



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 4BNW / pdb_00004bnw
Title : Crystal structure of 3-oxoacyl-(acyl-carrier-protein) reductase (FabG) from *Pseudomonas aeruginosa* in complex with an unknown ligand at 1.6 Å resolution
Authors : Cukier, C.D.; Schnell, R.; Lindqvist, Y.; Schneider, G.
Deposited on : 2013-05-17
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

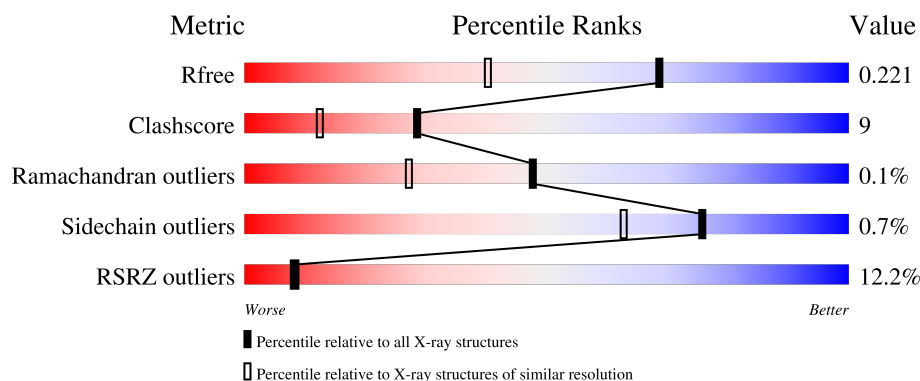
1 Overall quality at a glance

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	269	 7% 80% 10% 10%
1	B	269	 14% 76% 11% 12%
1	C	269	 12% 78% 14% 7%
1	D	269	 12% 78% 12% 9%

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
3	PG4	B	1248	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7741 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 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	10	0
			1805	1128	319	351	7			
1	B	238	Total	C	N	O	S	0	5	0
			1764	1108	312	338	6			
1	C	251	Total	C	N	O	S	0	8	0
			1886	1177	338	363	8			
1	D	246	Total	C	N	O	S	0	11	0
			1853	1164	326	355	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP O54438
A	-20	HIS	-	expression tag	UNP O54438
A	-19	HIS	-	expression tag	UNP O54438
A	-18	HIS	-	expression tag	UNP O54438
A	-17	HIS	-	expression tag	UNP O54438
A	-16	HIS	-	expression tag	UNP O54438
A	-15	HIS	-	expression tag	UNP O54438
A	-14	SER	-	expression tag	UNP O54438
A	-13	SER	-	expression tag	UNP O54438
A	-12	GLY	-	expression tag	UNP O54438
A	-11	VAL	-	expression tag	UNP O54438
A	-10	ASP	-	expression tag	UNP O54438
A	-9	LEU	-	expression tag	UNP O54438
A	-8	GLY	-	expression tag	UNP O54438
A	-7	THR	-	expression tag	UNP O54438
A	-6	GLU	-	expression tag	UNP O54438
A	-5	ASN	-	expression tag	UNP O54438
A	-4	LEU	-	expression tag	UNP O54438
A	-3	TYR	-	expression tag	UNP O54438
A	-2	PHE	-	expression tag	UNP O54438

