



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2024 – 02:20 PM EDT

PDB ID : 8UP6
Title : Structure of atypical asparaginase from *Rhodospirillum rubrum* (mutant K19A) in complex with L-Asp
Authors : Lubkowski, J.; Wlodawer, A.; Zhang, D.
Deposited on : 2023-10-21
Resolution : 1.70 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
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

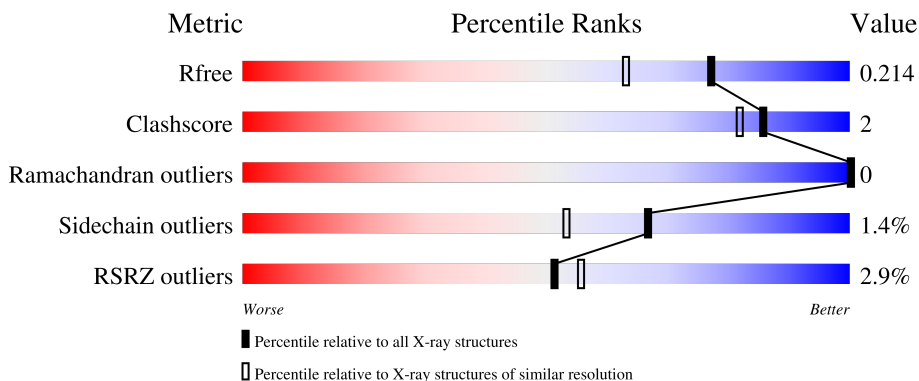
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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	185	 5% 86% 5% • 8%
1	B	185	 2% 83% 5% 12%
1	C	185	 85% • • 11%
1	D	185	 4% 86% 5% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5340 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 Asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	170	1248	788	219	235	6	0	1	0
1	B	163	1202	761	212	224	5	0	1	0
1	C	164	1208	765	213	225	5	0	1	0
1	D	169	1241	785	218	232	6	0	1	0

There are 56 discrepancies between the modelled and reference sequences:

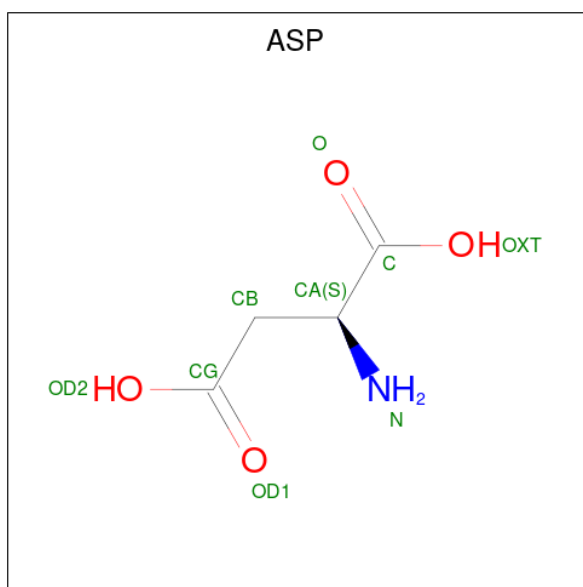
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q2RMX1
A	-11	HIS	-	expression tag	UNP Q2RMX1
A	-10	HIS	-	expression tag	UNP Q2RMX1
A	-9	HIS	-	expression tag	UNP Q2RMX1
A	-8	HIS	-	expression tag	UNP Q2RMX1
A	-7	HIS	-	expression tag	UNP Q2RMX1
A	-6	GLU	-	expression tag	UNP Q2RMX1
A	-5	ASN	-	expression tag	UNP Q2RMX1
A	-4	LEU	-	expression tag	UNP Q2RMX1
A	-3	TYR	-	expression tag	UNP Q2RMX1
A	-2	PHE	-	expression tag	UNP Q2RMX1
A	-1	GLN	-	expression tag	UNP Q2RMX1
A	0	SER	-	expression tag	UNP Q2RMX1
A	19	ALA	LYS	engineered mutation	UNP Q2RMX1
B	-12	HIS	-	expression tag	UNP Q2RMX1
B	-11	HIS	-	expression tag	UNP Q2RMX1
B	-10	HIS	-	expression tag	UNP Q2RMX1
B	-9	HIS	-	expression tag	UNP Q2RMX1
B	-8	HIS	-	expression tag	UNP Q2RMX1
B	-7	HIS	-	expression tag	UNP Q2RMX1
B	-6	GLU	-	expression tag	UNP Q2RMX1

