Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 09:49 AM EST

PDB ID	:	3T0J
Title	:	Crystal structure of inositol monophosphatase - II from Staphylococcus aureus MSSA476
Authors	:	Dutta, A.; Bhattacharyya, S.; Dutta, D.; Das, A.K.
Deposited on	:	2011-07-20
Resolution	:	2.59 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:

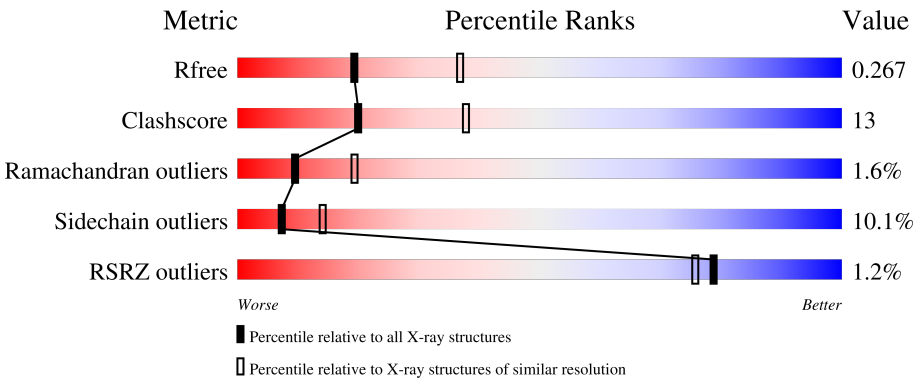
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	283	.% 73% 17% • • 6%
1	B	283	.% 65% 20% 6% • 8%
1	C	283	.% 71% 19% • • 6%
1	D	283	2% 64% 20% 6% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8500 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 Inositol monophosphatase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2070	1318	352	397	3	0	1	0
			Total	C	N	O	S			
1	B	260	2011	1280	337	390	4	0	2	0
			Total	C	N	O	S			
1	C	265	2050	1308	345	393	4	0	0	0
			Total	C	N	O	S			
1	D	257	1983	1262	332	385	4	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q6GAA7
A	-6	HIS	-	expression tag	UNP Q6GAA7
A	-5	HIS	-	expression tag	UNP Q6GAA7
A	-4	HIS	-	expression tag	UNP Q6GAA7
A	-3	HIS	-	expression tag	UNP Q6GAA7
A	-2	HIS	-	expression tag	UNP Q6GAA7
A	-1	GLY	-	expression tag	UNP Q6GAA7
A	0	SER	-	expression tag	UNP Q6GAA7
B	-7	HIS	-	expression tag	UNP Q6GAA7
B	-6	HIS	-	expression tag	UNP Q6GAA7
B	-5	HIS	-	expression tag	UNP Q6GAA7
B	-4	HIS	-	expression tag	UNP Q6GAA7
B	-3	HIS	-	expression tag	UNP Q6GAA7
B	-2	HIS	-	expression tag	UNP Q6GAA7
B	-1	GLY	-	expression tag	UNP Q6GAA7
B	0	SER	-	expression tag	UNP Q6GAA7
C	-7	HIS	-	expression tag	UNP Q6GAA7
C	-6	HIS	-	expression tag	UNP Q6GAA7
C	-5	HIS	-	expression tag	UNP Q6GAA7
C	-4	HIS	-	expression tag	UNP Q6GAA7
C	-3	HIS	-	expression tag	UNP Q6GAA7

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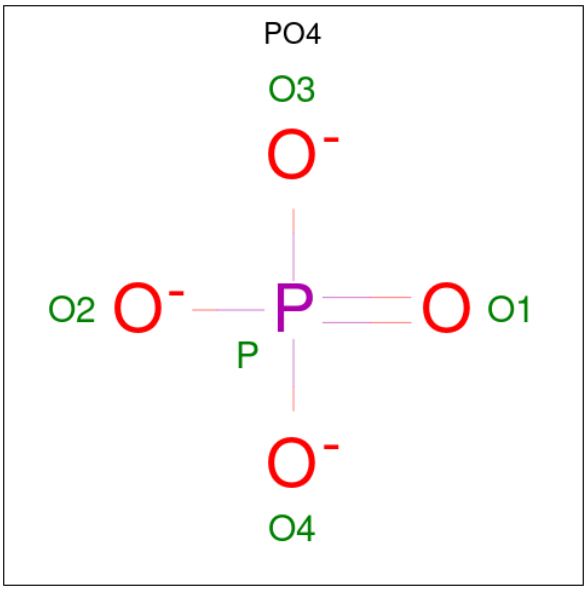
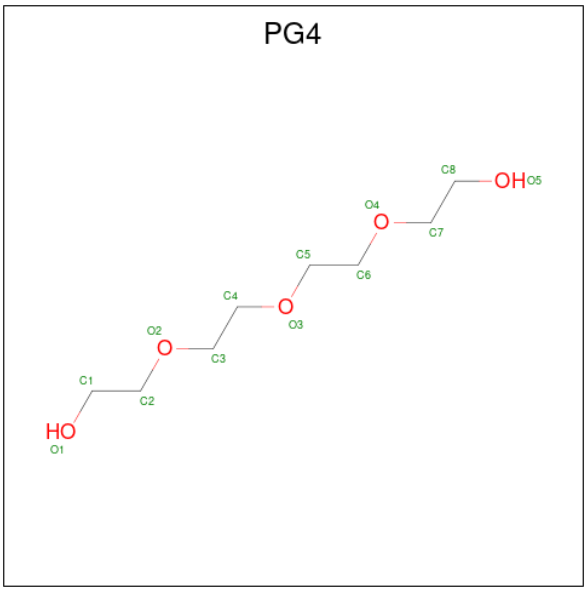
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q6GAA7
C	-1	GLY	-	expression tag	UNP Q6GAA7
C	0	SER	-	expression tag	UNP Q6GAA7
D	-7	HIS	-	expression tag	UNP Q6GAA7
D	-6	HIS	-	expression tag	UNP Q6GAA7
D	-5	HIS	-	expression tag	UNP Q6GAA7
D	-4	HIS	-	expression tag	UNP Q6GAA7
D	-3	HIS	-	expression tag	UNP Q6GAA7
D	-2	HIS	-	expression tag	UNP Q6GAA7
D	-1	GLY	-	expression tag	UNP Q6GAA7
D	0	SER	-	expression tag	UNP Q6GAA7