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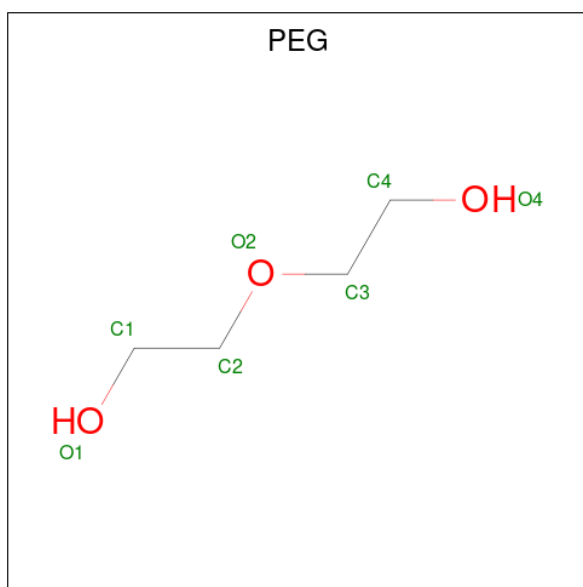
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP O54438
A	0	SER	-	expression tag	UNP O54438
B	-21	MET	-	expression tag	UNP O54438
B	-20	HIS	-	expression tag	UNP O54438
B	-19	HIS	-	expression tag	UNP O54438
B	-18	HIS	-	expression tag	UNP O54438
B	-17	HIS	-	expression tag	UNP O54438
B	-16	HIS	-	expression tag	UNP O54438
B	-15	HIS	-	expression tag	UNP O54438
B	-14	SER	-	expression tag	UNP O54438
B	-13	SER	-	expression tag	UNP O54438
B	-12	GLY	-	expression tag	UNP O54438
B	-11	VAL	-	expression tag	UNP O54438
B	-10	ASP	-	expression tag	UNP O54438
B	-9	LEU	-	expression tag	UNP O54438
B	-8	GLY	-	expression tag	UNP O54438
B	-7	THR	-	expression tag	UNP O54438
B	-6	GLU	-	expression tag	UNP O54438
B	-5	ASN	-	expression tag	UNP O54438
B	-4	LEU	-	expression tag	UNP O54438
B	-3	TYR	-	expression tag	UNP O54438
B	-2	PHE	-	expression tag	UNP O54438
B	-1	GLN	-	expression tag	UNP O54438
B	0	SER	-	expression tag	UNP O54438
C	-21	MET	-	expression tag	UNP O54438
C	-20	HIS	-	expression tag	UNP O54438
C	-19	HIS	-	expression tag	UNP O54438
C	-18	HIS	-	expression tag	UNP O54438
C	-17	HIS	-	expression tag	UNP O54438
C	-16	HIS	-	expression tag	UNP O54438
C	-15	HIS	-	expression tag	UNP O54438
C	-14	SER	-	expression tag	UNP O54438
C	-13	SER	-	expression tag	UNP O54438
C	-12	GLY	-	expression tag	UNP O54438
C	-11	VAL	-	expression tag	UNP O54438
C	-10	ASP	-	expression tag	UNP O54438
C	-9	LEU	-	expression tag	UNP O54438
C	-8	GLY	-	expression tag	UNP O54438
C	-7	THR	-	expression tag	UNP O54438
C	-6	GLU	-	expression tag	UNP O54438
C	-5	ASN	-	expression tag	UNP O54438
C	-4	LEU	-	expression tag	UNP O54438

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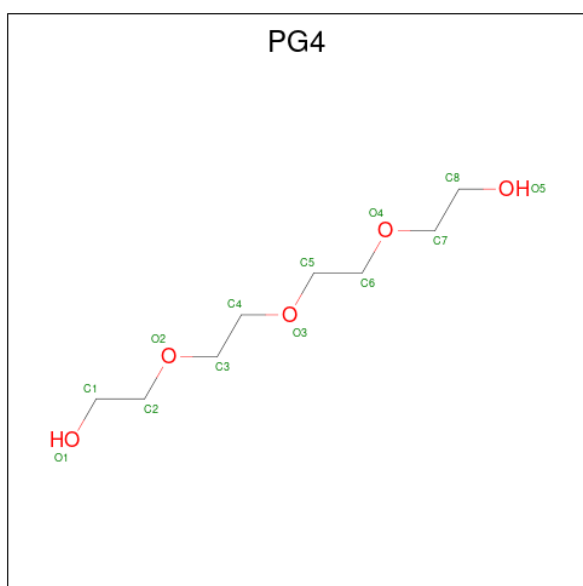
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP O54438
C	-2	PHE	-	expression tag	UNP O54438
C	-1	GLN	-	expression tag	UNP O54438
C	0	SER	-	expression tag	UNP O54438
D	-21	MET	-	expression tag	UNP O54438
D	-20	HIS	-	expression tag	UNP O54438
D	-19	HIS	-	expression tag	UNP O54438
D	-18	HIS	-	expression tag	UNP O54438
D	-17	HIS	-	expression tag	UNP O54438
D	-16	HIS	-	expression tag	UNP O54438
D	-15	HIS	-	expression tag	UNP O54438
D	-14	SER	-	expression tag	UNP O54438
D	-13	SER	-	expression tag	UNP O54438
D	-12	GLY	-	expression tag	UNP O54438
D	-11	VAL	-	expression tag	UNP O54438
D	-10	ASP	-	expression tag	UNP O54438
D	-9	LEU	-	expression tag	UNP O54438
D	-8	GLY	-	expression tag	UNP O54438
D	-7	THR	-	expression tag	UNP O54438
D	-6	GLU	-	expression tag	UNP O54438
D	-5	ASN	-	expression tag	UNP O54438
D	-4	LEU	-	expression tag	UNP O54438
D	-3	TYR	-	expression tag	UNP O54438
D	-2	PHE	-	expression tag	UNP O54438
D	-1	GLN	-	expression tag	UNP O54438
D	0	SER	-	expression tag	UNP O54438