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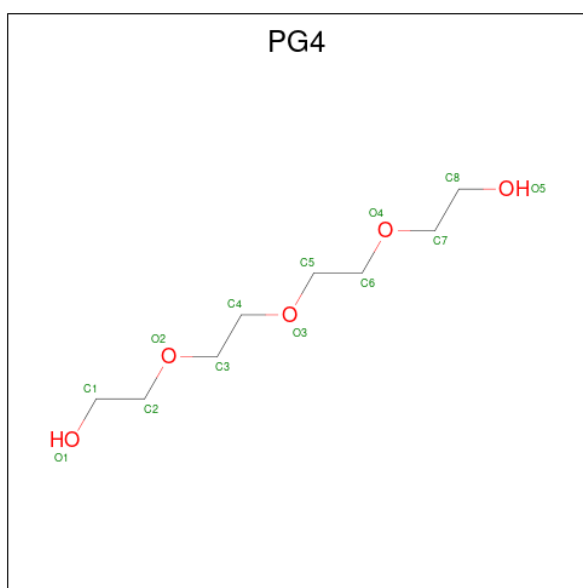
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ASN	-	expression tag	UNP Q2RMX1
B	-4	LEU	-	expression tag	UNP Q2RMX1
B	-3	TYR	-	expression tag	UNP Q2RMX1
B	-2	PHE	-	expression tag	UNP Q2RMX1
B	-1	GLN	-	expression tag	UNP Q2RMX1
B	0	SER	-	expression tag	UNP Q2RMX1
B	19	ALA	LYS	engineered mutation	UNP Q2RMX1
C	-12	HIS	-	expression tag	UNP Q2RMX1
C	-11	HIS	-	expression tag	UNP Q2RMX1
C	-10	HIS	-	expression tag	UNP Q2RMX1
C	-9	HIS	-	expression tag	UNP Q2RMX1
C	-8	HIS	-	expression tag	UNP Q2RMX1
C	-7	HIS	-	expression tag	UNP Q2RMX1
C	-6	GLU	-	expression tag	UNP Q2RMX1
C	-5	ASN	-	expression tag	UNP Q2RMX1
C	-4	LEU	-	expression tag	UNP Q2RMX1
C	-3	TYR	-	expression tag	UNP Q2RMX1
C	-2	PHE	-	expression tag	UNP Q2RMX1
C	-1	GLN	-	expression tag	UNP Q2RMX1
C	0	SER	-	expression tag	UNP Q2RMX1
C	19	ALA	LYS	engineered mutation	UNP Q2RMX1
D	-12	HIS	-	expression tag	UNP Q2RMX1
D	-11	HIS	-	expression tag	UNP Q2RMX1
D	-10	HIS	-	expression tag	UNP Q2RMX1
D	-9	HIS	-	expression tag	UNP Q2RMX1
D	-8	HIS	-	expression tag	UNP Q2RMX1
D	-7	HIS	-	expression tag	UNP Q2RMX1
D	-6	GLU	-	expression tag	UNP Q2RMX1
D	-5	ASN	-	expression tag	UNP Q2RMX1
D	-4	LEU	-	expression tag	UNP Q2RMX1
D	-3	TYR	-	expression tag	UNP Q2RMX1
D	-2	PHE	-	expression tag	UNP Q2RMX1
D	-1	GLN	-	expression tag	UNP Q2RMX1
D	0	SER	-	expression tag	UNP Q2RMX1
D	19	ALA	LYS	engineered mutation	UNP Q2RMX1

