



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 3NQI / pdb_00003nqi
Title : Crystal structure of a Putative lipoprotein (BF3042) from Bacteroides fragilis
NCTC 9343 at 1.87 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-06-29
Resolution : 1.87 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

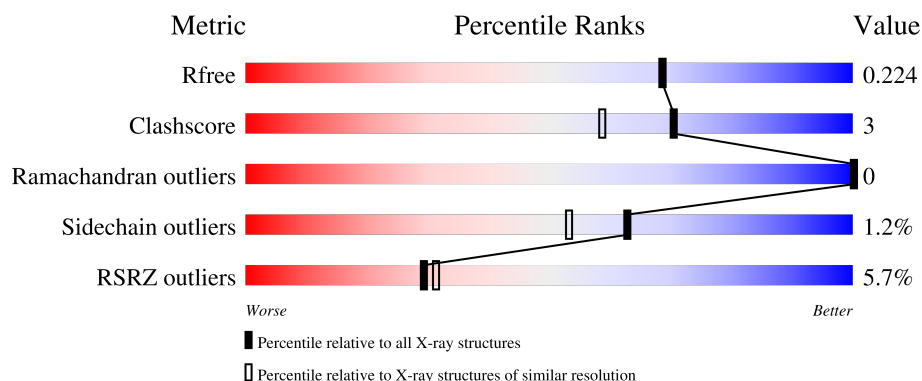
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	246	3% 90% 6%
1	B	246	6% 84% 9% 7%
1	C	246	2% 84% 9% 7%
1	D	246	10% 84% 10% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7821 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 Putative lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	11	0
			1831	1168	289	369	2	3			
1	B	230	Total	C	N	O	S	Se	0	14	0
			1849	1185	292	367	2	3			
1	C	230	Total	C	N	O	S	Se	0	11	0
			1832	1168	292	367	2	3			
1	D	230	Total	C	N	O	S	Se	0	9	0
			1813	1159	294	355	2	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q5LAY5
A	23	MSE	-	expression tag	UNP Q5LAY5
B	22	GLY	-	expression tag	UNP Q5LAY5
B	23	MSE	-	expression tag	UNP Q5LAY5
C	22	GLY	-	expression tag	UNP Q5LAY5
C	23	MSE	-	expression tag	UNP Q5LAY5
D	22	GLY	-	expression tag	UNP Q5LAY5
D	23	MSE	-	expression tag	UNP Q5LAY5

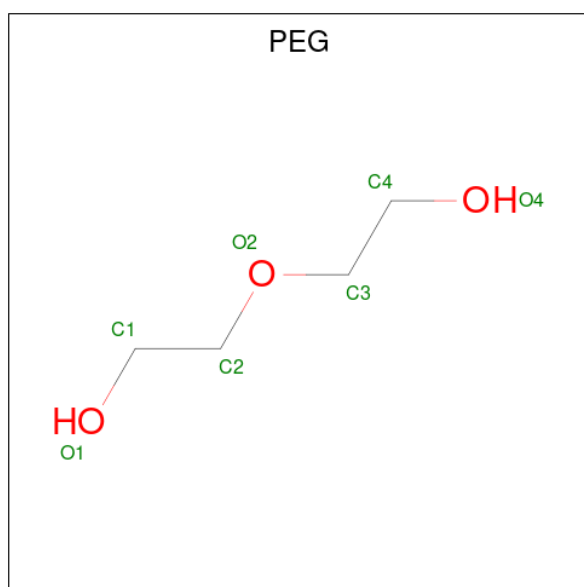
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	1
			5	5		
2	B	8	Total	Cd	0	4
			12	12		
2	C	4	Total	Cd	0	0
			4	4		
2	D	4	Total	Cd	0	1
			6	6		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	3	Total	Cl	0	0
			3	3		
3	C	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



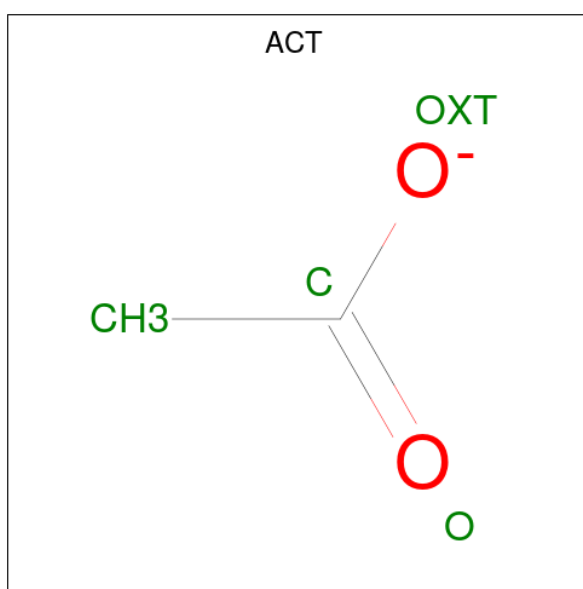
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		

Continued on next page...