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



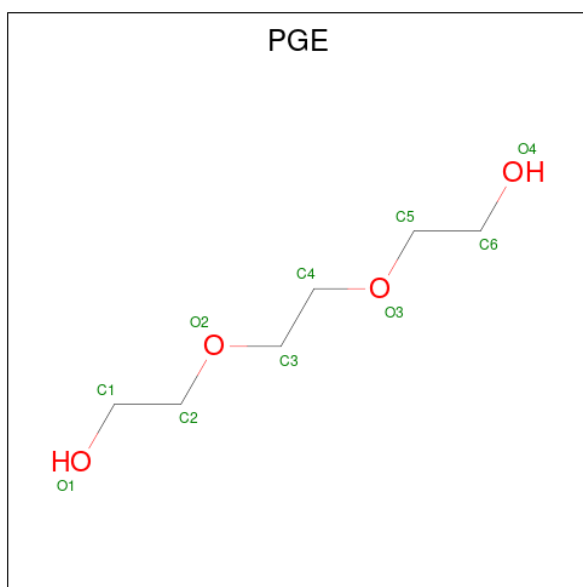
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	6	4		

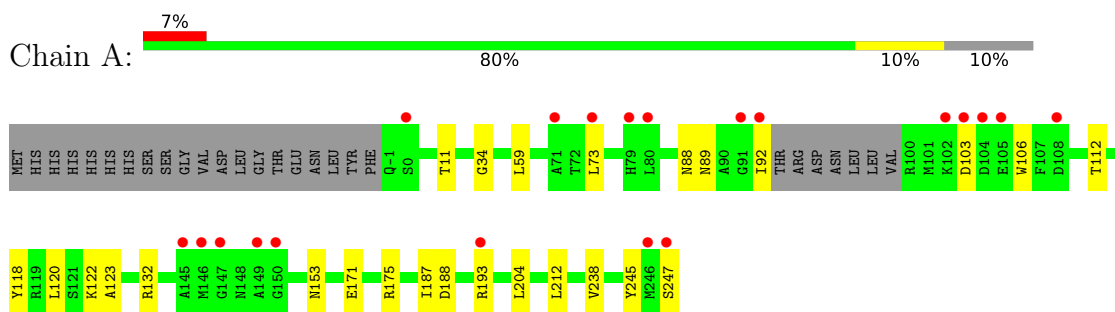
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total	O	0	0
			102	102		
5	B	97	Total	O	0	0
			97	97		
5	C	96	Total	O	0	0
			96	96		
5	D	101	Total	O	0	0
			101	101		

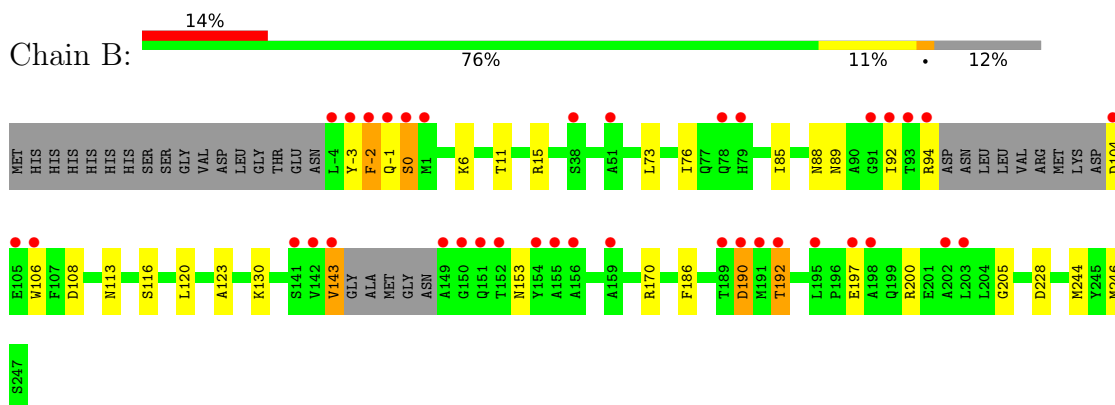
3 Residue-property plots

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.

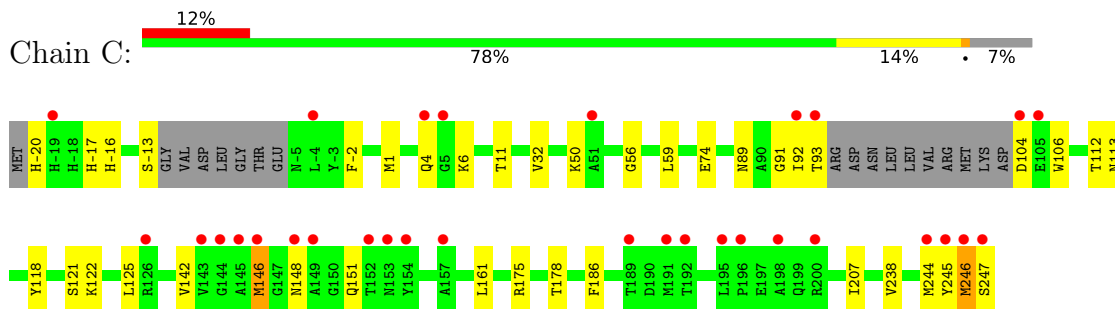
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



