



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:38 PM UTC

PDB ID : 8UOW / pdb_00008uow
Title : Structure of atypical asparaginase from *Rhodospirillum rubrum* (mutant Y21A)
Authors : Lubkowski, J.; Wlodawer, A.; Zhang, D.
Deposited on : 2023-10-20
Resolution : 1.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

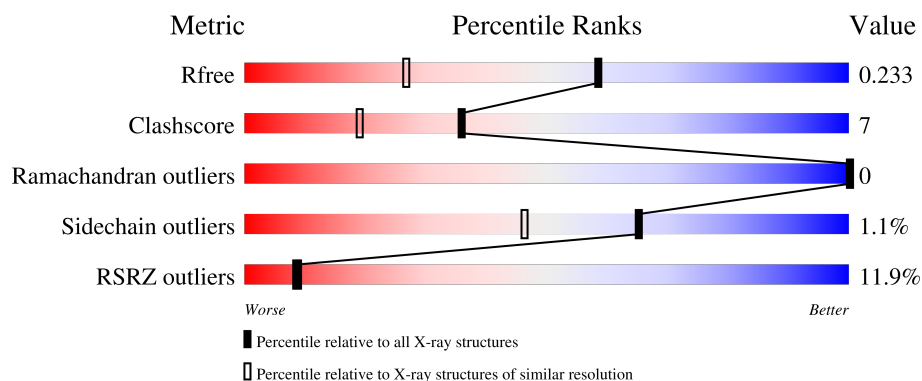
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	15% 79% 10% 11%
1	B	185	7% 77% 9% 14%
1	C	185	8% 81% 5% 14%
1	D	185	12% 84% 6% 10%

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
2	EPE	A	201	-	X	X	-
2	EPE	B	201	-	-	X	-
2	EPE	C	201	-	X	X	-
2	EPE	D	201	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5401 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
1	A	165	Total	C	N	O	S	0	2	0
			1209	766	214	222	7			
1	B	159	Total	C	N	O	S	0	1	0
			1165	738	208	214	5			
1	C	159	Total	C	N	O	S	0	1	0
			1165	738	208	214	5			
1	D	166	Total	C	N	O	S	0	1	0
			1209	765	215	223	6			

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	21	ALA	TYR	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	21	ALA	TYR	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	21	ALA	TYR	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	21	ALA	TYR	engineered mutation	UNP Q2RMX1

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

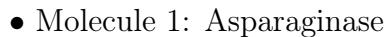
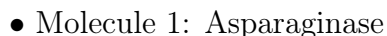
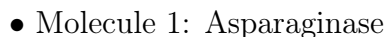


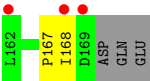
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			8	3	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			8	3	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			8	3	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			8	3	1	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	1
			153	153		
3	B	156	Total	O	0	3
			159	159		
3	C	155	Total	O	0	1
			156	156		
3	D	153	Total	O	0	0
			153	153		

- Molecule 1: Asparaginase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.83Å 77.12Å 114.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 1.60 38.80 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.80-1.60) 98.4 (38.80-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.186 , 0.221 0.198 , 0.233	Depositor DCC
R_{free} test set	2582 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5401	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.67 % 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 3.0569e-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: EPE

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	1.17	1/1233 (0.1%)	1.29	1/1666 (0.1%)
1	B	1.17	2/1185 (0.2%)	1.29	3/1601 (0.2%)
1	C	1.15	0/1185	1.27	1/1601 (0.1%)
1	D	1.10	0/1230	1.28	2/1663 (0.1%)
All	All	1.15	3/4833 (0.1%)	1.28	7/6531 (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	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	PRO	C-O	-5.77	1.16	1.24
1	A	45	ALA	C-O	5.72	1.30	1.24
1	B	92	GLU	C-O	5.07	1.29	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	HIS	CA-CB-CG	7.06	120.86	113.80
1	A	85	HIS	CA-CB-CG	6.96	120.76	113.80
1	B	123	ASP	CA-CB-CG	6.41	119.01	112.60
1	B	85	HIS	CA-CB-CG	5.86	119.66	113.80
1	C	85	HIS	CA-CB-CG	5.57	119.37	113.80
1	B	16	THR	CA-CB-OG1	-5.43	101.45	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	ASP	CA-CB-CG	5.12	117.72	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	167	PRO	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	1209	0	1252	24	0
1	B	1165	0	1200	20	0
1	C	1165	0	1200	14	0
1	D	1209	0	1245	18	0
2	A	8	0	5	8	0
2	B	8	0	5	10	0
2	C	8	0	5	10	0
2	D	8	0	5	13	0
3	A	153	0	0	3	0
3	B	159	0	0	0	0
3	C	156	0	0	0	0
3	D	153	0	0	0	0
All	All	5401	0	4917	71	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 7.