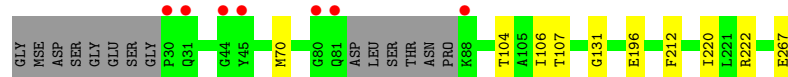
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	119	Total 119	O 119	0	0
6	C	80	Total 80	O 80	0	0
6	D	47	Total 47	O 47	0	0

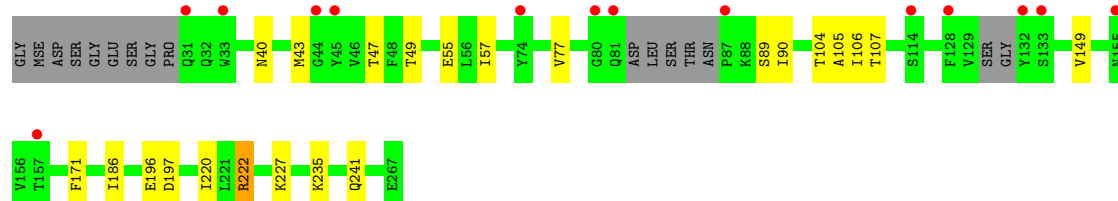
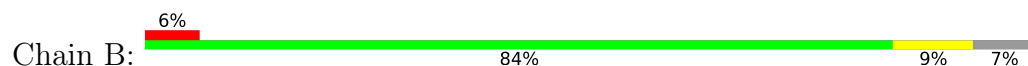
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

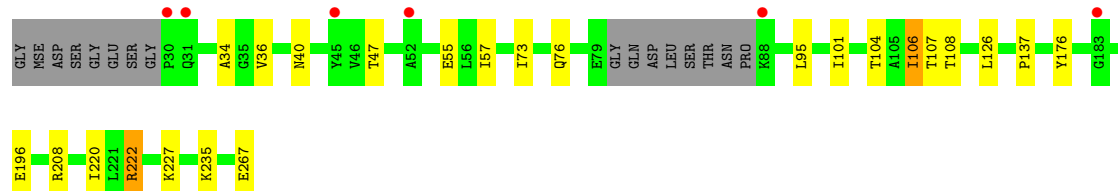
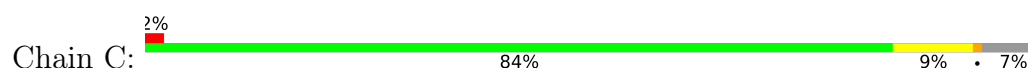
• Molecule 1: Putative lipoprotein



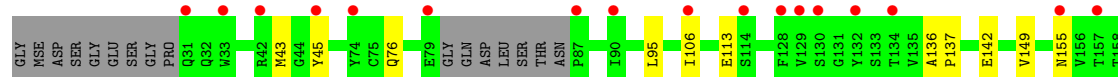
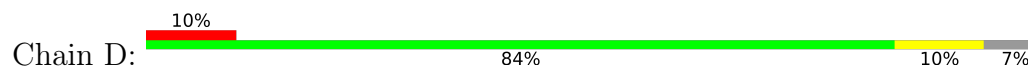
• Molecule 1: Putative lipoprotein

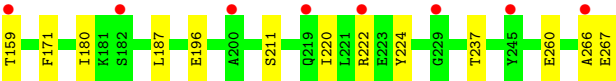


• Molecule 1: Putative lipoprotein



• Molecule 1: Putative lipoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.49Å 77.23Å 97.41Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	47.29 – 1.87 47.29 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.29-1.87) 99.6 (47.29-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0110, PHENIX	Depositor
R, R_{free}	0.191 , 0.220 0.195 , 0.224	Depositor DCC
R_{free} test set	4686 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.9	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	7821	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% 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: CL, ACT, CD, 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	1.03	1/1892 (0.1%)	0.93	1/2573 (0.0%)
1	B	0.91	0/1917	0.88	0/2606
1	C	0.80	0/1892	0.85	0/2570
1	D	0.74	0/1866	0.77	0/2536
All	All	0.88	1/7567 (0.0%)	0.86	1/10285 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	PHE	CA-CB	-5.19	1.45	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	MSE	CG-SE-CE	5.88	111.86	98.92