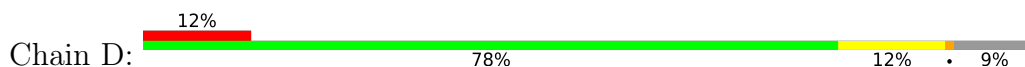
• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG

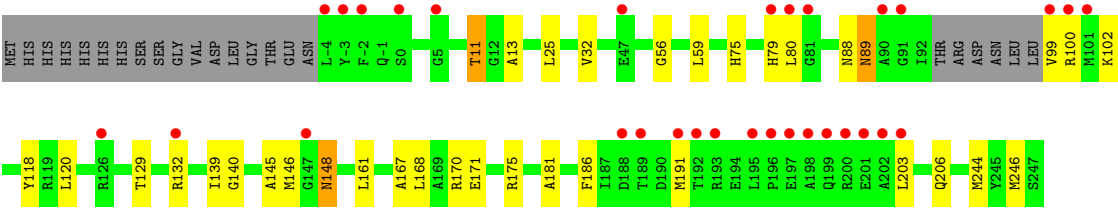


• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



• Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.95Å 107.98Å 146.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 1.60 29.96 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.96-1.60) 99.7 (29.96-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.178 , 0.209 0.190 , 0.221	Depositor DCC
R_{free} test set	5715 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7741	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 5.75% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PG4, PEG