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



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

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 10 6 4	0	0
3	D	1	Total C O 10 6 4	0	0
3	D	1	Total C O 13 8 5	0	0

- Molecule 4 is water.

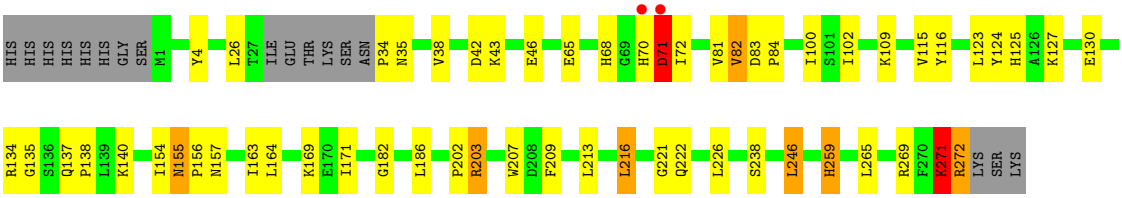
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	81	Total O 81 81	0	0
4	B	70	Total O 70 70	0	0
4	C	76	Total O 76 76	0	0
4	D	67	Total O 67 67	0	0

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.

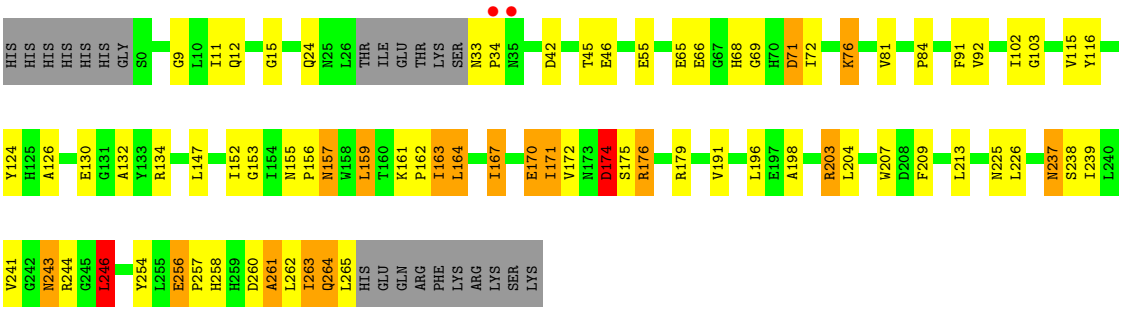
• Molecule 1: Inositol monophosphatase family protein

Chain A:



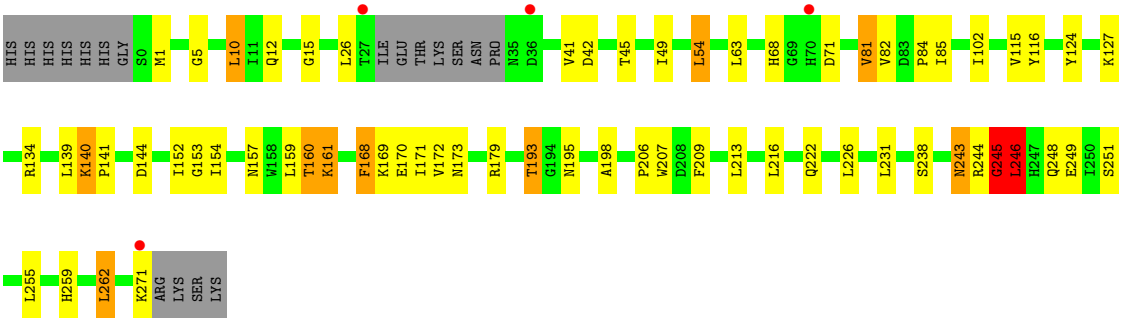
• Molecule 1: Inositol monophosphatase family protein

