



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 01:00 PM BST

PDB ID : 3UNV
Title : Pantoea agglomerans Phenylalanine Aminomutase
Authors : Geiger, J.; Strom, S.
Deposited on : 2011-11-16
Resolution : 1.54 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 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 : 2.14.4.dev1
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) : 2.14.4.dev1

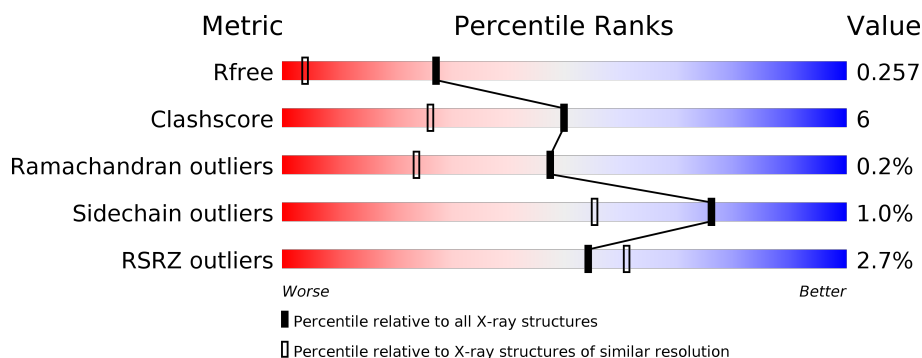
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	547	 3% 80% 13% 6%
1	B	547	 2% 83% 10% 6%

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
5	EDO	B	1003	-	-	X	-
5	EDO	B	1004	-	-	X	-
6	PO4	A	550	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8538 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.

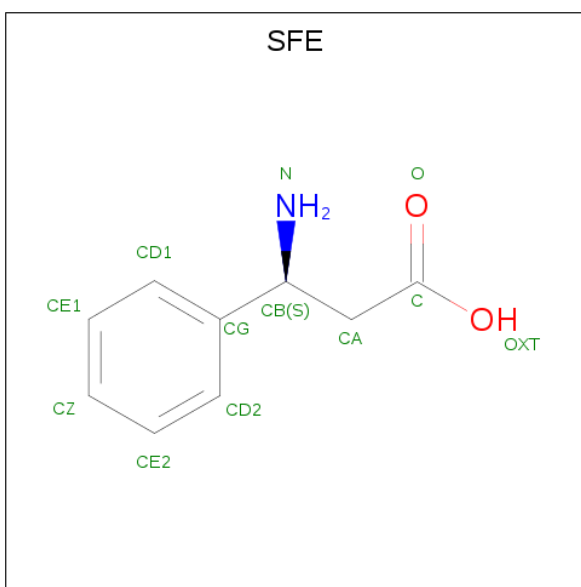
- Molecule 1 is a protein called AdmH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	1	3	0
			3981	2494	692	770	25			
1	B	514	Total	C	N	O	S	7	3	0
			3970	2489	689	767	25			

There are 16 discrepancies between the modelled and reference sequences:

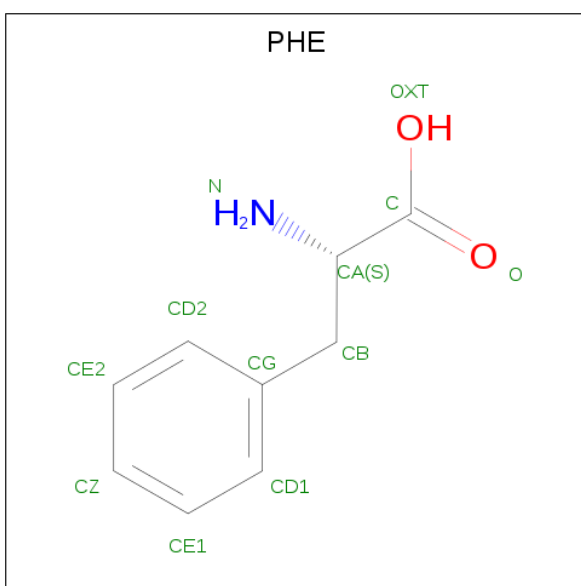
Chain	Residue	Modelled	Actual	Comment	Reference
A	542	LEU	-	EXPRESSION TAG	UNP Q84FL5
A	543	GLU	-	EXPRESSION TAG	UNP Q84FL5
A	544	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	545	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	546	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	547	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	548	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	549	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	542	LEU	-	EXPRESSION TAG	UNP Q84FL5
B	543	GLU	-	EXPRESSION TAG	UNP Q84FL5
B	544	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	545	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	546	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	547	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	548	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	549	HIS	-	EXPRESSION TAG	UNP Q84FL5

