1	A	85	GLU	CG-CD	7.86	1.63	1.51
1	B	141	TYR	CG-CD1	7.57	1.49	1.39
1	A	45	GLU	CG-CD	7.29	1.62	1.51
1	A	152	TYR	CD2-CE2	6.96	1.49	1.39
1	A	122	MSE	SE-CE	6.95	2.36	1.95
1	B	99	GLN	CG-CD	6.66	1.66	1.51
1	B	141	TYR	CE2-CZ	6.66	1.47	1.38
1	A	80	VAL	CB-CG1	6.38	1.66	1.52
1	A	45	GLU	CD-OE1	6.07	1.32	1.25
1	B	66	TYR	CG-CD1	5.98	1.47	1.39
1	B	139	PHE	CD2-CE2	5.87	1.50	1.39
1	B	95	ALA	CA-CB	5.86	1.64	1.52
1	A	220	MSE	SE-CE	5.69	2.29	1.95
1	B	122	MSE	SE-CE	5.64	2.28	1.95
1	B	211	GLU	CD-OE1	5.58	1.31	1.25
1	B	211	GLU	CG-CD	5.56	1.60	1.51
1	A	221	GLU	CD-OE2	5.52	1.31	1.25
1	B	90	VAL	CB-CG1	5.50	1.64	1.52
1	A	54	VAL	CA-CB	5.48	1.66	1.54
1	A	82	GLU	CG-CD	5.41	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	PHE	CD1-CE1	5.37	1.50	1.39
1	A	199	CYS	CB-SG	-5.34	1.73	1.81
1	B	66	TYR	CE1-CZ	5.30	1.45	1.38
1	A	72	PHE	CD2-CE2	5.28	1.49	1.39
1	A	111	TYR	CE1-CZ	5.26	1.45	1.38
1	B	107	GLU	CG-CD	5.25	1.59	1.51
1	B	53	THR	CB-CG2	5.24	1.69	1.52
1	A	159	TYR	CE2-CZ	5.21	1.45	1.38
1	A	66	TYR	CD1-CE1	5.20	1.47	1.39
1	B	66	TYR	CE2-CZ	5.13	1.45	1.38
1	A	220	MSE	CG-SE	5.05	2.12	1.95
1	A	189	TYR	CD2-CE2	5.02	1.46	1.39
1	B	60	GLY	C-O	5.02	1.31	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH1	16.23	128.42	120.30
1	B	215	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	B	51	LYS	CD-CE-NZ	-8.39	92.39	111.70
1	B	124	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	B	124	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	215	ARG	CD-NE-CZ	7.00	133.40	123.60
1	B	18	LEU	CB-CG-CD1	6.18	121.51	111.00
1	A	215	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	208	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	85	GLU	CG-CD-OE1	6.03	130.35	118.30
1	B	100	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	121	ILE	CA-CB-CG1	5.49	121.43	111.00
1	A	91	ILE	CA-CB-CG1	5.33	121.13	111.00
1	B	132	LYS	CD-CE-NZ	-5.20	99.74	111.70
1	A	1	MSE	CG-SE-CE	5.19	110.32	98.90
1	B	53	THR	CA-CB-CG2	5.15	119.62	112.40
1	B	97	LEU	CB-CG-CD1	-5.14	102.25	111.00
1	A	64	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	84	ILE	CA-CB-CG1	5.10	120.69	111.00

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	1716	0	1729	49	0
1	B	1716	0	1729	28	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	227	0	0	4	0
3	B	174	0	0	2	0
All	All	3848	0	3458	72	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 10.