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	1831	0	1851	7	1
1	B	1849	0	1883	19	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1832	0	1852	17	0
1	D	1813	0	1831	12	3
2	A	5	0	0	0	1
2	B	12	0	0	0	3
2	C	4	0	0	0	0
2	D	6	0	0	0	2
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	28	0	40	0	0
4	B	28	0	40	1	0
4	C	14	0	20	0	0
4	D	7	0	10	0	0
5	B	8	0	6	0	0
5	C	4	0	3	0	0
5	D	4	0	3	1	0
6	A	121	0	0	0	2
6	B	119	0	0	2	1
6	C	80	0	0	1	0
6	D	47	0	0	0	0
All	All	7821	0	7539	50	7

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 3.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222[A]:ARG:HB3	1:B:222[A]:ARG:CZ	2.11	0.80
1:B:40:ASN:HB2	1:B:47[A]:THR:HG22	1.65	0.77
1:C:47[B]:THR:HG21	1:C:55:GLU:OE2	1.89	0.73
1:C:222[A]:ARG:NH1	1:D:142:GLU:OE1	2.23	0.71
1:B:47[A]:THR:HG21	1:B:55:GLU:OE2	1.92	0.70
1:D:222[B]:ARG:HB3	1:D:222[B]:ARG:CZ	2.21	0.70
1:C:196:GLU:OE2	6:C:668:HOH:O	2.11	0.66
1:C:40:ASN:HB2	1:C:47[B]:THR:HG23	1.78	0.66
1:C:40:ASN:HB2	1:C:47[B]:THR:CG2	2.30	0.62
1:B:40:ASN:HB2	1:B:47[A]:THR:CG2	2.31	0.61
1:C:36:VAL:HG13	1:C:101:ILE:HD11	1.82	0.61
1:C:222[A]:ARG:HB3	1:C:222[A]:ARG:CZ	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LEU:HD21	1:D:220:ILE:HG22	1.89	0.54
1:D:149[A]:VAL:HG11	1:D:171:PHE:CE1	2.42	0.54
1:B:40:ASN:OD1	1:B:47[A]:THR:HG23	2.10	0.52
1:D:237:THR:HG22	1:D:260:GLU:HG2	1.92	0.52
1:B:197:ASP:OD1	6:B:579:HOH:O	2.19	0.50
1:B:107:THR:HG23	1:B:220[A]:ILE:HD13	1.93	0.49
1:B:222[A]:ARG:HB3	1:B:222[A]:ARG:NH2	2.28	0.49
1:A:267:GLU:OE2	1:B:227:LYS:NZ	2.44	0.48
1:D:155[B]:ASN:ND2	1:D:155[B]:ASN:H	2.13	0.46
1:B:186[A]:ILE:HD12	1:B:235:LYS:HB3	1.98	0.46
1:A:107:THR:HG23	1:A:220[A]:ILE:HD12	1.97	0.46
1:C:227:LYS:NZ	1:D:267:GLU:OE2	2.49	0.46
1:B:149[B]:VAL:HG11	1:B:171:PHE:CE1	2.51	0.46
1:D:136:ALA:HB1	1:D:137:PRO:HD2	1.97	0.46
1:B:104:THR:HG22	1:B:106:ILE:HG23	1.98	0.45
1:A:222[B]:ARG:HD2	1:B:222[B]:ARG:HD2	1.98	0.45
1:A:107:THR:HG23	1:A:220[A]:ILE:CD1	2.47	0.44
1:B:49:THR:HG21	4:B:331:PEG:H32	1.99	0.44
1:B:77[A]:VAL:HG23	1:B:90:ILE:CG2	2.47	0.44
1:B:47[B]:THR:HB	1:B:57[B]:ILE:HD13	2.00	0.44
1:C:107:THR:HG23	1:C:220:ILE:HG12	1.99	0.44
1:D:76:GLN:HB2	1:D:95:LEU:HD11	1.99	0.44
1:B:105:ALA:HB1	1:B:220[B]:ILE:CD1	2.47	0.44
1:D:266:ALA:HB3	5:D:340:ACT:OXT	2.18	0.44
1:B:241:GLN:NE2	6:B:655:HOH:O	2.44	0.43
1:C:108:THR:O	1:C:176:TYR:HA	2.19	0.43
1:A:104:THR:HG22	1:A:106:ILE:HG23	2.01	0.43
1:C:267:GLU:N	1:C:267:GLU:OE1	2.51	0.43
1:C:34:ALA:HA	1:C:73:ILE:O	2.19	0.43
1:C:126:LEU:O	1:C:137:PRO:HD3	2.20	0.42
1:D:180:ILE:HD13	1:D:224:TYR:HA	2.02	0.42
1:A:131:GLY:O	1:C:208:ARG:HD3	2.21	0.41
1:A:222[B]:ARG:HD2	1:A:222[B]:ARG:HA	1.89	0.41
1:C:47[B]:THR:OG1	1:C:57:ILE:HD13	2.21	0.41
1:B:47[B]:THR:HG21	1:B:57[B]:ILE:HD12	2.02	0.41
1:C:104:THR:HG22	1:C:106:ILE:HG23	2.03	0.40
1:D:43[A]:MSE:HE3	1:D:45:TYR:HE2	1.87	0.40
1:C:76:GLN:HG3	1:C:95:LEU:HD11	2.03	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:OE2	2:A:302[A]:CD:CD[2_555]	2.10	0.10
1:B:196:GLU:OE2	2:B:306[A]:CD:CD[2_555]	2.13	0.07
1:D:113:GLU:OE2	2:B:318[B]:CD:CD[1_545]	2.13	0.07
2:B:319[A]:CD:CD	6:A:429:HOH:O[4_455]	2.15	0.05
6:A:555:HOH:O	6:B:424:HOH:O[1_545]	2.15	0.05
1:D:196:GLU:OE2	2:D:315[B]:CD:CD[2_556]	2.16	0.04
1:D:196:GLU:OE1	2:D:315[A]:CD:CD[2_556]	2.17	0.03