- Molecule 2 is (3S)-3-amino-3-phenylpropanoic acid (three-letter code: SFE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			12	9	1	2		
2	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			12	9	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

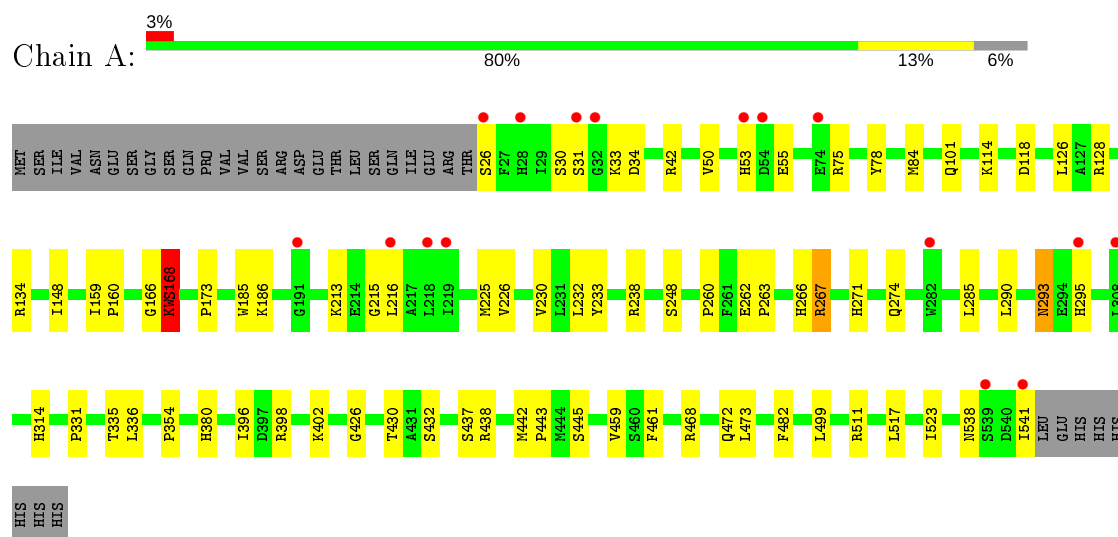
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	243	Total 243	O 243	0	0
7	B	248	Total 248	O 248	0	0