Chain B:



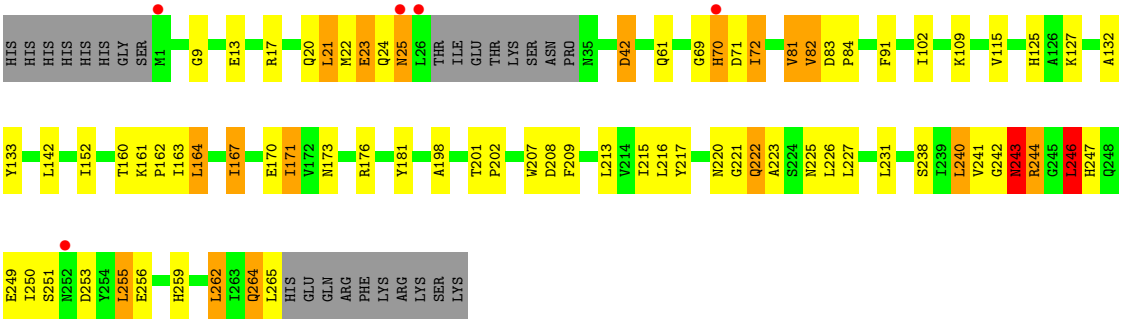
• Molecule 1: Inositol monophosphatase family protein

Chain C:



• Molecule 1: Inositol monophosphatase family protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.14Å 55.21Å 149.47Å 90.00° 124.33° 90.00°	Depositor
Resolution (Å)	19.74 – 2.59 19.74 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.74-2.59) 99.3 (19.74-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.183 , 0.268 0.184 , 0.267	Depositor DCC
R_{free} test set	1899 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8500	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 16.53% 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: PG4, 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	0.75	0/2118	0.80	1/2880 (0.0%)
1	B	0.75	1/2057 (0.0%)	0.83	1/2800 (0.0%)
1	C	0.69	0/2095	0.80	3/2849 (0.1%)
1	D	0.69	0/2026	0.79	1/2759 (0.0%)
All	All	0.72	1/8296 (0.0%)	0.81	6/11288 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	ASP	CB-CG	-5.35	1.40	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	LEU	CB-CG-CD1	-6.05	100.72	111.00
1	C	54	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	262	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	246	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	C	246	LEU	CA-CB-CG	-5.59	102.45	115.30
1	D	246	LEU	CB-CG-CD1	-5.19	102.18	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	LYS	Peptide
1	A	34	PRO	Peptide
1	C	245	GLY	Peptide

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	2070	0	2007	38	0
1	B	2011	0	1955	63	0
1	C	2050	0	1989	53	0
1	D	1983	0	1917	53	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	39	0	54	10	0
3	B	10	0	13	2	0
3	D	23	0	31	2	0
4	A	81	0	0	3	0
4	B	70	0	0	2	0
4	C	76	0	0	3	0
4	D	67	0	0	2	0
All	All	8500	0	7966	203	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 13.

