Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 03:24 PM EDT

PDB ID	:	2ABW
Title	:	Glutaminase subunit of the plasmodial PLP synthase (Vitamin B6 biosynthesis)
Authors	:	Gengenbacher, M.; Fitzpatrick, T.B.; Raschle, T.; Flicker, K.; Sinning, I.; Mueller, S.; Macheroux, P.; Tews, I.; Kappes, B.
Deposited on	:	2005-07-17
Resolution	:	1.62 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:

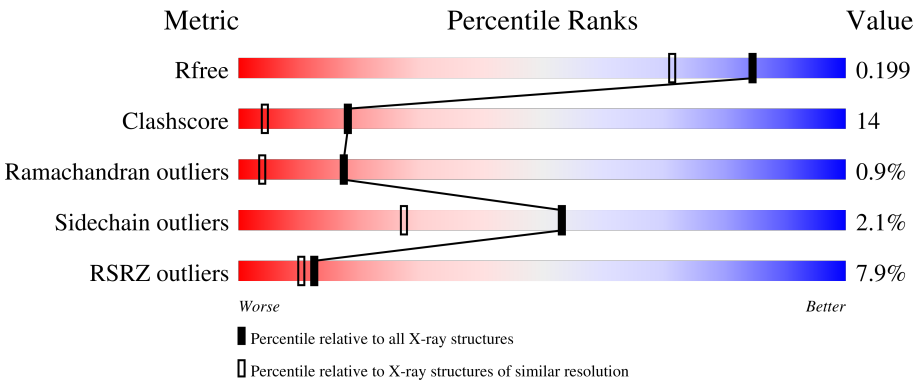
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.62 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	227	11% 80% 14% • 5%
1	B	227	4% 82% 16% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4130 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.

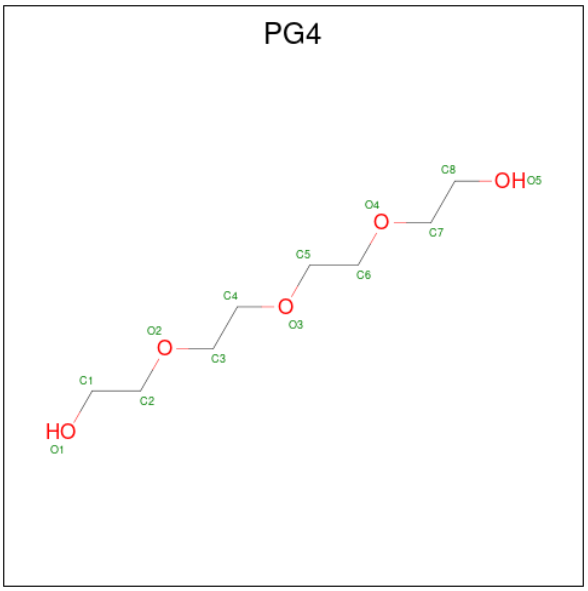
- Molecule 1 is a protein called Pdx2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1742	1118	290	323	11	0	16	0
1	B	226	1906	1215	328	353	10	0	21	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	LEU	-	expression tag	GB 56797978
A	221	GLU	-	expression tag	GB 56797978
A	222	HIS	-	expression tag	GB 56797978
A	223	HIS	-	expression tag	GB 56797978
A	224	HIS	-	expression tag	GB 56797978
A	225	HIS	-	expression tag	GB 56797978
A	226	HIS	-	expression tag	GB 56797978
A	227	HIS	-	expression tag	GB 56797978
B	220	LEU	-	expression tag	GB 56797978
B	221	GLU	-	expression tag	GB 56797978
B	222	HIS	-	expression tag	GB 56797978
B	223	HIS	-	expression tag	GB 56797978
B	224	HIS	-	expression tag	GB 56797978
B	225	HIS	-	expression tag	GB 56797978
B	226	HIS	-	expression tag	GB 56797978
B	227	HIS	-	expression tag	GB 56797978

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0

- Molecule 3 is water.

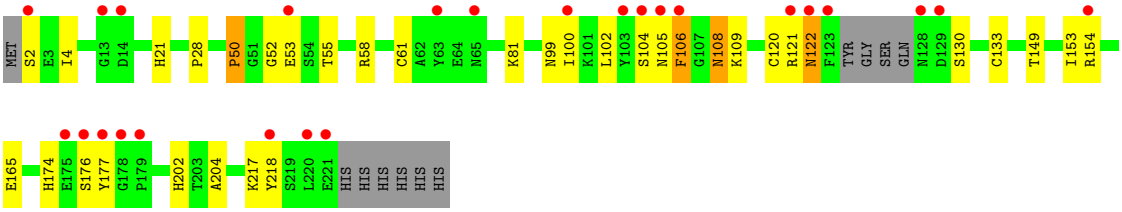
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	222	222	222	0	0
			Total	O		
3	B	247	247	247	0	0

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.