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	1.27	4/1852 (0.2%)	1.13	0/2502
1	B	1.28	4/1797 (0.2%)	1.19	4/2429 (0.2%)
1	C	1.37	3/1922 (0.2%)	1.22	2/2596 (0.1%)
1	D	1.26	5/1902 (0.3%)	1.17	2/2569 (0.1%)
All	All	1.30	16/7473 (0.2%)	1.18	8/10096 (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	B	0	1
1	C	1	2
All	All	1	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	167	ALA	N-CA	6.42	1.54	1.46
1	C	238	VAL	N-CA	6.34	1.51	1.46
1	C	74	GLU	CA-C	-6.23	1.44	1.52
1	A	238	VAL	CA-C	-6.19	1.48	1.53
1	D	139	ILE	N-CA	-6.08	1.38	1.46
1	A	34	GLY	CA-C	-6.06	1.48	1.52
1	C	178	THR	N-CA	-5.89	1.39	1.45
1	B	85	ILE	N-CA	5.81	1.53	1.46
1	A	187	ILE	C-O	-5.65	1.17	1.24
1	D	11	THR	N-CA	5.57	1.53	1.45
1	D	89	ASN	CA-C	5.34	1.59	1.52
1	D	25	LEU	N-CA	-5.33	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	ILE	CA-CB	5.14	1.60	1.54
1	A	188	ASP	N-CA	5.14	1.52	1.46
1	B	113	ASN	N-CA	-5.13	1.40	1.46
1	B	130	LYS	N-CA	5.02	1.52	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-2	PHE	N-CA-C	6.42	119.36	108.90
1	D	148	ASN	N-CA-C	6.35	118.21	111.28
1	D	13	ALA	N-CA-C	5.62	119.77	113.02
1	B	192	THR	N-CA-C	-5.61	105.94	112.89
1	C	175	ARG	N-CA-C	5.18	119.23	113.02
1	B	190	ASP	CA-C-N	5.03	127.03	120.28
1	B	190	ASP	C-N-CA	5.03	127.03	120.28
1	C	161	LEU	N-CA-C	-5.01	105.71	111.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	246[B]	MET	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	0	SER	Peptide
1	C	246[B]	MET	Peptide
1	C	91	GLY	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	1805	0	1864	21	0
1	B	1764	0	1818	40	0
1	C	1886	0	1904	57	0
1	D	1853	0	1917	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	10	0	0
2	C	7	0	10	1	0
3	B	13	0	18	9	0
4	D	10	0	14	0	0
5	A	102	0	0	2	0
5	B	97	0	0	5	0
5	C	96	0	0	5	0
5	D	101	0	0	4	0
All	All	7741	0	7555	131	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 9.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:PHE:CD2	1:C:244[A]:MET:HE1	1.64	1.30
1:C:186:PHE:CD2	1:C:244[A]:MET:CE	2.15	1.29
1:C:186:PHE:HD2	1:C:244[A]:MET:CE	1.46	1.28
1:C:207:ILE:HG12	1:C:244[A]:MET:SD	2.00	1.02
1:B:228[A]:ASP:OD2	3:B:1248:PG4:H61	1.59	1.01
1:C:186:PHE:HD2	1:C:244[A]:MET:HE1	0.86	1.01
5:B:2092:HOH:O	1:C:244[A]:MET:HE2	1.76	0.85
1:C:151:GLN:HB2	1:C:246[A]:MET:HE1	1.59	0.84
1:C:151:GLN:CD	1:C:246[A]:MET:HE2	2.05	0.82
1:C:186:PHE:CD2	1:C:244[A]:MET:SD	2.74	0.81
1:C:151:GLN:HB2	1:C:246[A]:MET:CE	2.10	0.81
1:C:186:PHE:CE2	1:C:244[A]:MET:SD	2.74	0.80
1:D:206[B]:GLN:HB3	1:D:244[B]:MET:SD	2.22	0.79
1:A:204:LEU:HD21	1:A:212:LEU:HD12	1.66	0.78
1:C:186:PHE:CE2	1:C:244[A]:MET:CE	2.68	0.77
1:C:186:PHE:CD2	1:C:244[A]:MET:HE3	2.19	0.76