All (203) 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:1:MET:HE1	1:C:127:LYS:HE2	1.29	1.13
1:C:1:MET:CE	1:C:127:LYS:HE2	1.81	1.09
1:B:261:ALA:O	1:B:263:ILE:N	1.99	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HD22	1:A:157:ASN:H	1.12	0.93
1:A:70:HIS:O	1:A:71:ASP:HB2	1.66	0.92
1:B:237[A]:ASN:HD22	1:B:237[A]:ASN:N	1.66	0.89
1:B:12:GLN:HE22	1:C:12:GLN:HE22	1.13	0.89
1:B:264:GLN:HE21	1:B:264:GLN:N	1.72	0.87
1:A:155:ASN:ND2	1:A:157:ASN:H	1.76	0.83
1:C:193:THR:CG2	1:C:195:ASN:HB2	2.09	0.82
1:C:160:THR:HG21	1:D:173:ASN:OD1	1.81	0.80
1:B:237[A]:ASN:N	1:B:237[A]:ASN:ND2	2.27	0.78
1:D:242:GLY:O	1:D:243:ASN:HB3	1.85	0.77
1:C:1:MET:HE3	1:C:127:LYS:HE2	1.67	0.76
1:B:237[A]:ASN:HD22	1:B:237[A]:ASN:H	1.35	0.75
1:D:22:MET:O	1:D:23:GLU:HG2	1.88	0.73
1:D:69:GLY:HA2	1:D:72:ILE:CD1	2.18	0.73
1:D:163:ILE:O	1:D:164:LEU:HB2	1.88	0.73
1:C:193:THR:HG22	1:C:195:ASN:HB2	1.70	0.72
1:A:271:LYS:HG3	1:A:272:ARG:HA	1.72	0.72
1:B:152:ILE:HD13	1:B:171:ILE:CD1	2.21	0.70
1:A:134:ARG:HE	3:A:277:PG4:H32	1.57	0.69
1:C:222:GLN:HG3	1:C:244:ARG:HG2	1.74	0.69
1:C:226:LEU:HG	1:C:238:SER:HB2	1.74	0.69
1:C:245:GLY:HA2	1:C:248:GLN:H	1.58	0.68
1:C:157:ASN:O	1:C:160:THR:HB	1.93	0.68
1:C:209:PHE:O	1:C:213:LEU:HB2	1.94	0.67
1:A:46:GLU:OE2	1:A:68:HIS:HD2	1.77	0.67
1:D:71:ASP:O	1:D:72:ILE:C	2.33	0.66
1:D:244:ARG:HG2	4:D:299:HOH:O	1.96	0.65
1:D:213:LEU:O	1:D:217:TYR:HD2	1.78	0.64
1:B:171:ILE:C	1:B:171:ILE:HD13	2.17	0.64
1:A:70:HIS:O	1:A:71:ASP:CB	2.41	0.64
1:D:69:GLY:HA2	1:D:72:ILE:HD11	1.80	0.64
1:C:1:MET:HE1	1:C:127:LYS:CE	2.19	0.63
1:D:198:ALA:HB2	1:D:246:LEU:HD21	1.81	0.63
1:A:156:PRO:HD3	1:B:156:PRO:HG3	1.82	0.62
1:C:10:LEU:HD11	1:C:49:ILE:HG23	1.82	0.61
1:D:216:LEU:HG	1:D:221:GLY:HA3	1.83	0.61
1:B:225:ASN:HB2	1:B:238[B]:SER:OG	2.00	0.61
1:D:81:VAL:HG23	1:D:207:TRP:HA	1.82	0.61
1:D:81:VAL:CG2	1:D:207:TRP:HA	2.32	0.60
1:D:42:ASP:OD2	1:D:84:PRO:HG2	2.01	0.60
1:B:196:LEU:O	4:B:301:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ILE:HD13	1:B:171:ILE:HD11	1.84	0.59
1:A:182:GLY:O	3:A:279:PG4:H61	2.03	0.59
1:D:264:GLN:HE21	1:D:264:GLN:HA	1.68	0.58
1:B:24:GLN:HG3	1:B:24:GLN:O	2.02	0.58
1:C:193:THR:HG22	1:C:195:ASN:H	1.67	0.58
1:D:69:GLY:HA2	1:D:72:ILE:HD12	1.85	0.58
1:D:244:ARG:CG	4:D:299:HOH:O	2.52	0.58
1:D:249:GLU:O	1:D:253:ASP:CB	2.52	0.58
1:B:198:ALA:HB2	1:B:246:LEU:HD21	1.86	0.58
1:B:81:VAL:HG12	1:B:103:GLY:O	2.04	0.57
1:D:9:GLY:O	1:D:13:GLU:HG3	2.04	0.57
1:D:164:LEU:HA	1:D:167:ILE:HG12	1.86	0.56
1:A:209:PHE:HB2	1:A:213:LEU:HD13	1.86	0.56
1:B:65:GLU:OE1	1:B:66:GLU:OE2	2.23	0.56
1:B:159:LEU:HD21	1:B:172:VAL:HG11	1.88	0.56
1:B:226:LEU:HG	1:B:238[B]:SER:HB2	1.86	0.56
1:B:256:GLU:HG3	1:B:257:PRO:HD3	1.87	0.56
1:D:222:GLN:O	1:D:241:VAL:HA	2.05	0.56
1:B:81:VAL:HG22	1:B:207:TRP:HA	1.85	0.56
1:D:69:GLY:O	1:D:70:HIS:HB3	2.06	0.56
1:B:203:ARG:HG3	4:B:282:HOH:O	2.06	0.56
1:B:226:LEU:HG	1:B:238[A]:SER:HB3	1.87	0.56
1:D:264:GLN:O	1:D:265:LEU:CB	2.54	0.56
1:D:152:ILE:HD13	1:D:171:ILE:HD13	1.87	0.56
1:C:139:LEU:O	1:C:140:LYS:CB	2.54	0.55
1:C:245:GLY:HA2	1:C:248:GLN:N	2.22	0.55
1:C:82:VAL:HB	1:C:102:ILE:HG12	1.90	0.54