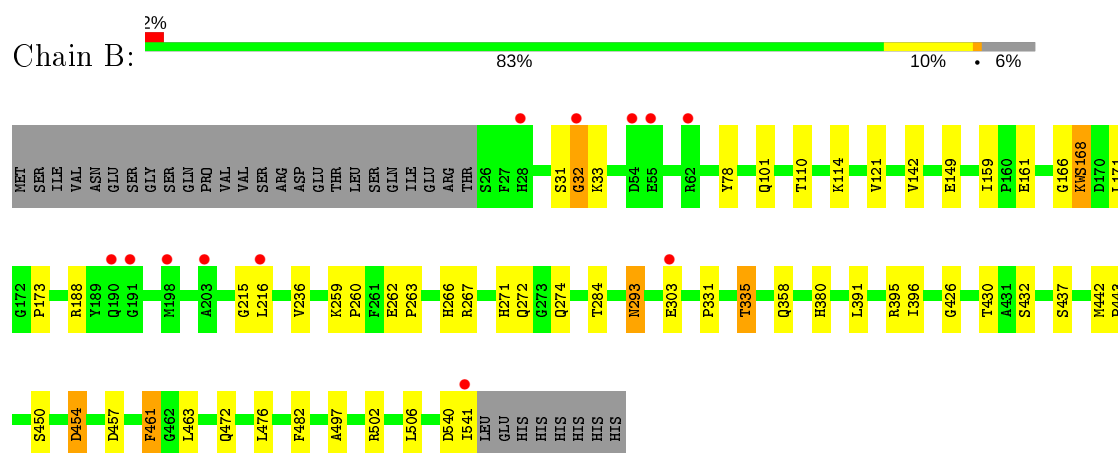
3 Residue-property plots

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: AdmH



• Molecule 1: AdmH



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.96 Å 185.84 Å 72.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.54 27.81 – 1.54	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-1.54) 91.1 (27.81-1.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.54 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.247 0.212 , 0.257	Depositor DCC
R_{free} test set	7034 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8538	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GOL, PO4, SFE, EDO, KWS

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	1.29	6/4016 (0.1%)	1.07	15/5433 (0.3%)
1	B	1.27	6/4023 (0.1%)	1.04	10/5444 (0.2%)
All	All	1.28	12/8039 (0.1%)	1.06	25/10877 (0.2%)

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	6
1	B	0	3
All	All	0	9

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	TYR	CD2-CE2	5.82	1.48	1.39
1	B	461	PHE	CE1-CZ	5.76	1.48	1.37
1	B	149	GLU	CG-CD	5.68	1.60	1.51
1	B	335	THR	CB-CG2	-5.64	1.33	1.52
1	B	236	VAL	CB-CG2	5.55	1.64	1.52
1	A	336	LEU	N-CA	5.49	1.57	1.46
1	A	55	GLU	CG-CD	5.43	1.60	1.51
1	B	272	GLN	CG-CD	5.27	1.63	1.51
1	A	398	ARG	CG-CD	5.23	1.65	1.51
1	A	445	SER	CB-OG	5.16	1.49	1.42
1	A	262	GLU	CD-OE2	-5.12	1.20	1.25
1	B	395	ARG	CZ-NH1	5.06	1.39	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	267[A]	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	267[B]	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	267[A]	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	267[B]	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	134	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	511	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	B	188	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	395	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	126	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	A	438	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	B	463	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	B	454	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	188	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	128	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	B	395	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	118	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	457	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	391	LEU	CB-CG-CD1	5.42	120.21	111.00
1	A	225	MET	CG-SD-CE	5.37	108.79	100.20
1	A	75	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	468	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	476	LEU	CB-CG-CD2	-5.23	102.10	111.00
1	A	34	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	506	LEU	CB-CG-CD2	-5.14	102.26	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	GLY	Mainchain
1	A	168[A]	KWS	Mainchain,Peptide
1	A	168[B]	KWS	Mainchain,Peptide
1	B	166	GLY	Mainchain
1	B	168	KWS	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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	3981	0	3997	52	0
1	B	3970	0	3988	40	0
2	A	12	0	8	4	0
2	B	12	0	9	1	0
3	A	12	0	8	1	0
4	A	6	0	8	1	0
4	B	12	0	16	1	0
5	A	16	0	24	5	0
5	B	16	0	24	11	0
6	A	10	0	0	1	0
7	A	243	0	0	6	0
7	B	248	0	0	2	0
All	All	8538	0	8082	94	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 6.