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	101	Total	O	0	0
			101	101		
4	C	91	Total	O	0	0
			91	91		
4	D	106	Total	O	0	0
			106	106		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.05Å 77.33Å 115.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.89 – 1.70 38.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.89-1.70) 99.3 (38.86-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.181 , 0.205 0.193 , 0.214	Depositor DCC
R_{free} test set	1431 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5340	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8622e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.75	0/1272	0.95	2/1723 (0.1%)
1	B	0.82	0/1224	0.90	0/1657
1	C	0.80	2/1232 (0.2%)	0.93	3/1668 (0.2%)
1	D	0.75	0/1264	0.94	1/1712 (0.1%)
All	All	0.78	2/4992 (0.0%)	0.93	6/6760 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	102	GLU	CD-OE1	5.54	1.31	1.25
1	C	92	GLU	CD-OE2	5.46	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	43	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	9	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	43	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	55	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	55	ARG	CG-CD-NE	-5.05	101.20	111.80

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	1248	0	1269	4	0
1	B	1202	0	1226	7	0
1	C	1208	0	1230	3	0
1	D	1241	0	1269	4	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
3	B	26	0	36	2	0
3	D	13	0	18	3	0
4	A	86	0	0	1	0
4	B	101	0	0	2	0
4	C	91	0	0	2	0
4	D	106	0	0	3	0
All	All	5340	0	5054	22	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 2.

All (22) 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:A:163:GLY:HA3	1:D:23:LEU:HD23	1.69	0.74
1:D:71:ARG:O	1:D:75:GLN:HG3	1.88	0.72
3:D:201:PG4:C2	4:D:391:HOH:O	2.42	0.68
1:C:37:GLU:OE2	4:C:301:HOH:O	2.13	0.66
1:A:24:GLU:HG3	4:A:242:HOH:O	1.97	0.64
3:D:201:PG4:H21	4:D:391:HOH:O	1.98	0.62
3:D:201:PG4:H22	4:D:391:HOH:O	2.07	0.53
1:D:57:ASP:HB2	1:D:60:ASP:OD2	2.09	0.53
1:B:38:VAL:HG21	1:B:128[A]:ILE:HD12	1.90	0.52
1:B:157:ARG:HD2	4:B:322:HOH:O	2.08	0.52
3:B:202:PG4:H21	4:B:385:HOH:O	2.09	0.52
3:B:202:PG4:H12	3:B:203:PG4:O5	2.10	0.52
1:A:57:ASP:HB2	1:A:60:ASP:OD2	2.15	0.47
1:C:25:GLU:HG3	1:C:29:VAL:CG1	2.46	0.45
1:B:9:ARG:HH11	1:B:9:ARG:HG2	1.82	0.45
1:B:101:PRO:HD2	1:B:102:GLU:OE1	2.16	0.44
1:B:89:THR:HA	1:B:92:GLU:OE2	2.19	0.42
1:A:62:THR:OG1	1:A:64:ALA:HB3	2.20	0.42
1:C:102:GLU:HG2	4:C:353:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASP:OD1	1:B:152:ASP:C	2.59	0.41
1:D:157:ARG:NE	1:D:166:GLU:OE1	2.51	0.41
1:B:38:VAL:HG21	1:B:128[A]:ILE:CD1	2.52	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	169/185 (91%)	169 (100%)	0	0	100	100
1	B	162/185 (88%)	162 (100%)	0	0	100	100
1	C	163/185 (88%)	162 (99%)	1 (1%)	0	100	100
1	D	168/185 (91%)	167 (99%)	1 (1%)	0	100	100
All	All	662/740 (90%)	660 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	127/141 (90%)	122 (96%)	5 (4%)	32	13
1	B	121/141 (86%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	122/141 (86%)	121 (99%)	1 (1%)	81	74
1	D	126/141 (89%)	125 (99%)	1 (1%)	81	74
All	All	496/564 (88%)	489 (99%)	7 (1%)	67	53