All (72) 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:24:MSE:CE	1:B:24:MSE:SE	2.17	1.42
1:B:193:MSE:SE	1:B:193:MSE:CE	2.16	1.40
1:B:122:MSE:CE	1:B:122:MSE:SE	2.28	1.31
1:A:220:MSE:SE	1:A:220:MSE:CE	2.29	1.31
1:A:122:MSE:CE	1:A:122:MSE:SE	2.36	1.23
1:A:1:MSE:CE	1:A:1:MSE:SE	2.44	1.16
1:B:1:MSE:SE	1:B:1:MSE:CE	2.51	1.09
1:A:190:LYS:HA	1:B:220:MSE:HE1	1.39	1.05
1:B:219:VAL:HG23	1:B:220:MSE:HE2	1.44	1.00
1:A:190:LYS:HA	1:B:220:MSE:CE	2.04	0.88
1:B:1:MSE:HE3	1:B:89:GLU:HG3	1.55	0.88
1:A:90:VAL:HG11	1:A:122:MSE:HE3	1.56	0.87
1:A:1:MSE:HE2	1:A:89:GLU:HG2	1.59	0.84
1:A:220:MSE:CE	1:A:220:MSE:HA	2.07	0.83
1:B:53:THR:HG22	1:B:54:VAL:HG23	1.61	0.82
1:A:121:ILE:CD1	1:A:139:PHE:HA	2.11	0.81
1:A:121:ILE:HD11	1:A:139:PHE:HA	1.66	0.78
1:A:163:PHE:HZ	1:A:188:MSE:HE3	1.49	0.77
1:B:219:VAL:HG23	1:B:220:MSE:CE	2.15	0.76
1:A:133:ASN:HD21	1:A:136:ARG:HH21	1.34	0.75
1:A:1:MSE:HE3	3:A:598:HOH:O	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PRO:O	1:A:15:ASP:HB2	1.89	0.71
1:A:190:LYS:HD2	1:B:220:MSE:CE	2.21	0.71
1:A:163:PHE:CZ	1:A:188:MSE:HE3	2.25	0.71
1:A:183:VAL:HA	1:A:188:MSE:HE2	1.75	0.69
1:B:4:HIS:HE1	3:B:609:HOH:O	1.79	0.65
1:A:190:LYS:HD2	1:B:220:MSE:HE2	1.79	0.65
1:A:156:GLN:NE2	3:A:634:HOH:O	2.31	0.62
1:A:3:PRO:HG2	1:A:37:VAL:HB	1.81	0.62
1:A:220:MSE:HE2	1:A:220:MSE:HA	1.82	0.62
1:A:84:ILE:HD12	1:A:116:ALA:HB2	1.80	0.62
1:B:85:GLU:OE1	3:B:629:HOH:O	2.16	0.60
1:B:1:MSE:HG3	1:B:89:GLU:HB3	1.84	0.60
1:A:90:VAL:HG11	1:A:122:MSE:CE	2.34	0.57
1:A:18:LEU:HD13	1:A:27:MSE:HE3	1.87	0.56
1:A:214:LYS:O	1:A:218:GLN:HG2	2.06	0.55
1:B:95:ALA:HB3	1:B:123:ALA:HB1	1.87	0.55
1:A:121:ILE:HD13	1:A:139:PHE:HA	1.89	0.55
1:A:122:MSE:CE	1:A:122:MSE:HB2	2.37	0.54
1:A:18:LEU:CD1	1:A:27:MSE:HE3	2.38	0.54
1:A:190:LYS:HD2	1:B:220:MSE:HE1	1.91	0.53
1:A:14:PRO:O	1:A:15:ASP:CB	2.51	0.53
1:B:95:ALA:CB	1:B:123:ALA:HB1	2.38	0.53
1:B:48:LEU:O	1:B:52:GLU:HG2	2.09	0.53
1:A:133:ASN:ND2	1:A:136:ARG:HH21	2.05	0.52
1:A:212:ILE:HD13	1:A:212:ILE:N	2.25	0.51
1:A:121:ILE:HD13	1:A:139:PHE:CD1	2.45	0.51
1:B:216:PHE:O	1:B:219:VAL:HG22	2.12	0.50
1:B:18:LEU:HB3	1:B:24:MSE:CE	2.44	0.48
1:B:181:GLY:O	1:B:182:ASN:HB2	2.15	0.47
1:B:122:MSE:HE3	1:B:143:GLY:HA3	1.97	0.46
1:A:9:SER:HA	1:A:40:ARG:HB2	1.96	0.46
1:A:2:LEU:HD11	1:A:122:MSE:HE1	1.98	0.46
1:A:90:VAL:CG1	1:A:122:MSE:HE3	2.39	0.46
1:B:18:LEU:HB3	1:B:24:MSE:HE3	1.99	0.45
1:A:204:GLY:O	1:A:212:ILE:HD11	2.18	0.44
1:A:216:PHE:O	1:A:219:VAL:HG22	2.18	0.44
1:B:39:ILE:CD1	1:B:56:LEU:HD12	2.47	0.44
1:A:160:GLN:OE1	3:A:557:HOH:O	2.21	0.43
1:A:59:ILE:CD1	1:A:122:MSE:HE1	2.49	0.43
1:A:185:THR:OG1	1:A:188:MSE:HG3	2.19	0.43
1:B:125:ILE:HG13	1:B:143:GLY:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HE21	1:A:171:GLN:HB2	1.54	0.42
1:A:188:MSE:HE1	3:A:672:HOH:O	2.19	0.42
1:A:49:ALA:O	1:A:52:GLU:HB2	2.19	0.42
1:A:183:VAL:HA	1:A:188:MSE:CE	2.45	0.42
1:A:218:GLN:HB2	1:A:218:GLN:HE21	1.65	0.42
1:B:7:ILE:HB	1:B:201:VAL:HG22	2.02	0.41
1:A:157:LEU:HD13	1:A:159:TYR:OH	2.20	0.41
1:A:220:MSE:HE3	1:A:220:MSE:HA	1.95	0.41
1:B:5:GLY:O	1:B:199:CYS:HB2	2.21	0.41
1:A:148:GLY:HA2	1:A:153:THR:O	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	220/223 (99%)	212 (96%)	7 (3%)	1 (0%)	34	21
1	B	220/223 (99%)	214 (97%)	5 (2%)	1 (0%)	34	21
All	All	440/446 (99%)	426 (97%)	12 (3%)	2 (0%)	34	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	B	20	SER