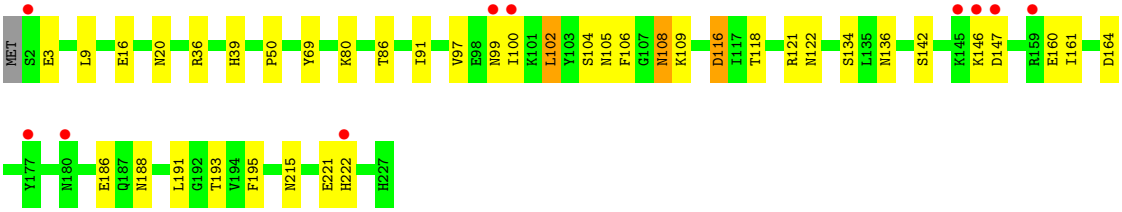
- Molecule 1: Pdx2 protein

Chain A:



- Molecule 1: Pdx2 protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.04Å 67.92Å 70.33Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	25.00 – 1.62 24.90 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-1.62) 99.9 (24.90-1.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.62Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.151 , 0.189 0.165 , 0.199	Depositor DCC
R_{free} test set	2676 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4130	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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

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	1.12	8/1834 (0.4%)	1.02	1/2485 (0.0%)
1	B	1.07	4/2014 (0.2%)	0.98	5/2727 (0.2%)
All	All	1.09	12/3848 (0.3%)	1.00	6/5212 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GLU	CB-CG	6.29	1.64	1.52
1	A	133	CYS	CB-SG	-6.23	1.71	1.82
1	A	120[A]	CYS	CB-SG	-6.19	1.71	1.82
1	A	120[B]	CYS	CB-SG	-6.19	1.71	1.82
1	B	16	GLU	CG-CD	6.13	1.61	1.51
1	B	116	ASP	CB-CG	5.78	1.63	1.51
1	B	69	TYR	CD1-CE1	5.37	1.47	1.39
1	A	218	TYR	CD1-CE1	5.32	1.47	1.39
1	A	61	CYS	CB-SG	-5.31	1.73	1.81
1	A	109	LYS	CE-NZ	5.29	1.62	1.49
1	A	81	LYS	CD-CE	-5.23	1.38	1.51
1	A	165	GLU	CG-CD	5.13	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	ASP	CB-CG-OD1	10.57	127.81	118.30
1	A	58	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	36	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	116	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	164	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	B	80	LYS	CD-CE-NZ	-5.08	100.02	111.70

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	1742	0	1710	27	0
1	B	1906	0	1846	68	0
2	A	13	0	18	0	0
3	A	222	0	0	16	1
3	B	247	0	0	31	2
All	All	4130	0	3574	99	2

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 14.