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	40	LYS
1	A	57	ASP
1	A	166	GLU
1	A	169	ASP
1	C	102	GLU
1	D	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

5 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	ASP	B	201	-	6,8,8	1.24	1 (16%)	8,10,10	1.73	2 (25%)
2	ASP	C	200	-	6,8,8	0.97	0	8,10,10	1.22	0
3	PG4	B	203	-	12,12,12	0.33	0	11,11,11	0.26	0
3	PG4	B	202	-	12,12,12	0.22	0	11,11,11	0.32	0
3	PG4	D	201	-	12,12,12	0.20	0	11,11,11	0.56	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	ASP	B	201	-	-	2/8/8/8	-
2	ASP	C	200	-	-	2/8/8/8	-
3	PG4	B	203	-	-	5/10/10/10	-
3	PG4	B	202	-	-	3/10/10/10	-
3	PG4	D	201	-	-	6/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	ASP	OD1-CG	2.20	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	ASP	OXT-C-CA	2.92	123.33	113.38
2	B	201	ASP	OXT-C-O	-2.81	117.72	124.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	ASP	O-C-CA-N
2	C	200	ASP	O-C-CA-N
2	B	201	ASP	OXT-C-CA-N
3	B	203	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
2	C	200	ASP	OXT-C-CA-N
3	B	203	PG4	O1-C1-C2-O2
3	D	201	PG4	O1-C1-C2-O2
3	D	201	PG4	O4-C7-C8-O5
3	B	202	PG4	O2-C3-C4-O3
3	B	202	PG4	O1-C1-C2-O2
3	B	202	PG4	C4-C3-O2-C2
3	B	203	PG4	C5-C6-O4-C7
3	D	201	PG4	C5-C6-O4-C7
3	D	201	PG4	C8-C7-O4-C6
3	D	201	PG4	O3-C5-C6-O4
3	B	203	PG4	C3-C4-O3-C5
3	D	201	PG4	C4-C3-O2-C2
3	B	203	PG4	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	PG4	1	0
3	B	202	PG4	2	0
3	D	201	PG4	3	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

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, 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	170/185 (91%)	0.19	9 (5%) 26 29	6, 18, 43, 58	0
1	B	163/185 (88%)	-0.01	3 (1%) 68 72	5, 14, 36, 47	0
1	C	164/185 (88%)	-0.05	0 100 100	5, 13, 31, 42	0
1	D	169/185 (91%)	0.10	7 (4%) 37 41	5, 15, 44, 55	0
All	All	666/740 (90%)	0.06	19 (2%) 51 56	5, 15, 40, 58	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	3.9
1	D	59	LEU	3.4
1	A	169	ASP	3.0
1	D	63	GLU	3.0
1	A	59	LEU	3.0
1	A	160	ARG	2.9
1	A	60	ASP	2.9
1	D	62	THR	2.9
1	B	57	ASP	2.8
1	A	1	MET	2.8
1	A	0	SER	2.7
1	A	57	ASP	2.5
1	B	59	LEU	2.5
1	D	24	GLU	2.4
1	A	62	THR	2.4
1	D	58	SER	2.2
1	B	168	ILE	2.2
1	D	57	ASP	2.1
1	D	160	ARG	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	B	203	13/13	0.69	0.21	38,46,50,51	0
3	PG4	B	202	13/13	0.88	0.17	25,38,47,48	0
3	PG4	D	201	13/13	0.90	0.17	23,36,47,51	0
2	ASP	B	201	9/9	0.92	0.18	19,25,31,37	0
2	ASP	C	200	9/9	0.96	0.14	18,20,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.