1:C:170:GLU:HA	1:C:170:GLU:OE1	2.08	0.54
1:C:244:ARG:O	1:C:245:GLY:O	2.26	0.54
1:A:134:ARG:HH21	3:A:277:PG4:H22	1.73	0.53
1:C:152:ILE:HG22	1:C:198:ALA:HB3	1.90	0.53
1:D:70:HIS:C	1:D:72:ILE:H	2.11	0.53
1:D:249:GLU:O	1:D:253:ASP:HB3	2.08	0.53
1:A:155:ASN:HD22	1:A:157:ASN:N	1.92	0.53
1:C:245:GLY:HA2	1:C:248:GLN:HB2	1.89	0.53
1:C:81:VAL:CG2	1:C:207:TRP:HA	2.39	0.52
1:A:271:LYS:HG3	1:A:272:ARG:CA	2.40	0.52
1:B:69:GLY:O	1:B:72:ILE:HG12	2.09	0.52
1:C:271:LYS:HA	4:C:306:HOH:O	2.09	0.52
1:D:83:ASP:OD2	1:D:208:ASP:OD1	2.26	0.52
1:D:251:SER:HA	1:D:255:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:MET:C	1:D:23:GLU:HG2	2.28	0.52
1:D:125:HIS:CE1	1:D:133:TYR:HB2	2.45	0.52
1:D:21:LEU:C	1:D:23:GLU:H	2.12	0.52
1:B:155:ASN:OD1	1:B:157:ASN:HB2	2.11	0.51
1:A:269:ARG:HB2	3:A:278:PG4:H71	1.93	0.51
1:B:147:LEU:O	1:B:175:SER:HA	2.10	0.51
1:C:169:LYS:HB2	1:D:160:THR:HG22	1.91	0.51
1:B:33:ASN:N	1:B:34:PRO:HD2	2.26	0.51
1:C:160:THR:HG22	1:C:161:LYS:HD2	1.92	0.51
1:D:249:GLU:O	1:D:253:ASP:HB2	2.12	0.50
1:C:15:GLY:HA3	1:C:116:TYR:HE2	1.76	0.50
1:B:204:LEU:HD22	1:B:239:ILE:HG13	1.94	0.50
3:D:277:PG4:H51	3:D:278:PG4:H22	1.93	0.50
1:B:163:ILE:O	1:B:167:ILE:HG23	2.12	0.50
1:A:265:LEU:HD22	3:A:278:PG4:H81	1.93	0.50
1:B:153:GLY:HA2	1:B:179:ARG:O	2.11	0.49
1:A:83:ASP:HB2	1:A:207:TRP:HB2	1.94	0.49
1:B:243:ASN:ND2	1:B:246:LEU:H	2.10	0.49
1:D:226:LEU:HG	1:D:238:SER:HB2	1.95	0.49
1:B:171:ILE:HD13	1:B:171:ILE:O	2.12	0.49
1:D:82:VAL:HB	1:D:102:ILE:HG12	1.94	0.49
1:A:4:TYR:CE2	4:A:280:HOH:O	2.55	0.49
1:B:76:LYS:HA	1:B:76:LYS:HD2	1.64	0.49
1:A:163:ILE:HG22	1:A:265:LEU:HD11	1.94	0.48
1:B:9:GLY:HA3	1:C:5:GLY:O	2.13	0.48
3:A:279:PG4:H62	4:A:295:HOH:O	2.13	0.48
1:B:126:ALA:HB2	1:B:132:ALA:HA	1.97	0.47
1:B:34:PRO:HB2	1:B:92:VAL:HG13	1.97	0.47
1:D:223:ALA:HB1	1:D:231:LEU:HD12	1.94	0.47
1:A:226:LEU:HD12	1:A:238:SER:HB2	1.96	0.47
1:C:124:TYR:CE1	1:C:134:ARG:HG3	2.50	0.47
1:B:124:TYR:CE1	1:B:134:ARG:HG3	2.49	0.47
1:C:206:PRO:HA	1:C:209:PHE:CZ	2.50	0.47
1:C:251:SER:HA	1:C:255:LEU:HD12	1.97	0.47
1:C:139:LEU:HD12	1:C:139:LEU:HA	1.68	0.47
1:C:168:PHE:O	1:C:172:VAL:HG23	2.15	0.46
1:C:245:GLY:HA2	1:C:248:GLN:CB	2.44	0.46
1:B:134:ARG:HD2	3:B:277:PG4:O1	2.16	0.46
1:C:41:VAL:HG12	1:C:85:ILE:HD11	1.97	0.46
1:C:68:HIS:HE1	4:C:302:HOH:O	1.98	0.46
1:B:45:THR:HG22	1:B:84:PRO:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ILE:HG22	1:D:198:ALA:HB3	1.99	0.45
1:D:181:TYR:CE2	3:D:278:PG4:H12	2.51	0.45
1:D:250:ILE:HG22	1:D:255:LEU:HD22	1.98	0.45
1:B:45:THR:CG2	1:B:84:PRO:HB3	2.47	0.45
1:A:116:TYR:HB2	1:A:123:LEU:HD13	1.99	0.45
1:B:170:GLU:OE1	1:B:170:GLU:HA	2.17	0.45
1:B:263:ILE:C	1:B:264:GLN:HE21	2.20	0.45
1:D:213:LEU:HG	1:D:217:TYR:HE2	1.82	0.45
1:A:134:ARG:HH21	3:A:277:PG4:C2	2.30	0.45
1:D:152:ILE:HA	1:D:198:ALA:O	2.17	0.45
1:A:46:GLU:OE2	1:A:68:HIS:CD2	2.65	0.44
1:C:140:LYS:HA	1:C:141:PRO:HD3	1.86	0.44
1:C:193:THR:HG22	1:C:195:ASN:CB	2.44	0.44
1:D:209:PHE:O	1:D:213:LEU:HB2	2.18	0.44
1:B:170:GLU:OE1	1:B:170:GLU:CA	2.66	0.44
1:D:91:PHE:CD2	1:D:91:PHE:C	2.90	0.44
1:B:91:PHE:C	1:B:91:PHE:CD2	2.91	0.44