All (99) 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:39[B]:HIS:CD2	3:B:313:HOH:O	2.02	1.12
1:B:222:HIS:HB2	3:B:377:HOH:O	1.59	1.03
1:B:105[B]:ASN:HB3	3:B:350:HOH:O	1.59	1.01
1:B:9:LEU:HD23	3:B:422:HOH:O	1.60	1.01
1:B:104[B]:SER:OG	3:B:273:HOH:O	1.78	0.98
1:A:53:GLU:HG2	3:A:1275:HOH:O	1.64	0.97
1:B:186:GLU:HG3	3:B:453:HOH:O	1.66	0.95
1:A:106:PHE:HB2	3:A:1279:HOH:O	1.66	0.94
1:B:116:ASP:HB3	3:B:386:HOH:O	1.69	0.91
1:B:191:LEU:HB2	3:B:453:HOH:O	1.73	0.88
1:B:221[B]:GLU:HG3	1:B:222:HIS:O	1.73	0.88
1:A:153:ILE:HG23	3:A:1253:HOH:O	1.74	0.88
1:B:109[B]:LYS:HE2	3:B:282:HOH:O	1.75	0.85
1:B:193[B]:THR:OG1	1:B:195:PHE:CE2	2.34	0.79
1:B:121[B]:ARG:HD3	1:B:121[B]:ARG:H	1.49	0.77
1:B:97:VAL:HB	3:B:353:HOH:O	1.87	0.75
1:B:147:ASP:HA	3:B:433:HOH:O	1.87	0.75
1:B:102:LEU:HB2	1:B:121[B]:ARG:HH22	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:HB3	3:A:1253:HOH:O	1.88	0.73
1:B:222:HIS:HD2	3:B:449:HOH:O	1.72	0.71
1:A:202:HIS:HD2	1:A:204:ALA:H	1.39	0.69
1:B:136[B]:ASN:ND2	3:B:473:HOH:O	2.14	0.69
1:B:188:ASN:HB3	3:B:409:HOH:O	1.93	0.68
1:B:134[A]:SER:OG	3:B:433:HOH:O	2.10	0.68
1:B:121[B]:ARG:CG	1:B:121[B]:ARG:HH11	2.09	0.66
1:A:52:GLY:HA2	3:A:1314:HOH:O	1.95	0.65
1:B:222:HIS:CD2	3:B:449:HOH:O	2.46	0.65
1:A:99:ASN:HD22	1:A:122:ASN:CA	2.10	0.65
1:B:121[B]:ARG:HH11	1:B:121[B]:ARG:HG2	1.60	0.65
1:B:136[A]:ASN:OD1	3:B:420:HOH:O	2.14	0.64
1:B:91:ILE:HD13	1:B:121[A]:ARG:HD3	1.79	0.64
1:B:116:ASP:CB	3:B:386:HOH:O	2.35	0.63
1:B:106:PHE:HE2	3:B:298:HOH:O	1.82	0.61
1:A:55[B]:THR:HG23	3:A:1257:HOH:O	1.99	0.61
1:B:105[A]:ASN:HB3	3:B:350:HOH:O	1.99	0.61
1:B:193[B]:THR:OG1	1:B:195:PHE:CD2	2.54	0.61
1:A:108:ASN:C	1:A:108:ASN:HD22	2.04	0.60
1:B:118:THR:HB	1:B:160[B]:GLU:CG	2.33	0.59
1:A:105:ASN:OD1	1:A:106:PHE:CZ	2.57	0.58
1:B:109[B]:LYS:NZ	3:B:239:HOH:O	2.04	0.57
1:B:97:VAL:O	3:B:353:HOH:O	2.17	0.57
1:B:160[B]:GLU:CA	1:B:161:ILE:N	2.66	0.57
1:B:121[B]:ARG:HD3	1:B:121[B]:ARG:N	2.19	0.57
1:A:28[A]:PRO:O	3:A:1157:HOH:O	2.09	0.55
1:B:20:ASN:ND2	3:B:441:HOH:O	2.39	0.54
1:B:86:THR:OG1	1:B:193[B]:THR:CG2	2.55	0.54
1:B:121[A]:ARG:O	1:B:122[A]:ASN:C	2.45	0.54
1:B:99:ASN:ND2	1:B:122[A]:ASN:O	2.41	0.54
1:B:97:VAL:CG1	1:B:121[B]:ARG:CG	2.86	0.54
1:A:2[A]:SER:N	3:A:1269:HOH:O	2.39	0.54
1:A:4[A]:ILE:HD13	1:A:217:LYS:HD3	1.89	0.53
1:A:174:HIS:HD2	1:A:176:SER:O	1.92	0.53
1:B:118:THR:HB	1:B:160[B]:GLU:HG3	1.90	0.52
1:B:91:ILE:HD13	1:B:121[A]:ARG:CG	2.39	0.52
1:A:108:ASN:O	3:A:1270:HOH:O	2.19	0.51
1:B:121[A]:ARG:CZ	3:B:452:HOH:O	2.59	0.51
1:A:53:GLU:CG	3:A:1275:HOH:O	2.38	0.50
1:A:4[A]:ILE:HD13	1:A:217:LYS:CD	2.41	0.50
1:A:153:ILE:O	1:A:154:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4[A]:ILE:CD1	1:A:217:LYS:HD3	2.41	0.50
1:B:86:THR:OG1	1:B:193[B]:THR:HG23	2.11	0.50
1:B:146:LYS:HG2	1:B:147:ASP:CG	2.32	0.49
1:A:149:THR:O	1:A:202:HIS:HE1	1.95	0.49
1:B:102:LEU:HB2	1:B:121[B]:ARG:NH2	2.25	0.49
1:A:100[A]:ILE:O	1:A:102:LEU:N	2.45	0.49
1:B:91:ILE:HD13	1:B:121[A]:ARG:CD	2.43	0.49
1:B:108:ASN:C	1:B:108:ASN:HD22	2.16	0.49
1:B:215:ASN:ND2	3:B:400:HOH:O	2.39	0.48
1:B:121[B]:ARG:HG2	1:B:121[B]:ARG:NH1	2.27	0.48
1:B:146:LYS:HG2	1:B:147:ASP:OD1	2.14	0.48
1:A:130:SER:CB	3:A:1253:HOH:O	2.53	0.47
1:B:118:THR:HB	1:B:160[B]:GLU:HG2	1.95	0.47
1:B:121[B]:ARG:HH11	1:B:121[B]:ARG:CB	2.26	0.47
1:B:109[B]:LYS:CE	3:B:239:HOH:O	2.57	0.47
1:A:28[B]:PRO:HA	3:A:1157:HOH:O	2.15	0.47
1:B:121[B]:ARG:CD	1:B:121[B]:ARG:N	2.77	0.47
1:B:105[A]:ASN:HB3	3:B:382:HOH:O	2.15	0.47
1:B:142:SER:CB	3:B:467:HOH:O	2.64	0.46
1:A:105:ASN:OD1	1:A:106:PHE:CE2	2.69	0.46
1:A:99:ASN:ND2	1:A:122:ASN:CA	2.77	0.45
1:B:191:LEU:CA	3:B:453:HOH:O	2.66	0.43
1:B:100:ILE:HG22	1:B:121[B]:ARG:NH2	2.33	0.43
1:A:55[B]:THR:HG21	1:A:102:LEU:HD12	2.00	0.43
1:B:100:ILE:HB	1:B:121[B]:ARG:CZ	2.49	0.43
1:B:100:ILE:C	1:B:121[B]:ARG:HH21	2.23	0.42
1:B:97:VAL:CG1	1:B:121[B]:ARG:HG2	2.49	0.42
1:B:109[B]:LYS:NZ	3:B:247:HOH:O	2.03	0.42
1:B:142:SER:HB2	3:B:467:HOH:O	2.20	0.42
1:B:91:ILE:HD13	1:B:121[A]:ARG:HG2	2.01	0.41
1:B:97:VAL:HG13	1:B:121[B]:ARG:CG	2.50	0.41
1:B:97:VAL:HG12	1:B:121[B]:ARG:CD	2.51	0.40