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	239/246 (97%)	234 (98%)	5 (2%)	0	100	100
1	B	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
1	C	237/246 (96%)	231 (98%)	6 (2%)	0	100	100
1	D	235/246 (96%)	232 (99%)	3 (1%)	0	100	100
All	All	949/984 (96%)	929 (98%)	20 (2%)	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	206/210 (98%)	206 (100%)	0	100	100
1	B	208/210 (99%)	203 (98%)	5 (2%)	43	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	206/210 (98%)	202 (98%)	4 (2%)	50	36
1	D	199/210 (95%)	196 (98%)	3 (2%)	57	46
All	All	819/840 (98%)	807 (98%)	12 (2%)	63	46

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43[A]	MSE
1	B	43[B]	MSE
1	B	89	SER
1	B	222[A]	ARG
1	B	222[B]	ARG
1	C	106	ILE
1	C	222[A]	ARG
1	C	222[B]	ARG
1	C	235	LYS
1	D	106	ILE
1	D	159	THR
1	D	211	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	76	GLN
1	D	40	ASN
1	D	67	ASN
1	D	76	GLN
1	D	242	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 36 are monoatomic - leaving 15 for Mogul analysis.

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	$\# Z > 2$
4	PEG	A	332	-	6,6,6	0.49	0	5,5,5	0.14	0
4	PEG	C	334	-	6,6,6	0.41	0	5,5,5	0.49	0
4	PEG	A	333	-	6,6,6	0.33	0	5,5,5	0.34	0
4	PEG	A	337	-	6,6,6	0.30	0	5,5,5	0.49	0
4	PEG	B	331	-	6,6,6	0.40	0	5,5,5	0.25	0
4	PEG	C	338	-	6,6,6	0.51	0	5,5,5	0.31	0
5	ACT	B	342	2	3,3,3	0.94	0	3,3,3	2.11	2 (66%)
5	ACT	C	343	2	3,3,3	0.95	0	3,3,3	2.22	2 (66%)
5	ACT	D	340	2	3,3,3	0.91	0	3,3,3	1.78	1 (33%)
5	ACT	B	341	-	3,3,3	0.85	0	3,3,3	1.40	0
4	PEG	B	336	-	6,6,6	0.53	0	5,5,5	0.57	0
4	PEG	D	339	-	6,6,6	0.54	0	5,5,5	0.16	0
4	PEG	B	335	-	6,6,6	0.52	0	5,5,5	0.26	0
4	PEG	B	330	-	6,6,6	0.34	0	5,5,5	0.37	0
4	PEG	A	329	-	6,6,6	0.40	0	5,5,5	0.58	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
4	PEG	A	332	-	-	3/4/4/4	-
4	PEG	C	334	-	-	1/4/4/4	-
4	PEG	A	333	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	337	-	-	4/4/4/4	-
4	PEG	B	331	-	-	2/4/4/4	-
4	PEG	C	338	-	-	1/4/4/4	-
4	PEG	B	336	-	-	3/4/4/4	-
4	PEG	D	339	-	-	1/4/4/4	-
4	PEG	B	335	-	-	1/4/4/4	-
4	PEG	B	330	-	-	1/4/4/4	-
4	PEG	A	329	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	343	ACT	OXT-C-O	-2.82	111.58	122.03
5	B	342	ACT	OXT-C-O	-2.72	111.93	122.03
5	C	343	ACT	OXT-C-CH3	2.62	126.03	115.05
5	D	340	ACT	OXT-C-O	-2.46	112.89	122.03
5	B	342	ACT	OXT-C-CH3	2.43	125.23	115.05