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	189/183 (103%)	180 (95%)	9 (5%)	31 15
1	B	189/183 (103%)	181 (96%)	8 (4%)	36 21
All	All	378/366 (103%)	361 (96%)	17 (4%)	34 18

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	94	ASP
1	A	121	ILE
1	A	122	MSE
1	A	156	GLN
1	A	171	GLN
1	A	212	ILE
1	A	218	GLN
1	A	220	MSE
1	B	14	PRO
1	B	18	LEU
1	B	39	ILE
1	B	45	GLU
1	B	51	LYS
1	B	93	LEU
1	B	106	ASP
1	B	110	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	133	ASN
1	A	156	GLN
1	A	171	GLN
1	A	218	GLN
1	B	115	HIS
1	B	164	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

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	$\#\|Z\| > 2$
2	PO4	A	501	-	4,4,4	0.40	0	6,6,6	0.29	0
2	PO4	A	502	-	4,4,4	1.19	0	6,6,6	0.36	0
2	PO4	B	503	-	4,4,4	0.45	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
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	B	503	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	215/223 (96%)	-0.06	2 (0%) 85 90	19, 25, 37, 54	0
1	B	215/223 (96%)	0.15	8 (3%) 45 56	20, 30, 42, 51	0
All	All	430/446 (96%)	0.05	10 (2%) 64 73	19, 28, 39, 54	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	HIS	4.0
1	B	196	GLY	3.6
1	B	174	ASP	3.5
1	A	221	GLU	3.5
1	B	195	LEU	3.0
1	B	171	GLN	3.0
1	B	175	ALA	2.5
1	B	198	HIS	2.2
1	A	219	VAL	2.1
1	B	191	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	PO4	B	503	5/5	0.99	0.06	-1.87	31,37,40,41	0
2	PO4	A	502	5/5	0.99	0.06	-2.34	27,28,29,31	0
2	PO4	A	501	5/5	0.99	0.06	-3.37	34,36,38,43	0

6.5 Other polymers

There are no such residues in this entry.