All (94) 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)
7:A:779:HOH:O	5:B:550:EDO:H22	1.59	1.01
1:B:454:ASP:OD1	5:B:1003:EDO:H21	1.68	0.92
1:A:538:ASN:O	1:A:541:ILE:HG22	1.81	0.81
1:B:266:HIS:HD2	1:B:274:GLN:HE21	1.33	0.77
1:A:266:HIS:HD2	1:A:274:GLN:HE21	1.32	0.74
1:A:271:HIS:HD2	4:A:1002:GOL:O2	1.70	0.74
1:B:78:TYR:OH	2:B:1000:SFE:HA2C	1.88	0.73
1:A:168[A]:KWS:HB2A	2:A:1000[A]:SFE:HD1	1.73	0.70
7:A:779:HOH:O	5:B:550:EDO:C2	2.25	0.70
1:A:538:ASN:O	1:A:541:ILE:CG2	2.41	0.69
1:A:238:ARG:HH22	5:A:1005:EDO:H22	1.57	0.68
1:B:259:LYS:O	1:B:262[B]:GLU:HG3	1.94	0.68
1:A:260:PRO:O	1:A:266:HIS:HE1	1.79	0.66
7:A:627:HOH:O	5:B:1003:EDO:H22	1.98	0.64
1:B:271:HIS:HD2	4:B:1001:GOL:O2	1.80	0.63
1:B:497:ALA:HB2	5:B:1004:EDO:H12	1.79	0.62
1:A:168[A]:KWS:HB2A	2:A:1000[A]:SFE:CD1	2.28	0.62
1:B:497:ALA:CB	5:B:1004:EDO:H12	2.30	0.61
1:A:168[A]:KWS:CB2	2:A:1000[A]:SFE:CD1	2.80	0.59
1:A:266:HIS:CD2	1:A:274:GLN:HE21	2.16	0.59
1:A:101:GLN:HE21	1:A:215:GLY:H	1.50	0.59
1:A:232:LEU:HD23	1:A:541:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLN:HE21	1:B:215:GLY:H	1.51	0.58
1:A:523:ILE:HG12	1:B:110:THR:HG22	1.86	0.58
1:A:42:ARG:HH21	5:A:1005:EDO:C1	2.17	0.57
1:A:314:HIS:HE1	7:A:769:HOH:O	1.89	0.55
1:A:380:HIS:HD2	7:A:750:HOH:O	1.89	0.55
1:A:293:ASN:HD22	1:A:295:HIS:H	1.54	0.55
1:A:293:ASN:HD21	1:A:295:HIS:HB3	1.71	0.54
1:B:114:LYS:O	1:B:161:GLU:HG3	2.07	0.54
1:A:437:SER:HA	1:A:472:GLN:HE22	1.73	0.54
1:B:31:SER:O	1:B:32:GLY:O	2.25	0.53
1:A:78:TYR:OH	2:A:1000[A]:SFE:HA2C	2.08	0.53
1:A:232:LEU:HD23	1:A:541:ILE:HD11	1.91	0.53
1:A:293:ASN:ND2	1:A:295:HIS:H	2.08	0.52
1:B:101:GLN:HE21	1:B:215:GLY:N	2.07	0.52
1:B:442:MET:SD	1:B:443:PRO:HD2	2.50	0.52
1:B:260:PRO:O	1:B:266:HIS:HE1	1.93	0.51
1:A:101:GLN:HE21	1:A:215:GLY:N	2.08	0.51
1:A:248:SER:HB3	1:A:285:LEU:HD21	1.93	0.51
1:A:293:ASN:HD22	1:A:293:ASN:C	2.15	0.50
1:A:30:SER:HA	1:A:53:HIS:HB3	1.92	0.50
1:A:442:MET:SD	1:A:443:PRO:HD2	2.52	0.49
7:A:627:HOH:O	5:B:1003:EDO:C2	2.55	0.49
1:B:380:HIS:HD2	7:B:635:HOH:O	1.95	0.49
1:B:497:ALA:H	5:B:1004:EDO:C1	2.26	0.49
1:B:266:HIS:CD2	1:B:274:GLN:HE21	2.22	0.49
1:A:232:LEU:CD2	1:A:541:ILE:HD11	2.44	0.47
1:A:78:TYR:CE1	1:A:84:MET:HA	2.50	0.46
1:A:293:ASN:HD22	1:A:295:HIS:N	2.13	0.46