All (2) 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)
3:B:468:HOH:O	3:B:468:HOH:O[2_556]	1.97	0.23
3:A:1202:HOH:O	3:B:382:HOH:O[4_556]	2.13	0.07

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	227/227 (100%)	216 (95%)	8 (4%)	3 (1%)	12 2
1	B	245/227 (108%)	235 (96%)	9 (4%)	1 (0%)	34 15
All	All	472/454 (104%)	451 (96%)	17 (4%)	4 (1%)	17 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	A	122	ASN
1	B	50	PRO
1	A	50	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	204/202 (101%)	198 (97%)	6 (3%)	42 16
1	B	222/202 (110%)	220 (99%)	2 (1%)	78 64
All	All	426/404 (105%)	418 (98%)	8 (2%)	53 32

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	50	PRO

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Mol	Chain	Res	Type
1	A	104	SER
1	A	106	PHE
1	A	108	ASN
1	A	121	ARG
1	B	102	LEU
1	B	108	ASN

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	108	ASN
1	A	174	HIS
1	A	202	HIS
1	B	96	ASN
1	B	108	ASN
1	B	127	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)

1 ligand is 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	PG4	A	1101	-	12,12,12	0.54	0	11,11,11	0.59	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	PG4	A	1101	-	-	0/10/10/10	-

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 (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	216/227 (95%)	0.35	25 (11%)	4	3	14, 19, 42, 52	0
1	B	226/227 (99%)	0.30	10 (4%)	34	30	16, 24, 35, 43	0
All	All	442/454 (97%)	0.33	35 (7%)	12	10	14, 22, 39, 52	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	TYR	7.7
1	A	176	SER	7.2
1	A	123	PHE	6.7
1	B	146	LYS	5.3
1	A	105	ASN	5.3
1	B	147	ASP	4.3
1	B	99	ASN	4.0
1	A	221	GLU	3.9
1	A	128	ASN	3.9
1	A	106	PHE	3.9
1	B	222	HIS	3.7
1	A	154	ARG	3.7
1	A	175	GLU	3.7
1	B	2	SER	3.5
1	A	122	ASN	3.5
1	A	220	LEU	3.2
1	A	129	ASP	3.2
1	A	63	TYR	3.0
1	B	100	ILE	3.0
1	B	177	TYR	3.0
1	A	14	ASP	2.7
1	A	103	TYR	2.7
1	A	178	GLY	2.7
1	A	218	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	104	SER	2.6
1	A	13	GLY	2.5
1	A	100[A]	ILE	2.5
1	A	53	GLU	2.4
1	A	121	ARG	2.3
1	A	2[A]	SER	2.3
1	B	180[A]	ASN	2.3
1	B	159[A]	ARG	2.1
1	A	179	PRO	2.1
1	B	145	LYS	2.0
1	A	65	ASN	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
2	PG4	A	1101	13/13	0.94	0.11	23,27,43,45	0

6.5 Other polymers (i)

There are no such residues in this entry.