1:C:151:GLN:CG	1:C:246[A]:MET:HE2	2.16	0.74
5:B:2092:HOH:O	1:C:244[A]:MET:CE	2.32	0.73
1:C:151:GLN:OE1	1:C:247[B]:SER:HB3	1.88	0.72
1:C:207:ILE:CG1	1:C:244[A]:MET:SD	2.77	0.72
1:A:247:SER:OG	1:C:247[A]:SER:HB2	1.91	0.71
1:B:143:VAL:HB	1:B:186:PHE:CE1	2.26	0.71
1:A:171[B]:GLU:OE2	1:B:104:ASP:N	2.24	0.70
1:D:161[B]:LEU:HD21	1:D:181:ALA:HB1	1.74	0.70
1:B:143:VAL:HG11	1:B:186:PHE:CZ	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244[B]:MET:SD	5:C:2069:HOH:O	2.51	0.68
1:B:186:PHE:CE2	1:B:244[B]:MET:SD	2.88	0.66
1:C:186:PHE:HD2	1:C:244[A]:MET:SD	2.17	0.65
1:B:186:PHE:HE2	1:B:244[B]:MET:SD	2.19	0.65
1:B:143:VAL:HB	1:B:186:PHE:CD1	2.32	0.65
1:C:186:PHE:HE2	1:C:244[A]:MET:SD	2.20	0.63
1:C:104:ASP:CG	1:D:118:TYR:OH	2.42	0.62
1:B:228[A]:ASP:CG	3:B:1248:PG4:H61	2.23	0.61
1:D:161[B]:LEU:CD2	5:D:2086:HOH:O	2.49	0.61
1:B:92:ILE:HD11	1:B:116:SER:OG	2.00	0.61
1:B:6[B]:LYS:NZ	3:B:1248:PG4:O4	2.34	0.60
1:B:244[A]:MET:SD	1:B:246:MET:HG3	2.41	0.60
1:C:106:TRP:CG	1:D:171[A]:GLU:HG3	2.36	0.60
1:B:92:ILE:CD1	1:B:116:SER:OG	2.49	0.60
1:C:-13:SER:HB3	5:C:2004:HOH:O	2.02	0.59
1:D:102[B]:LYS:HG3	5:D:2052:HOH:O	2.04	0.58
1:B:116:SER:HB2	5:B:2042:HOH:O	2.04	0.57
1:D:145:ALA:HA	1:D:191:MET:HE3	1.87	0.56
1:C:186:PHE:CE2	1:C:244[A]:MET:HE3	2.38	0.56
1:D:244[A]:MET:SD	1:D:246:MET:HE2	2.45	0.56
1:C:113:ASN:CG	1:C:142:VAL:O	2.49	0.56
1:C:151:GLN:CB	1:C:246[A]:MET:CE	2.81	0.56
1:C:151:GLN:CB	1:C:246[A]:MET:HE2	2.35	0.56
1:A:245:TYR:HB2	1:D:170[A]:ARG:HH22	1.71	0.56
1:C:106:TRP:CD1	1:D:171[A]:GLU:HG3	2.40	0.56
1:A:193:ARG:HA	5:A:2079:HOH:O	2.05	0.55
1:C:-13:SER:O	1:C:50:LYS:HE2	2.06	0.55
1:A:247:SER:OG	1:C:247[A]:SER:CB	2.53	0.55
1:B:0:SER:HB2	3:B:1248:PG4:H71	1.88	0.54
1:B:143:VAL:CG1	1:B:186:PHE:CE1	2.90	0.54
1:C:-16:HIS:ND1	1:C:59:LEU:HD21	2.23	0.53
1:A:122:LYS:NZ	1:A:171[A]:GLU:OE2	2.40	0.53
1:C:151:GLN:OE1	1:C:247[B]:SER:CB	2.54	0.53
1:D:132:ARG:NH1	1:D:175:ARG:HG2	2.24	0.53
1:D:146:MET:HE1	1:D:203:LEU:HD13	1.91	0.52
1:A:118:TYR:CE1	1:A:122:LYS:HE3	2.45	0.52
1:D:161[B]:LEU:HD22	5:D:2086:HOH:O	2.10	0.52
1:A:132:ARG:NH2	5:A:2050:HOH:O	2.41	0.52
1:B:197:GLU:HA	5:B:2073:HOH:O	2.08	0.52
1:A:92:ILE:HD13	1:A:112:THR:HG21	1.93	0.51
1:C:-17:HIS:HE1	5:C:2006:HOH:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HG2	1:B:15:ARG:HH11	1.75	0.51
1:C:118:TYR:OH	1:C:122:LYS:HE2	2.12	0.50
1:B:-2:PHE:CZ	1:C:-2:PHE:CE1	2.98	0.50
1:B:88:ASN:OD1	1:B:120:LEU:HD23	2.11	0.50
1:A:11:THR:O	1:A:89:ASN:HB3	2.12	0.50
1:B:94:ARG:CG	1:B:108:ASP:HB3	2.43	0.49
1:B:143:VAL:CB	1:B:186:PHE:CE1	2.93	0.49
1:C:-16:HIS:CD2	1:C:-16:HIS:C	2.90	0.49
1:D:161[B]:LEU:HD23	5:D:2086:HOH:O	2.11	0.49
1:A:106:TRP:HA	1:A:153:ASN:OD1	2.12	0.49