1:B:331:PRO:O	1:B:335:THR:HG22	2.15	0.46
1:A:473:LEU:HD23	1:A:541:ILE:HD11	1.98	0.45
1:A:232:LEU:HD23	1:A:541:ILE:HD12	1.97	0.45
5:A:1007:EDO:H21	6:A:1008:PO4:O3	2.15	0.45
1:B:142:VAL:HG23	7:B:681:HOH:O	2.15	0.45
1:B:426:GLY:HA3	1:B:482:PHE:CZ	2.51	0.45
1:B:284:THR:HG23	1:B:502:ARG:HB3	1.99	0.45
1:A:263:PRO:O	1:A:267[B]:ARG:HG3	2.17	0.45
1:B:437:SER:HA	1:B:472:GLN:HE22	1.82	0.45
1:B:454:ASP:OD1	5:B:1003:EDO:C2	2.53	0.44
1:A:213:LYS:HE2	1:A:354:PRO:HD2	1.99	0.44
1:A:426:GLY:HA3	1:A:482:PHE:CZ	2.52	0.44
1:B:101:GLN:HE22	1:B:216:LEU:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:SER:HA	1:B:461:PHE:CE1	2.53	0.43
1:A:226:VAL:O	1:A:230:VAL:HG13	2.18	0.43
1:A:159:ILE:HA	1:A:160:PRO:HD3	1.88	0.43
1:B:159:ILE:HG21	1:B:173:PRO:HB3	2.01	0.43
1:A:168[A]:KWS:HG2	1:A:459:VAL:HA	2.01	0.42
1:A:42:ARG:HH21	5:A:1005:EDO:H11	1.84	0.42
1:A:159:ILE:HG23	1:A:173:PRO:HA	2.01	0.42
1:A:396:ILE:HD13	1:A:430:THR:HG21	2.01	0.42
1:A:461:PHE:CE1	1:B:432:SER:HA	2.55	0.42
1:B:262[B]:GLU:HA	1:B:263:PRO:HD3	1.93	0.42
1:B:259:LYS:N	1:B:260:PRO:CD	2.83	0.42
1:B:497:ALA:H	5:B:1004:EDO:H11	1.85	0.41
1:B:450:SER:O	5:B:1003:EDO:O1	2.34	0.41
1:A:168[B]:KWS:HB2	3:A:1001[B]:PHE:HB2	1.83	0.41
1:A:50:VAL:HB	1:A:148:ILE:HG23	2.02	0.41
1:B:396:ILE:HD13	1:B:430:THR:HG21	2.03	0.41
1:A:260:PRO:O	1:A:266:HIS:CE1	2.67	0.41
1:A:331:PRO:O	1:A:335:THR:HG22	2.21	0.41
1:B:267[B]:ARG:HD2	1:B:267[B]:ARG:HH21	1.62	0.41
1:A:185:TRP:CG	1:A:186:LYS:N	2.88	0.41
1:B:541:ILE:HG23	1:B:541:ILE:O	2.20	0.41
1:A:168[B]:KWS:HG2	1:A:459:VAL:HA	2.02	0.41
1:A:101:GLN:NE2	1:A:216:LEU:H	2.19	0.41
1:B:358:GLN:HE21	1:B:358:GLN:HB3	1.72	0.41
1:B:159:ILE:HG23	1:B:173:PRO:HA	2.03	0.41
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.94	0.40
1:B:121:VAL:HG22	1:B:159:ILE:HD12	2.03	0.40
1:A:114:LYS:H	5:A:1006:EDO:C2	2.34	0.40
1:B:101:GLN:NE2	1:B:216:LEU:H	2.20	0.40
1:A:290:LEU:HD12	1:A:499:LEU:HD23	2.04	0.40
1:B:293:ASN:HD22	1:B:293:ASN:C	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	513/547 (94%)	503 (98%)	10 (2%)	0	100	100
1	B	514/547 (94%)	502 (98%)	10 (2%)	2 (0%)	34	13
All	All	1027/1094 (94%)	1005 (98%)	20 (2%)	2 (0%)	47	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	LYS
1	B	32	GLY