All (71) 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:D:87:THR:H	2:D:201:EPE:H92	1.25	0.98
1:A:87:THR:H	2:A:201:EPE:H92	1.26	0.97
1:D:87:THR:H	2:D:201:EPE:C9	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:THR:H	2:D:201:EPE:H101	1.33	0.92
1:A:21:ALA:HB2	1:A:28:LEU:CD2	1.99	0.91
1:D:16:THR:H	2:D:201:EPE:C10	1.91	0.84
1:D:87:THR:N	2:D:201:EPE:H92	1.93	0.83
1:C:87:THR:H	2:C:201:EPE:H92	1.45	0.82
1:D:16:THR:OG1	2:D:201:EPE:H102	1.80	0.81
1:B:21:ALA:HB2	1:B:28:LEU:HD23	1.60	0.80
1:C:16:THR:H	2:C:201:EPE:C10	1.96	0.77
1:A:87:THR:H	2:A:201:EPE:C9	1.99	0.75
1:A:87:THR:N	2:A:201:EPE:H92	2.00	0.74
1:A:16:THR:OG1	2:A:201:EPE:H102	1.88	0.74
1:A:16:THR:H	2:A:201:EPE:C10	2.00	0.74
1:A:16:THR:H	2:A:201:EPE:H101	1.52	0.74
1:A:19:LYS:HB3	1:A:28:LEU:HB3	1.70	0.72
1:B:21:ALA:HB2	1:B:28:LEU:CD2	2.19	0.71
1:B:16:THR:H	2:B:201:EPE:C10	2.04	0.70
1:A:21:ALA:HB2	1:A:28:LEU:HD21	1.74	0.69
1:D:86:GLY:HA2	2:D:201:EPE:H92	1.74	0.69
1:A:146[B]:MET:HA	1:A:146[B]:MET:HE2	1.75	0.69
1:B:28:LEU:HG	1:C:28:LEU:HG	1.76	0.68
1:B:28:LEU:HD13	1:B:116:PRO:HG2	1.75	0.68
1:B:87:THR:H	2:B:201:EPE:H92	1.58	0.67
1:C:19:LYS:HB3	1:C:28:LEU:HB3	1.77	0.66
1:C:16:THR:H	2:C:201:EPE:H101	1.62	0.64
1:D:16:THR:N	2:D:201:EPE:H101	2.09	0.63
1:C:87:THR:H	2:C:201:EPE:C9	2.12	0.61
1:B:16:THR:H	2:B:201:EPE:H102	1.66	0.60
1:C:16:THR:H	2:C:201:EPE:H102	1.65	0.60
1:A:57:ASP:HB2	3:A:327:HOH:O	2.02	0.60
1:A:92:GLU:HG2	3:A:396:HOH:O	2.02	0.59
1:D:87:THR:H	2:D:201:EPE:H91	1.67	0.59
1:C:16:THR:OG1	2:C:201:EPE:H102	2.02	0.59
1:B:87:THR:H	2:B:201:EPE:C9	2.16	0.59
1:B:19:LYS:HB3	1:B:28:LEU:HB3	1.84	0.58
1:B:86:GLY:HA2	2:B:201:EPE:H101	1.86	0.58
1:A:28:LEU:CD1	1:A:116:PRO:HG2	2.36	0.55
1:D:86:GLY:CA	2:D:201:EPE:H92	2.36	0.54
1:B:16:THR:OG1	2:B:201:EPE:H102	2.07	0.54
1:A:146[B]:MET:HE2	1:A:146[B]:MET:CA	2.37	0.54
1:B:16:THR:N	2:B:201:EPE:H102	2.23	0.53
1:B:28:LEU:CD1	1:B:116:PRO:HG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:THR:N	2:C:201:EPE:H102	2.24	0.53
1:A:16:THR:H	2:A:201:EPE:H102	1.75	0.52
1:B:10:ILE:CD1	1:B:39:LEU:HD11	2.40	0.52
1:B:16:THR:H	2:B:201:EPE:H101	1.73	0.51
1:D:102:GLU:H	1:D:102:GLU:CD	2.18	0.50
1:A:28:LEU:HD12	1:A:116:PRO:HG2	1.93	0.50
1:C:157:ARG:NE	1:C:166:GLU:OE1	2.46	0.47
1:D:16:THR:HB	2:D:201:EPE:N1	2.33	0.44
1:B:87:THR:OG1	2:B:201:EPE:C6	2.65	0.44
1:C:87:THR:N	2:C:201:EPE:H92	2.22	0.44
1:A:28:LEU:HD21	1:D:28:LEU:HD11	1.98	0.44
1:A:86:GLY:HA2	2:A:201:EPE:H101	1.99	0.43
1:A:28:LEU:HG	1:D:28:LEU:HG	2.01	0.43
1:A:33:PRO:HG3	3:A:411:HOH:O	2.18	0.43
1:A:163:GLY:O	1:B:43:ARG:NH1	2.48	0.43
1:C:86:GLY:HA2	2:C:201:EPE:H101	2.00	0.43
1:D:152:ASP:OD1	1:D:152:ASP:C	2.62	0.43
1:D:15:GLY:HA2	2:D:201:EPE:H101	2.01	0.43
1:B:38:VAL:HG21	1:B:128[A]:ILE:HD12	2.02	0.42
1:C:16:THR:N	2:C:201:EPE:C10	2.73	0.42
1:A:28:LEU:HD11	1:D:28:LEU:HD21	2.02	0.41
1:C:159:ASN:HD22	1:C:166:GLU:CD	2.28	0.41
1:A:145:ALA:O	1:A:146[B]:MET:HE2	2.19	0.41
1:A:152:ASP:OD1	1:A:152:ASP:C	2.61	0.41
1:B:86:GLY:CA	2:B:201:EPE:H101	2.49	0.41
1:B:152:ASP:OD1	1:B:152:ASP:C	2.64	0.40
1:D:16:THR:N	2:D:201:EPE:C10	2.71	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	163/185 (88%)	163 (100%)	0	0	100	100
1	B	156/185 (84%)	156 (100%)	0	0	100	100
1	C	156/185 (84%)	156 (100%)	0	0	100	100
1	D	163/185 (88%)	162 (99%)	1 (1%)	0	100	100
All	All	638/740 (86%)	637 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	123/141 (87%)	120 (98%)	3 (2%)	43	19
1	B	117/141 (83%)	117 (100%)	0	100	100
1	C	117/141 (83%)	116 (99%)	1 (1%)	70	55
1	D	122/141 (86%)	121 (99%)	1 (1%)	73	59
All	All	479/564 (85%)	474 (99%)	5 (1%)	65	50