1:B:228[A]:ASP:OD1	3:B:1248:PG4:H62	2.14	0.48
1:C:146:MET:HE2	1:C:148:ASN:HB2	1.95	0.48
1:C:121:SER:O	1:C:125:LEU:HG	2.14	0.47
1:B:228[A]:ASP:OD1	3:B:1248:PG4:C6	2.63	0.47
1:C:11:THR:O	1:C:89:ASN:HB3	2.15	0.47
1:A:132:ARG:CZ	1:A:175:ARG:HG2	2.45	0.47
1:D:79:HIS:C	1:D:80:LEU:HD12	2.40	0.46
1:D:11:THR:O	1:D:89:ASN:HB3	2.15	0.46
1:C:151:GLN:HB2	1:C:246[A]:MET:HE2	1.88	0.46
1:B:6[B]:LYS:NZ	3:B:1248:PG4:C6	2.78	0.46
1:D:88:ASN:OD1	1:D:120:LEU:HD23	2.16	0.46
1:D:186:PHE:CE2	1:D:203:LEU:HD11	2.51	0.46
1:A:245:TYR:O	1:C:247[A]:SER:HB3	2.16	0.46
1:B:192:THR:O	1:B:200:ARG:NH2	2.44	0.46
1:B:11:THR:O	1:B:89:ASN:HB3	2.16	0.45
1:A:73[A]:LEU:HD12	1:A:123:ALA:HB1	1.98	0.45
1:B:-2:PHE:CZ	1:C:-2:PHE:HE1	2.35	0.45
1:A:73[A]:LEU:CD1	1:A:123:ALA:HB1	2.47	0.45
1:B:94:ARG:HG2	1:B:108:ASP:HB3	1.99	0.45
1:C:247[B]:SER:O	1:C:247[B]:SER:OG	2.20	0.45
1:A:247:SER:CB	1:C:247[A]:SER:HB2	2.46	0.45
1:B:-3:TYR:CE1	1:C:1:MET:HE3	2.52	0.45
1:D:32:VAL:O	1:D:56:GLY:HA3	2.17	0.44
1:C:146:MET:HE2	1:C:148:ASN:CG	2.42	0.44
1:A:88:ASN:OD1	1:A:120:LEU:HD23	2.18	0.44
1:D:100:ARG:O	1:D:102[A]:LYS:HG2	2.17	0.44
1:B:170:ARG:NH2	1:C:245[A]:TYR:HB2	2.31	0.44
1:B:106:TRP:HB3	1:B:153:ASN:OD1	2.18	0.43
1:B:6[B]:LYS:HZ3	3:B:1248:PG4:H62	1.82	0.43
1:D:129:THR:O	1:D:132:ARG:HD2	2.19	0.43
5:C:2066:HOH:O	1:D:170[A]:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-1:GLN:CG	1:B:0:SER:N	2.82	0.43
1:C:6:LYS:NZ	2:C:1248:PEG:H21	2.34	0.42
1:C:106:TRP:CZ2	1:D:168:LEU:HD13	2.54	0.42
1:A:59[A]:LEU:HA	1:A:59[A]:LEU:HD23	1.67	0.42
1:B:143:VAL:CG1	1:B:186:PHE:CZ	3.00	0.42
1:B:186:PHE:CE2	1:B:244[A]:MET:HE2	2.53	0.42
1:C:151:GLN:CD	1:C:247[B]:SER:HB3	2.44	0.42
1:B:228[A]:ASP:CG	3:B:1248:PG4:C6	2.91	0.42
1:A:245:TYR:HB2	1:D:170[A]:ARG:NH2	2.34	0.42
1:B:73[A]:LEU:HD12	1:B:123:ALA:HB1	2.02	0.42
1:B:73[A]:LEU:CD1	1:B:123:ALA:HB1	2.49	0.42
1:D:170[B]:ARG:HE	1:D:170[B]:ARG:HB3	1.62	0.42
1:D:59:LEU:HD22	1:D:75:HIS:CE1	2.55	0.41
1:C:4:GLN:O	1:C:4:GLN:CG	2.68	0.41
5:B:2092:HOH:O	1:C:244[A]:MET:HE1	2.10	0.41
1:C:32:VAL:O	1:C:56:GLY:HA3	2.19	0.41
1:B:205:GLY:O	1:D:148:ASN:ND2	2.52	0.41
1:C:104:ASP:N	5:C:2046:HOH:O	2.53	0.41
1:C:92:ILE:HG22	1:C:93:THR:N	2.35	0.40
1:C:92:ILE:HD12	1:C:112:THR:HG21	2.03	0.40
1:D:140:GLY:HA2	1:D:161[B]:LEU:HD13	2.03	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	248/269 (92%)	245 (99%)	3 (1%)	0	100	100
1	B	237/269 (88%)	231 (98%)	5 (2%)	1 (0%)	30	14
1	C	252/269 (94%)	247 (98%)	5 (2%)	0	100	100
1	D	253/269 (94%)	249 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	990/1076 (92%)	972 (98%)	17 (2%)	1 (0%)	48 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	ASP