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	437/469 (93%)	431 (99%)	6 (1%)	67	39
1	B	436/469 (93%)	433 (99%)	3 (1%)	84	68
All	All	873/938 (93%)	864 (99%)	9 (1%)	76	55

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	31	SER
1	A	33	LYS
1	A	293	ASN
1	A	402	LYS
1	A	517	LEU
1	B	293	ASN
1	B	303	GLU
1	B	540	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	58	ASN
1	A	101	GLN
1	A	102	ASN
1	A	143	ASN
1	A	184	GLN
1	A	266	HIS
1	A	271	HIS
1	A	293	ASN
1	A	314	HIS
1	A	358	GLN
1	A	380	HIS
1	A	404	ASN
1	A	456	GLN
1	A	472	GLN
1	B	48	GLN
1	B	58	ASN
1	B	101	GLN
1	B	102	ASN
1	B	136	ASN
1	B	184	GLN
1	B	266	HIS
1	B	271	HIS
1	B	293	ASN
1	B	295	HIS
1	B	358	GLN
1	B	380	HIS
1	B	404	ASN
1	B	456	GLN
1	B	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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
1	KWS	A	168[B]	1,3	14,15,16	3.80	5 (35%)	18,21,23	6.19	11 (61%)
1	KWS	A	168[A]	1,2	14,15,16	3.47	5 (35%)	18,21,23	7.53	11 (61%)
1	KWS	B	168	1,2	14,15,16	3.58	4 (28%)	18,21,23	6.27	9 (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
1	KWS	A	168[B]	1,3	-	3/8/27/28	0/1/1/1
1	KWS	A	168[A]	1,2	-	2/8/27/28	0/1/1/1
1	KWS	B	168	1,2	-	3/8/27/28	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	KWS	O2-C2	11.56	1.47	1.23
1	A	168[B]	KWS	O2-C2	11.27	1.46	1.23
1	A	168[A]	KWS	O2-C2	10.82	1.45	1.23
1	A	168[B]	KWS	CA-N	5.10	1.62	1.47
1	A	168[B]	KWS	C2-N3	-3.94	1.30	1.39
1	B	168	KWS	CA-C1	-3.88	1.45	1.51
1	A	168[A]	KWS	CA-C1	-3.85	1.45	1.51
1	A	168[B]	KWS	CA-C1	-3.84	1.46	1.51
1	A	168[A]	KWS	C2-N3	-3.53	1.31	1.39
1	B	168	KWS	C2-N3	-3.49	1.31	1.39
1	A	168[A]	KWS	CA2-C2	-3.40	1.36	1.43
1	B	168	KWS	CA2-C2	-2.87	1.37	1.43
1	A	168[B]	KWS	CA2-N2	-2.67	1.34	1.39
1	A	168[A]	KWS	C1-N3	-2.42	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168[A]	KWS	CA2-C2-N3	25.72	115.53	103.37
1	B	168	KWS	CA2-C2-N3	21.99	113.77	103.37
1	A	168[B]	KWS	CA2-C2-N3	19.64	112.66	103.37
1	A	168[A]	KWS	C2-CA2-N2	-11.24	101.06	108.93
1	A	168[B]	KWS	C2-CA2-N2	-10.49	101.58	108.93
1	A	168[A]	KWS	C2-N3-C1	-10.42	102.69	107.97
1	B	168	KWS	C2-CA2-N2	-9.14	102.53	108.93
1	A	168[B]	KWS	C2-N3-C1	-9.02	103.40	107.97
1	B	168	KWS	C2-N3-C1	-7.50	104.17	107.97
1	A	168[A]	KWS	O2-C2-CA2	-6.38	127.38	130.96
1	A	168[B]	KWS	C1-CA-N	-4.95	101.92	109.96
1	A	168[A]	KWS	CB2-CA2-C2	4.94	131.81	122.76
1	B	168	KWS	O2-C2-CA2	-4.89	128.21	130.96
1	A	168[B]	KWS	CB2-CA2-C2	4.62	131.22	122.76
1	A	168[B]	KWS	O2-C2-CA2	-4.43	128.47	130.96
1	B	168	KWS	CA2-N2-C1	4.21	109.21	105.40
1	A	168[A]	KWS	CA2-N2-C1	3.98	109.00	105.40
1	A	168[B]	KWS	CA2-N2-C1	3.87	108.91	105.40
1	A	168[A]	KWS	O2-C2-N3	-3.69	117.02	124.35
1	B	168	KWS	O2-C2-N3	-3.21	117.96	124.35
1	A	168[A]	KWS	OG1-CB-CA	2.93	115.31	109.04
1	B	168	KWS	CB2-CA2-C2	2.91	128.10	122.76
1	A	168[B]	KWS	O2-C2-N3	-2.78	118.82	124.35
1	A	168[B]	KWS	CA3-N3-C1	2.73	130.44	127.16
1	A	168[B]	KWS	CG2-CB-CA	-2.70	105.80	112.16
1	B	168	KWS	CA3-N3-C1	2.65	130.35	127.16
1	A	168[A]	KWS	CA3-N3-C1	2.63	130.32	127.16
1	A	168[B]	KWS	N3-C1-N2	2.59	113.25	111.45
1	B	168	KWS	OG1-CB-CA	-2.58	103.53	109.04
1	A	168[A]	KWS	C1-CA-N	-2.46	105.97	109.96
1	A	168[A]	KWS	CG2-CB-CA	-2.45	106.39	112.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	168[B]	KWS	N2-C1-CA-CB
1	A	168[B]	KWS	N3-C1-CA-CB
1	A	168[A]	KWS	N2-C1-CA-CB
1	A	168[A]	KWS	N3-C1-CA-CB
1	B	168	KWS	N2-C1-CA-CB
1	B	168	KWS	N3-C1-CA-CB
1	B	168	KWS	C-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
1	A	168[B]	KWS	C-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	168[B]	KWS	2	0