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	67	GLU
1	A	166	GLU
1	C	102	GLU
1	D	168	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	EPE	D	201	-	7,7,15	3.82	2 (28%)	8,9,20	3.32	2 (25%)
2	EPE	C	201	-	7,7,15	4.41	1 (14%)	8,9,20	2.32	5 (62%)
2	EPE	A	201	-	7,7,15	4.27	1 (14%)	8,9,20	2.79	4 (50%)
2	EPE	B	201	-	7,7,15	4.27	1 (14%)	8,9,20	2.67	4 (50%)

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	EPE	D	201	-	-	3/5/5/19	-
2	EPE	C	201	-	-	4/5/5/19	-
2	EPE	A	201	-	-	4/5/5/19	-
2	EPE	B	201	-	-	2/5/5/19	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	EPE	C10-S	-11.50	1.61	1.77
2	B	201	EPE	C10-S	-11.07	1.62	1.77
2	A	201	EPE	C10-S	-10.97	1.62	1.77
2	D	201	EPE	C10-S	-9.63	1.64	1.77
2	D	201	EPE	O1S-S	2.29	1.51	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	EPE	C10-C9-N1	7.90	133.96	111.40
2	A	201	EPE	C6-N1-C9	-4.83	98.54	112.01
2	B	201	EPE	C6-N1-C9	-4.45	99.61	112.01
2	D	201	EPE	O2S-S-C10	4.06	112.87	106.73
2	A	201	EPE	C10-C9-N1	3.79	122.23	111.40
2	A	201	EPE	O2S-S-C10	3.61	112.18	106.73
2	B	201	EPE	C10-C9-N1	3.54	121.51	111.40
2	C	201	EPE	C10-C9-N1	3.43	121.18	111.40
2	B	201	EPE	O3S-S-O2S	-3.21	103.36	111.40
2	C	201	EPE	O3S-S-C10	2.85	111.58	106.00
2	C	201	EPE	O3S-S-O2S	-2.81	104.36	111.40
2	A	201	EPE	O2S-S-O1S	-2.57	105.47	113.82
2	C	201	EPE	O1S-S-C10	2.56	110.59	106.73
2	C	201	EPE	C6-N1-C9	-2.44	105.23	112.01
2	B	201	EPE	O1S-S-C10	2.29	110.18	106.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	EPE	C10-C9-N1-C6
2	A	201	EPE	C9-C10-S-O2S
2	B	201	EPE	C10-C9-N1-C6
2	C	201	EPE	C10-C9-N1-C6
2	D	201	EPE	C9-C10-S-O1S
2	D	201	EPE	C9-C10-S-O3S
2	A	201	EPE	C9-C10-S-O3S
2	C	201	EPE	C9-C10-S-O3S
2	A	201	EPE	C9-C10-S-O1S
2	D	201	EPE	C9-C10-S-O2S
2	B	201	EPE	C9-C10-S-O3S
2	C	201	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
2	C	201	EPE	C9-C10-S-O2S