1:C:206:PRO:HA	1:C:209:PHE:CE2	2.52	0.44
1:D:167:ILE:HD13	1:D:262:LEU:HD13	1.98	0.44
1:B:11:ILE:HD12	1:B:102:ILE:HD12	1.98	0.44
1:D:227:LEU:HD21	1:D:262:LEU:HB3	2.00	0.44
1:B:170:GLU:O	1:B:174:ASP:HB2	2.18	0.44
1:B:204:LEU:CD2	1:B:239:ILE:HG13	2.47	0.44
1:C:10:LEU:CD1	1:C:49:ILE:HG23	2.47	0.43
3:B:277:PG4:H62	3:B:277:PG4:H41	1.88	0.43
1:B:260:ASP:O	1:B:261:ALA:HB3	2.18	0.43
1:B:209:PHE:O	1:B:213:LEU:HB2	2.19	0.43
1:B:15:GLY:HA3	1:B:116:TYR:HE2	1.82	0.43
1:A:82:VAL:HB	1:A:102:ILE:HG12	2.00	0.43
1:B:191:VAL:HG21	1:B:241:VAL:HG23	2.01	0.43
1:C:45:THR:HB	1:C:84:PRO:HB3	2.00	0.43
1:C:134:ARG:HD2	4:C:338:HOH:O	2.18	0.43
1:C:245:GLY:CA	1:C:248:GLN:H	2.30	0.43
1:C:153:GLY:HA2	1:C:179:ARG:O	2.19	0.42
1:C:226:LEU:HG	1:C:238:SER:CB	2.46	0.42
1:A:124:TYR:CE1	1:A:134:ARG:HG3	2.54	0.42
1:A:155:ASN:HD22	1:A:155:ASN:C	2.23	0.42
1:B:170:GLU:HB3	1:B:254:TYR:CD2	2.54	0.42
1:C:246:LEU:H	1:C:249:GLU:H	1.67	0.42
1:B:225:ASN:HB2	1:B:238[A]:SER:HB2	1.99	0.42
1:A:259:HIS:HE1	4:A:308:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.74	0.42
1:B:226:LEU:H	1:B:238[A]:SER:HB2	1.85	0.42
1:C:63:LEU:O	1:C:81:VAL:HA	2.19	0.42
1:D:163:ILE:HG22	1:D:164:LEU:N	2.35	0.42
1:B:258:HIS:O	1:B:260:ASP:O	2.38	0.42
1:C:213:LEU:HD11	1:C:231:LEU:HD12	2.02	0.42
1:D:167:ILE:HD13	1:D:262:LEU:CD1	2.49	0.42
1:C:209:PHE:HB2	1:C:213:LEU:HD13	2.02	0.42
1:A:186:LEU:HB3	3:A:277:PG4:H81	2.01	0.41
1:A:216:LEU:HD22	1:A:221:GLY:HA3	2.02	0.41
1:D:132:ALA:HB1	1:D:215:ILE:HG23	2.02	0.41
1:B:46:GLU:HG2	1:B:68:HIS:HD2	1.85	0.41
1:C:152:ILE:HD12	1:C:154:ILE:HG22	2.01	0.41
1:B:162:PRO:C	1:B:164:LEU:H	2.24	0.41
1:C:173:ASN:OD1	1:D:160:THR:HB	2.21	0.41
1:B:152:ILE:O	1:B:152:ILE:HG13	2.20	0.41
1:B:159:LEU:HD12	1:B:159:LEU:HA	1.84	0.41
1:A:125:HIS:NE2	1:A:135:GLY:O	2.53	0.41
1:A:127:LYS:HE3	1:A:130:GLU:OE2	2.19	0.41
1:A:154:ILE:O	1:A:154:ILE:HG23	2.20	0.41
1:D:69:GLY:O	1:D:70:HIS:CB	2.68	0.41
1:A:137:GLN:HA	1:A:138:PRO:HD2	1.94	0.41
1:A:164:LEU:HD21	1:A:202:PRO:HG3	2.02	0.41
1:C:144:ASP:HA	1:C:243:ASN:ND2	2.35	0.41
1:A:35:ASN:O	1:A:38:VAL:HG12	2.19	0.41
1:A:134:ARG:NH2	3:A:277:PG4:H22	2.35	0.41
1:B:12:GLN:HE22	1:C:12:GLN:NE2	1.97	0.41
1:D:201:THR:OG1	1:D:202:PRO:HD2	2.21	0.41
1:D:240:LEU:HD13	1:D:247:HIS:CD2	2.55	0.41
1:D:225:ASN:HB2	1:D:238:SER:OG	2.20	0.41
1:A:65:GLU:HA	1:A:207:TRP:CE2	2.55	0.40
1:B:71:ASP:OD2	1:B:71:ASP:N	2.54	0.40
1:B:161:LYS:HA	1:B:162:PRO:HD2	1.86	0.40
1:A:84:PRO:O	1:A:100:ILE:HG12	2.21	0.40
1:A:203:ARG:HH11	1:A:203:ARG:HD3	1.75	0.40
3:A:279:PG4:H21	1:B:176:ARG:NH2	2.36	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	263/283 (93%)	251 (95%)	10 (4%)	2 (1%)	19 39
1	B	258/283 (91%)	245 (95%)	9 (4%)	4 (2%)	9 19
1	C	261/283 (92%)	244 (94%)	13 (5%)	4 (2%)	10 21
1	D	253/283 (89%)	229 (90%)	17 (7%)	7 (3%)	5 7
All	All	1035/1132 (91%)	969 (94%)	49 (5%)	17 (2%)	9 19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	LEU
1	C	246	LEU
1	D	70	HIS
1	A	71	ASP
1	B	261	ALA
1	C	245	GLY
1	D	24	GLN
1	D	72	ILE
1	D	162	PRO
1	D	243	ASN
1	A	26	LEU
1	B	263	ILE
1	C	140	LYS
1	D	25	ASN
1	D	164	LEU
1	C	54	LEU
1	B	163	ILE