1	A	168[A]	KWS	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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$
5	EDO	A	1004	-	3,3,3	0.71	0	2,2,2	0.82	0
5	EDO	A	1005	-	3,3,3	0.41	0	2,2,2	0.83	0
5	EDO	B	1005	-	3,3,3	0.45	0	2,2,2	1.15	0
5	EDO	B	1003	-	3,3,3	1.02	0	2,2,2	0.79	0
2	SFE	A	1000[A]	1	9,12,12	1.51	1 (11%)	9,15,15	1.71	3 (33%)
5	EDO	A	1006	-	3,3,3	0.16	0	2,2,2	1.22	0
2	SFE	B	1000	1	9,12,12	1.25	1 (11%)	9,15,15	1.52	2 (22%)
5	EDO	B	1004	-	3,3,3	0.41	0	2,2,2	1.16	0
4	GOL	A	1002	-	5,5,5	0.64	0	5,5,5	0.36	0
6	PO4	A	550	-	4,4,4	2.39	3 (75%)	6,6,6	1.53	1 (16%)
5	EDO	A	1007	-	3,3,3	0.58	0	2,2,2	0.30	0
5	EDO	B	550	-	3,3,3	0.19	0	2,2,2	0.79	0
4	GOL	B	1002	-	5,5,5	0.23	0	5,5,5	0.84	0
3	PHE	A	1001[B]	1	9,12,12	0.59	0	10,15,15	1.56	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1001	-	5,5,5	0.94	0	5,5,5	0.65	0
6	PO4	A	1008	-	4,4,4	0.88	0	6,6,6	1.03	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
5	EDO	A	1004	-	-	0/1/1/1	-
5	EDO	A	1005	-	-	1/1/1/1	-
5	EDO	B	1005	-	-	1/1/1/1	-
5	EDO	B	1003	-	-	0/1/1/1	-
2	SFE	A	1000[A]	1	-	1/6/8/8	0/1/1/1
5	EDO	A	1006	-	-	0/1/1/1	-
2	SFE	B	1000	1	-	1/6/8/8	0/1/1/1
5	EDO	B	1004	-	-	1/1/1/1	-
4	GOL	A	1002	-	-	0/4/4/4	-
5	EDO	A	1007	-	-	0/1/1/1	-
5	EDO	B	550	-	-	1/1/1/1	-
4	GOL	B	1002	-	-	0/4/4/4	-
3	PHE	A	1001[B]	1	-	4/4/8/8	0/1/1/1
4	GOL	B	1001	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000[A]	SFE	CG-CB	-4.06	1.46	1.52
6	A	550	PO4	P-O3	-3.33	1.44	1.54
2	B	1000	SFE	CG-CB	-2.77	1.48	1.52
6	A	550	PO4	P-O1	-2.53	1.44	1.50
6	A	550	PO4	P-O4	-2.25	1.47	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001[B]	PHE	CB-CA-C	-3.18	105.55	110.69
2	A	1000[A]	SFE	CA-CB-CG	-2.96	104.94	111.61
2	A	1000[A]	SFE	CD1-CG-CD2	2.94	121.96	118.29
3	A	1001[B]	PHE	CG-CB-CA	-2.84	108.31	114.22
6	A	550	PO4	O3-P-O1	2.81	121.18	110.89
2	B	1000	SFE	CE2-CD2-CG	-2.80	117.18	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	SFE	CD1-CG-CD2	2.18	121.01	118.29
2	A	1000[A]	SFE	CD1-CG-CB	-2.16	117.30	120.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001[B]	PHE	C-CA-CB-CG
3	A	1001[B]	PHE	CA-CB-CG-CD1
5	A	1005	EDO	O1-C1-C2-O2
3	A	1001[B]	PHE	CA-CB-CG-CD2
2	A	1000[A]	SFE	C-CA-CB-N
3	A	1001[B]	PHE	N-CA-CB-CG
5	B	1005	EDO	O1-C1-C2-O2
2	B	1000	SFE	C-CA-CB-N
5	B	1004	EDO	O1-C1-C2-O2
5	B	550	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	EDO	3	0
5	B	1003	EDO	5	0
2	A	1000[A]	SFE	4	0
5	A	1006	EDO	1	0
2	B	1000	SFE	1	0
5	B	1004	EDO	4	0
4	A	1002	GOL	1	0
5	A	1007	EDO	1	0
5	B	550	EDO	2	0
3	A	1001[B]	PHE	1	0
4	B	1001	GOL	1	0
6	A	1008	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	513/547 (93%)	-0.01	16 (3%)	49	56	12, 19, 33, 42	1 (0%)
1	B	513/547 (93%)	0.00	12 (2%)	60	66	12, 20, 33, 44	2 (0%)
All	All	1026/1094 (93%)	-0.00	28 (2%)	54	61	12, 20, 33, 44	3 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ILE	11.4
1	B	541	ILE	9.9
1	B	54	ASP	6.2
1	B	32	GLY	4.2
1	B	191	GLY	3.5
1	B	55	GLU	3.5
1	A	191	GLY	3.2
1	A	54	ASP	3.0
1	A	539	SER	3.0
1	B	28	HIS	2.9
1	A	295	HIS	2.9
1	B	190	GLN	2.7
1	A	218	LEU	2.6
1	A	219	ILE	2.6
1	B	216	LEU	2.5
1	A	216	LEU	2.5
1	A	53	HIS	2.4
1	A	308	LEU	2.3
1	B	198	MET	2.3
1	A	31	SER	2.3
1	A	26	SER	2.2
1	A	28	HIS	2.2
1	A	282	TRP	2.2
1	B	203	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	303	GLU	2.1
1	A	32	GLY	2.1
1	B	62	ARG	2.0
1	A	74	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KWS	A	168[B]	15/16	0.94	0.11	19,20,23,27	15
1	KWS	A	168[A]	15/16	0.94	0.11	7,13,19,22	15
1	KWS	B	168	15/16	0.94	0.09	16,20,24,31	0