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	333	PEG	O2-C3-C4-O4
4	A	337	PEG	O2-C3-C4-O4
4	A	337	PEG	O1-C1-C2-O2
4	B	331	PEG	O1-C1-C2-O2
4	C	334	PEG	O2-C3-C4-O4
4	D	339	PEG	O1-C1-C2-O2
4	B	335	PEG	O2-C3-C4-O4
4	C	338	PEG	O1-C1-C2-O2
4	A	333	PEG	O1-C1-C2-O2
4	B	336	PEG	O2-C3-C4-O4
4	B	336	PEG	C1-C2-O2-C3
4	A	332	PEG	O1-C1-C2-O2
4	B	331	PEG	O2-C3-C4-O4
4	A	332	PEG	C1-C2-O2-C3
4	B	336	PEG	O1-C1-C2-O2
4	B	330	PEG	O1-C1-C2-O2
4	A	337	PEG	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	333	PEG	C1-C2-O2-C3
4	A	332	PEG	O2-C3-C4-O4
4	A	337	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	331	PEG	1	0
5	D	340	ACT	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	230/246 (93%)	-0.08	7 (3%) 52 57	12, 28, 58, 92	10 (4%)
1	B	228/246 (92%)	0.11	14 (6%) 27 29	13, 30, 58, 101	13 (5%)
1	C	228/246 (92%)	0.38	6 (2%) 57 62	20, 39, 66, 91	10 (4%)
1	D	228/246 (92%)	0.73	25 (10%) 10 12	23, 46, 71, 91	8 (3%)
All	All	914/984 (92%)	0.28	52 (5%) 29 31	12, 37, 67, 101	41 (4%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	PRO	5.7
1	B	132	TYR	4.6
1	D	79	GLU	4.6
1	D	87	PRO	4.0
1	B	81	GLN	3.8
1	A	30	PRO	3.7
1	C	183	GLY	3.7
1	D	31	GLN	3.6
1	B	133	SER	3.6
1	D	129	VAL	3.3
1	D	134	THR	3.3
1	D	155[A]	ASN	3.3
1	A	45	TYR	3.2
1	A	81	GLN	3.2
1	B	80	GLY	3.0
1	C	31	GLN	3.0
1	C	52	ALA	3.0
1	D	42[A]	ARG	3.0
1	C	88	LYS	2.9
1	B	157	THR	2.9
1	D	74[A]	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	132	TYR	2.8
1	B	44	GLY	2.8
1	D	90	ILE	2.8
1	D	130	SER	2.8
1	C	30	PRO	2.8
1	C	45	TYR	2.7
1	B	31	GLN	2.6
1	D	33	TRP	2.6
1	B	114	SER	2.5
1	D	159	THR	2.5
1	D	157	THR	2.4
1	B	74[A]	TYR	2.4
1	D	266	ALA	2.4
1	A	44	GLY	2.4
1	D	182	SER	2.4
1	A	31	GLN	2.4
1	D	128	PHE	2.3
1	A	88	LYS	2.3
1	D	229	GLY	2.2
1	B	128	PHE	2.1
1	D	106	ILE	2.1
1	A	80	GLY	2.1
1	D	45	TYR	2.1
1	B	155	ASN	2.1
1	D	219	GLN	2.1
1	D	222[A]	ARG	2.1
1	D	114	SER	2.0
1	B	45	TYR	2.0
1	B	33	TRP	2.0
1	D	200	ALA	2.0
1	D	245	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
4	PEG	B	336	7/7	0.73	0.21	61,61,65,69	0
4	PEG	A	337	7/7	0.81	0.16	42,50,57,61	0