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	218/239 (91%)	199 (91%)	19 (9%)	10 20
1	B	214/239 (90%)	191 (89%)	23 (11%)	6 12
1	C	216/239 (90%)	200 (93%)	16 (7%)	13 28
1	D	210/239 (88%)	181 (86%)	29 (14%)	3 6
All	All	858/956 (90%)	771 (90%)	87 (10%)	7 14

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	43	LYS
1	A	71	ASP
1	A	72	ILE
1	A	81	VAL
1	A	82	VAL
1	A	109	LYS
1	A	115	VAL
1	A	140	LYS
1	A	155	ASN
1	A	169	LYS
1	A	171	ILE
1	A	203	ARG
1	A	216	LEU
1	A	222	GLN
1	A	246	LEU
1	A	259	HIS
1	A	271	LYS
1	A	272	ARG
1	B	42	ASP
1	B	55	GLU
1	B	71	ASP
1	B	76	LYS
1	B	115	VAL
1	B	130	GLU
1	B	157	ASN
1	B	159	LEU
1	B	164	LEU

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Mol	Chain	Res	Type
1	B	167	ILE
1	B	170	GLU
1	B	171	ILE
1	B	174	ASP
1	B	176	ARG
1	B	203	ARG
1	B	237[A]	ASN
1	B	237[B]	ASN
1	B	243	ASN
1	B	244	ARG
1	B	246	LEU
1	B	256	GLU
1	B	264	GLN
1	B	265	LEU
1	C	10	LEU
1	C	26	LEU
1	C	42	ASP
1	C	71	ASP
1	C	81	VAL
1	C	115	VAL
1	C	159	LEU
1	C	160	THR
1	C	161	LYS
1	C	168	PHE
1	C	171	ILE
1	C	193	THR
1	C	216	LEU
1	C	243	ASN
1	C	259	HIS
1	C	262	LEU
1	D	17	ARG
1	D	20	GLN
1	D	21	LEU
1	D	23	GLU
1	D	25	ASN
1	D	42	ASP
1	D	61	GLN
1	D	81	VAL
1	D	82	VAL
1	D	109	LYS
1	D	115	VAL
1	D	127	LYS

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Mol	Chain	Res	Type
1	D	142	LEU
1	D	161	LYS
1	D	167	ILE
1	D	170	GLU
1	D	171	ILE
1	D	176	ARG
1	D	220	ASN
1	D	222	GLN
1	D	240	LEU
1	D	243	ASN
1	D	244	ARG
1	D	246	LEU
1	D	255	LEU
1	D	256	GLU
1	D	259	HIS
1	D	262	LEU
1	D	264	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	68	HIS
1	A	93	HIS
1	A	155	ASN
1	A	157	ASN
1	A	220	ASN
1	A	259	HIS
1	A	268	GLN
1	B	12	GLN
1	B	25	ASN
1	B	40	ASN
1	B	59	ASN
1	B	68	HIS
1	B	243	ASN
1	B	264	GLN
1	C	25	ASN
1	C	40	ASN
1	C	61	GLN
1	C	68	HIS
1	C	70	HIS
1	C	146	ASN

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Mol	Chain	Res	Type
1	C	195	ASN
1	C	243	ASN
1	D	20	GLN
1	D	25	ASN
1	D	40	ASN
1	D	59	ASN
1	D	157	ASN
1	D	264	GLN