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
5	EDO	A	1007	4/4	0.62	0.16	48,53,54,56	0
5	EDO	B	1005	4/4	0.63	0.23	58,59,60,60	0
5	EDO	B	1004	4/4	0.80	0.16	31,37,39,45	0
5	EDO	B	1003	4/4	0.85	0.17	29,31,32,32	0
5	EDO	A	1005	4/4	0.89	0.09	41,42,45,45	0
3	PHE	A	1001[B]	12/12	0.90	0.12	24,35,38,38	12
2	SFE	A	1000[A]	12/12	0.91	0.12	23,26,27,27	12
5	EDO	A	1006	4/4	0.91	0.12	29,30,31,33	0
4	GOL	B	1002	6/6	0.91	0.12	26,32,33,37	0
2	SFE	B	1000	12/12	0.91	0.12	24,32,37,38	0
4	GOL	A	1002	6/6	0.92	0.10	18,24,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	1001	6/6	0.92	0.10	22,27,29,29	0
6	PO4	A	550	5/5	0.93	0.26	8,10,15,20	5
5	EDO	A	1004	4/4	0.94	0.08	24,25,27,28	0
5	EDO	B	550	4/4	0.95	0.11	25,28,30,32	0
6	PO4	A	1008	5/5	0.95	0.27	53,54,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.