4	PEG	D	339	7/7	0.84	0.15	59,63,66,69	0
5	ACT	B	341	4/4	0.84	0.17	62,62,63,64	0
4	PEG	B	335	7/7	0.85	0.14	47,54,56,59	0
4	PEG	A	329	7/7	0.85	0.16	35,51,58,59	0
4	PEG	B	330	7/7	0.86	0.14	49,50,55,56	0
4	PEG	C	338	7/7	0.86	0.16	55,61,64,65	0
4	PEG	C	334	7/7	0.87	0.13	49,52,58,59	0
4	PEG	A	332	7/7	0.87	0.14	51,60,65,68	0
2	CD	B	318[B]	1/1	0.88	0.10	70,70,70,70	1
2	CD	D	317	1/1	0.88	0.11	72,72,72,72	1
2	CD	B	318[A]	1/1	0.88	0.10	84,84,84,84	1
4	PEG	A	333	7/7	0.89	0.14	39,49,55,61	0
4	PEG	B	331	7/7	0.89	0.12	55,59,61,67	0
3	CL	A	321	1/1	0.90	0.14	53,53,53,53	0
3	CL	C	324	1/1	0.91	0.10	47,47,47,47	0
5	ACT	B	342	4/4	0.92	0.13	33,44,47,51	0
5	ACT	C	343	4/4	0.92	0.15	54,58,59,62	0
2	CD	B	308[B]	1/1	0.94	0.07	96,96,96,96	1
2	CD	B	308[A]	1/1	0.94	0.07	60,60,60,60	1
5	ACT	D	340	4/4	0.94	0.14	68,68,68,69	0
3	CL	C	326	1/1	0.96	0.09	43,43,43,43	0
2	CD	B	309	1/1	0.96	0.06	73,73,73,73	1
3	CL	B	322	1/1	0.97	0.06	38,38,38,38	0
2	CD	D	315[B]	1/1	0.97	0.05	43,43,43,43	1
2	CD	D	315[C]	1/1	0.97	0.05	45,45,45,45	1
2	CD	C	313	1/1	0.97	0.05	49,49,49,49	1
2	CD	D	315[A]	1/1	0.97	0.05	47,47,47,47	1
3	CL	B	320	1/1	0.97	0.06	35,35,35,35	0
3	CL	A	328	1/1	0.98	0.04	33,33,33,33	0
2	CD	C	316	1/1	0.98	0.07	46,46,46,46	0
2	CD	A	300	1/1	0.98	0.06	41,41,41,41	1
2	CD	B	304	1/1	0.98	0.07	38,38,38,38	1
3	CL	A	323	1/1	0.98	0.04	36,36,36,36	0
2	CD	B	319[B]	1/1	0.99	0.02	35,35,35,35	1
2	CD	C	310	1/1	0.99	0.04	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	C	311	1/1	0.99	0.04	52,52,52,52	0
2	CD	A	307	1/1	0.99	0.02	29,29,29,29	0
2	CD	A	301	1/1	0.99	0.03	31,31,31,31	0
3	CL	B	325	1/1	0.99	0.03	30,30,30,30	0
2	CD	D	312	1/1	0.99	0.03	50,50,50,50	0
2	CD	B	305	1/1	0.99	0.03	29,29,29,29	0
3	CL	D	327	1/1	0.99	0.05	42,42,42,42	0
2	CD	B	306[A]	1/1	0.99	0.04	42,42,42,42	1
2	CD	B	306[B]	1/1	0.99	0.04	44,44,44,44	1
2	CD	B	319[A]	1/1	0.99	0.02	22,22,22,22	1
2	CD	A	302[A]	1/1	1.00	0.03	28,28,28,28	1
2	CD	B	303	1/1	1.00	0.02	29,29,29,29	0
2	CD	A	302[C]	1/1	1.00	0.03	41,41,41,41	1
2	CD	D	314	1/1	1.00	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.