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)

10 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	PG4	A	278	-	12,12,12	0.70	0	11,11,11	0.47	0
3	PG4	A	277	-	12,12,12	0.55	0	11,11,11	0.25	0
3	PG4	D	278	-	12,12,12	0.57	0	11,11,11	0.66	0
2	PO4	D	276	-	4,4,4	0.65	0	6,6,6	0.80	0
3	PG4	A	279	-	12,12,12	0.56	0	11,11,11	0.46	0
2	PO4	C	276	-	4,4,4	0.68	0	6,6,6	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	B	276	-	4,4,4	1.08	0	6,6,6	0.78	0
3	PG4	B	277	-	9,9,12	0.56	0	8,8,11	0.35	0
2	PO4	A	276	-	4,4,4	1.37	0	6,6,6	1.01	0
3	PG4	D	277	-	9,9,12	0.60	0	8,8,11	0.28	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	PG4	A	278	-	-	6/10/10/10	-
3	PG4	A	277	-	-	6/10/10/10	-
3	PG4	D	278	-	-	5/10/10/10	-
3	PG4	A	279	-	-	3/10/10/10	-
3	PG4	B	277	-	-	6/7/7/10	-
3	PG4	D	277	-	-	4/7/7/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	277	PG4	O3-C5-C6-O4
3	B	277	PG4	O2-C3-C4-O3
3	A	279	PG4	O3-C5-C6-O4
3	A	277	PG4	O1-C1-C2-O2
3	D	277	PG4	O1-C1-C2-O2
3	D	278	PG4	C5-C6-O4-C7
3	A	278	PG4	O2-C3-C4-O3
3	D	278	PG4	O2-C3-C4-O3
3	A	278	PG4	C8-C7-O4-C6
3	A	279	PG4	C6-C5-O3-C4
3	A	277	PG4	C4-C3-O2-C2
3	D	278	PG4	C8-C7-O4-C6
3	A	278	PG4	O4-C7-C8-O5
3	A	278	PG4	C6-C5-O3-C4
3	A	277	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
3	D	277	PG4	C1-C2-O2-C3
3	A	277	PG4	C3-C4-O3-C5
3	A	279	PG4	C4-C3-O2-C2
3	A	278	PG4	C5-C6-O4-C7
3	D	278	PG4	C6-C5-O3-C4
3	B	277	PG4	C1-C2-O2-C3
3	B	277	PG4	C6-C5-O3-C4
3	A	278	PG4	O1-C1-C2-O2
3	B	277	PG4	C3-C4-O3-C5
3	A	277	PG4	C1-C2-O2-C3
3	D	277	PG4	C3-C4-O3-C5
3	B	277	PG4	O1-C1-C2-O2
3	D	278	PG4	O1-C1-C2-O2
3	D	277	PG4	O2-C3-C4-O3
3	B	277	PG4	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	278	PG4	2	0
3	A	277	PG4	5	0
3	D	278	PG4	2	0
3	A	279	PG4	3	0
3	B	277	PG4	2	0
3	D	277	PG4	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 (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	266/283 (93%)	-0.50	2 (0%)	86	84	12, 24, 45, 63	1 (0%)
1	B	260/283 (91%)	-0.45	2 (0%)	86	84	12, 25, 52, 75	1 (0%)
1	C	265/283 (93%)	-0.41	4 (1%)	73	70	16, 29, 47, 67	1 (0%)
1	D	257/283 (90%)	-0.27	5 (1%)	66	62	18, 32, 60, 74	1 (0%)
All	All	1048/1132 (92%)	-0.41	13 (1%)	79	76	12, 28, 54, 75	4 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	ASN	3.9
1	D	26	LEU	3.2
1	A	70	HIS	2.7
1	B	34	PRO	2.6
1	A	71	ASP	2.6
1	D	70	HIS	2.5
1	D	1	MET	2.5
1	C	36	ASP	2.4
1	C	70	HIS	2.4
1	D	252	ASN	2.1
1	C	27	THR	2.0
1	B	35	ASN	2.0
1	C	271	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, 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	PG4	A	278	13/13	0.70	0.27	65,70,73,73	0
3	PG4	B	277	10/13	0.73	0.26	55,60,67,67	0
3	PG4	D	278	13/13	0.81	0.24	57,63,67,68	0
3	PG4	A	277	13/13	0.83	0.23	64,68,76,76	0
3	PG4	D	277	10/13	0.84	0.20	44,52,55,56	0
3	PG4	A	279	13/13	0.84	0.23	55,66,70,71	0
2	PO4	C	276	5/5	0.98	0.08	28,32,33,34	0
2	PO4	B	276	5/5	0.99	0.08	23,26,28,28	0
2	PO4	D	276	5/5	0.99	0.07	26,26,28,30	0
2	PO4	A	276	5/5	1.00	0.06	19,20,20,21	0

6.5 Other polymers (i)

There are no such residues in this entry.