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	186/201 (92%)	185 (100%)	1 (0%)	81 70
1	B	180/201 (90%)	179 (99%)	1 (1%)	78 66
1	C	193/201 (96%)	191 (99%)	2 (1%)	68 50
1	D	190/201 (94%)	189 (100%)	1 (0%)	81 70
All	All	749/804 (93%)	744 (99%)	5 (1%)	76 63

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

Mol	Chain	Res	Type
1	A	103	ASP
1	B	143	VAL
1	C	-20	HIS
1	C	146	MET
1	D	99	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	148	ASN
1	A	151	GLN
1	A	206	GLN

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Mol	Chain	Res	Type
1	B	82	GLN
1	B	111	ASN
1	B	206	GLN
1	C	79	HIS
1	C	88	ASN
1	C	111	ASN
1	C	115	ASN
1	C	138	ASN
1	C	206	GLN
1	D	19	GLN
1	D	79	HIS
1	D	111	ASN
1	D	115	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	PG4	B	1248	-	12,12,12	0.53	0	11,11,11	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	A	1248	-	6,6,6	0.34	0	5,5,5	0.46	0
2	PEG	C	1248	-	6,6,6	0.79	0	5,5,5	1.67	1 (20%)
4	PGE	D	1248	-	9,9,9	0.44	0	8,8,8	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	B	1248	-	-	1/10/10/10	-
2	PEG	A	1248	-	-	2/4/4/4	-
2	PEG	C	1248	-	-	0/4/4/4	-
4	PGE	D	1248	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1248	PEG	O2-C2-C1	3.16	124.05	110.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1248	PG4	O1-C1-C2-O2
4	D	1248	PGE	O3-C5-C6-O4
2	A	1248	PEG	C1-C2-O2-C3
4	D	1248	PGE	O2-C3-C4-O3
4	D	1248	PGE	C4-C3-O2-C2
2	A	1248	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1248	PG4	9	0
2	C	1248	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	242/269 (89%)	0.31	20 (8%)	17 17	10, 19, 54, 79	10 (4%)
1	B	238/269 (88%)	0.53	37 (15%)	5 4	9, 21, 49, 76	5 (2%)
1	C	251/269 (93%)	0.43	31 (12%)	8 8	8, 18, 44, 67	8 (3%)
1	D	246/269 (91%)	0.56	31 (12%)	8 7	9, 20, 54, 90	11 (4%)
All	All	977/1076 (90%)	0.46	119 (12%)	8 8	8, 20, 51, 90	34 (3%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244[A]	MET	6.5
1	D	-3	TYR	6.2
1	A	92	ILE	5.9
1	D	196	PRO	5.9
1	B	-2	PHE	5.4
1	D	-4	LEU	5.4
1	C	189	THR	5.2
1	D	-2	PHE	5.0
1	D	195	LEU	5.0
1	B	-3	TYR	5.0
1	A	0	SER	4.9
1	D	198	ALA	4.3
1	D	189	THR	4.2
1	D	191	MET	4.2
1	C	245[A]	TYR	4.1
1	A	104	ASP	4.1
1	B	93	THR	4.0
1	B	143	VAL	4.0
1	D	188	ASP	4.0
1	C	-4	LEU	4.0
1	D	197	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	149	ALA	3.9
1	B	142	VAL	3.8
1	D	0	SER	3.8
1	D	80	LEU	3.7
1	B	141	SER	3.6
1	D	202	ALA	3.5
1	C	246[A]	MET	3.5
1	A	145	ALA	3.4
1	C	92	ILE	3.4
1	D	203	LEU	3.4
1	D	99	VAL	3.3
1	B	191	MET	3.2
1	B	51	ALA	3.2
1	B	-1	GLN	3.2
1	D	200	ARG	3.2
1	C	5	GLY	3.2
1	C	157	ALA	3.2
1	B	91	GLY	3.1
1	A	149	ALA	3.0
1	C	247[A]	SER	3.0
1	C	196	PRO	3.0
1	B	106	TRP	3.0
1	C	149	ALA	3.0
1	D	192	THR	3.0
1	C	146	MET	3.0
1	A	91	GLY	3.0
1	B	92	ILE	2.9
1	C	93	THR	2.9
1	C	152	THR	2.8
1	B	0	SER	2.8
1	A	71	ALA	2.8
1	C	51	ALA	2.8
1	D	126	ARG	2.8
1	D	132	ARG	2.8
1	C	148	ASN	2.8
1	B	105	GLU	2.8
1	C	154	TYR	2.8
1	D	199	GLN	2.8
1	C	200	ARG	2.7
1	B	79	HIS	2.7
1	D	201	GLU	2.7
1	B	104	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	2.7
1	B	192	THR	2.6
1	A	246	MET	2.6
1	B	152	THR	2.6
1	D	81	GLY	2.6
1	A	80	LEU	2.6
1	D	79	HIS	2.6
1	A	247	SER	2.6
1	B	202	ALA	2.6
1	C	153	ASN	2.6
1	A	147	GLY	2.5
1	B	159	ALA	2.5
1	B	198	ALA	2.5
1	D	193	ARG	2.5
1	B	151	GLN	2.5
1	A	150	GLY	2.5
1	B	150	GLY	2.5
1	B	-4	LEU	2.5
1	A	102	LYS	2.5
1	B	154	TYR	2.4
1	C	4	GLN	2.4
1	A	79	HIS	2.4
1	C	192	THR	2.4
1	C	105	GLU	2.4
1	A	193	ARG	2.4
1	C	191	MET	2.4
1	C	144	GLY	2.3
1	A	103	ASP	2.3
1	B	190	ASP	2.3
1	D	100	ARG	2.3
1	C	145	ALA	2.3
1	C	195	LEU	2.3
1	C	-19	HIS	2.3
1	D	5	GLY	2.3
1	D	91	GLY	2.3
1	B	78	GLN	2.2
1	B	94	ARG	2.2
1	A	73[A]	LEU	2.2
1	C	143	VAL	2.2
1	D	47	GLU	2.2
1	B	38	SER	2.2
1	B	1	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	GLY	2.1
1	A	146	MET	2.1
1	B	197	GLU	2.1
1	B	156	ALA	2.1
1	B	195	LEU	2.1
1	B	203	LEU	2.1
1	D	101	MET	2.1
1	A	105	GLU	2.1
1	B	189	THR	2.0
1	C	126	ARG	2.0
1	A	108	ASP	2.0
1	C	104	ASP	2.0
1	C	198	ALA	2.0
1	D	90[A]	ALA	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(Å ²)	Q<0.9
2	PEG	C	1248	7/7	0.82	0.15	40,45,49,52	0
3	PG4	B	1248	13/13	0.82	0.14	38,41,44,45	0
2	PEG	A	1248	7/7	0.85	0.11	42,45,48,49	0
4	PGE	D	1248	10/10	0.85	0.11	40,48,51,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.