There are no ring outliers.

4 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	EPE	13	0
2	C	201	EPE	10	0
2	A	201	EPE	8	0
2	B	201	EPE	10	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	165/185 (89%)	0.76	27 (16%) 4 4	4, 17, 40, 58	2 (1%)
1	B	159/185 (85%)	0.28	13 (8%) 17 17	3, 13, 32, 53	1 (0%)
1	C	159/185 (85%)	0.30	15 (9%) 14 14	3, 13, 32, 55	1 (0%)
1	D	166/185 (89%)	0.55	22 (13%) 7 7	3, 16, 39, 53	1 (0%)
All	All	649/740 (87%)	0.48	77 (11%) 9 8	3, 15, 37, 58	5 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	5.6
1	A	28	LEU	5.5
1	C	162	LEU	4.5
1	B	28	LEU	4.5
1	D	168	ILE	4.3
1	A	29	VAL	3.9
1	A	168	ILE	3.9
1	B	162	LEU	3.9
1	A	27	GLY	3.7
1	D	169	ASP	3.7
1	B	21	ALA	3.6
1	C	21	ALA	3.5
1	D	59	LEU	3.4
1	B	22	ARG	3.4
1	C	161	GLY	3.3
1	A	59	LEU	3.3
1	D	62	THR	3.2
1	D	101	PRO	3.2
1	D	67	GLU	3.2
1	B	29	VAL	3.2
1	D	21	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	62	THR	3.1
1	C	168	ILE	3.1
1	C	22	ARG	3.0
1	B	168	ILE	3.0
1	A	101	PRO	2.9
1	C	102	GLU	2.9
1	A	30	VAL	2.9
1	D	71	ARG	2.9
1	A	161	GLY	2.9
1	C	160	ARG	2.9
1	B	47	ALA	2.8
1	B	161	GLY	2.8
1	C	27	GLY	2.8
1	B	27	GLY	2.8
1	D	162	LEU	2.8
1	D	161	GLY	2.8
1	A	77	VAL	2.8
1	C	29	VAL	2.8
1	D	28	LEU	2.7
1	B	160	ARG	2.7
1	A	61	PHE	2.7
1	A	160	ARG	2.7
1	A	0	SER	2.7
1	A	32	ASP	2.7
1	D	57	ASP	2.7
1	A	167	PRO	2.6
1	A	60	ASP	2.6
1	A	73	VAL	2.6
1	A	162	LEU	2.6
1	C	6	SER	2.6
1	D	64	ALA	2.6
1	A	96	TYR	2.5
1	B	101	PRO	2.5
1	A	58	SER	2.5
1	A	1	MET	2.4
1	D	96	TYR	2.4
1	B	102	GLU	2.4
1	C	47	ALA	2.3
1	B	6	SER	2.3
1	D	0	SER	2.3
1	D	160	ARG	2.3
1	A	57	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	63	GLU	2.2
1	C	159	ASN	2.2
1	C	163	GLY	2.2
1	D	30	VAL	2.1
1	A	154	ALA	2.1
1	A	71	ARG	2.1
1	A	67	GLU	2.1
1	A	76	ALA	2.1
1	D	29	VAL	2.1
1	D	32	ASP	2.1
1	A	100	LEU	2.1
1	D	61	PHE	2.1
1	C	77	VAL	2.0
1	D	92	GLU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	EPE	A	201	8/15	0.90	0.12	22,22,24,29	8
2	EPE	D	201	8/15	0.90	0.12	17,19,22,25	8
2	EPE	C	201	8/15	0.91	0.14	19,22,23,28	8
2	EPE	B	201	8/15	0.92	0.13	15,18,20,23	8

6.5 Other polymers [i](#)

There are no such residues in this entry.