Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 08:25 AM EST

PDB ID	:	3P24
Title	:	Structure of profragilysin-3 from Bacteroides fragilis
Authors	:	Goulas, T.; Arolas, J.L.; Gomis-Ruth, F.X.
Deposited on	:	2010-10-01
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

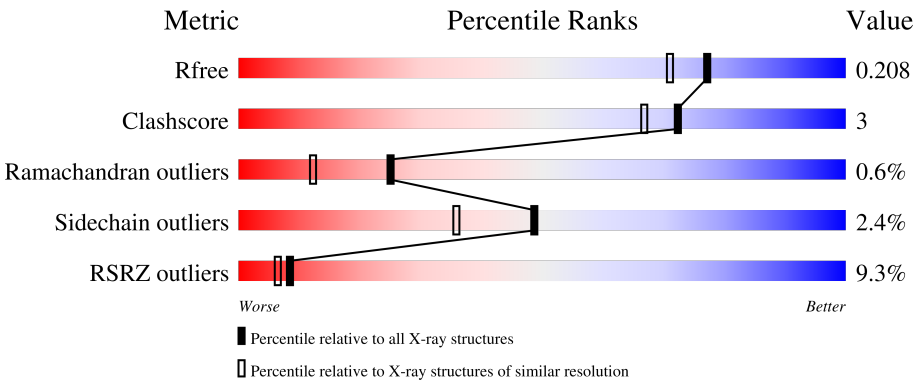
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	397	7%, 82%, 7% • 10%
1	B	397	9%, 81%, 8% • 11%
1	C	397	8%, 82%, 7% • 11%
1	D	397	9%, 80%, 9% • 10%

2 Entry composition (i)

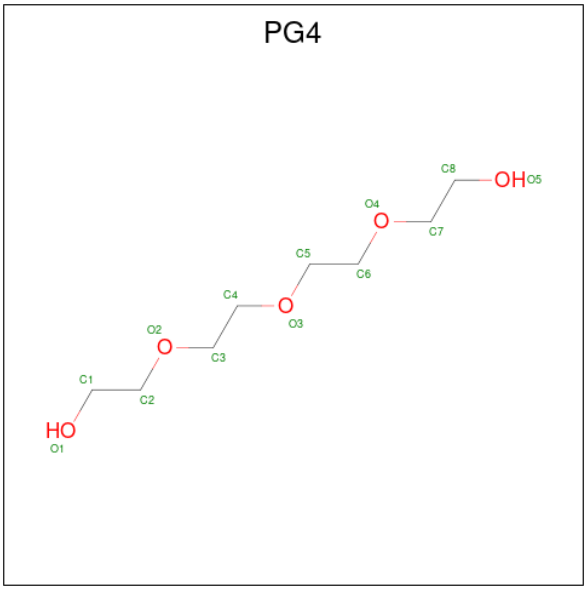
There are 6 unique types of molecules in this entry. The entry contains 12617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BFT-3.

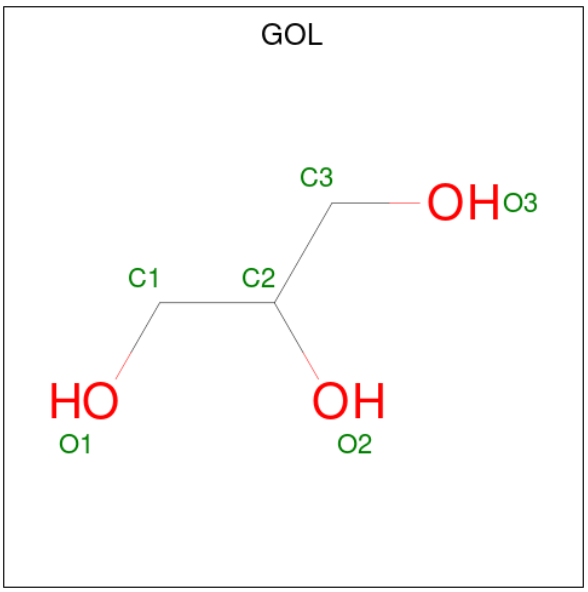
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2852	1809	475	554	14	0	3	0
1	B	355	2836	1797	474	551	14	0	3	0
1	C	354	2847	1809	472	552	14	0	7	0
1	D	357	2860	1814	475	556	15	0	6	0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



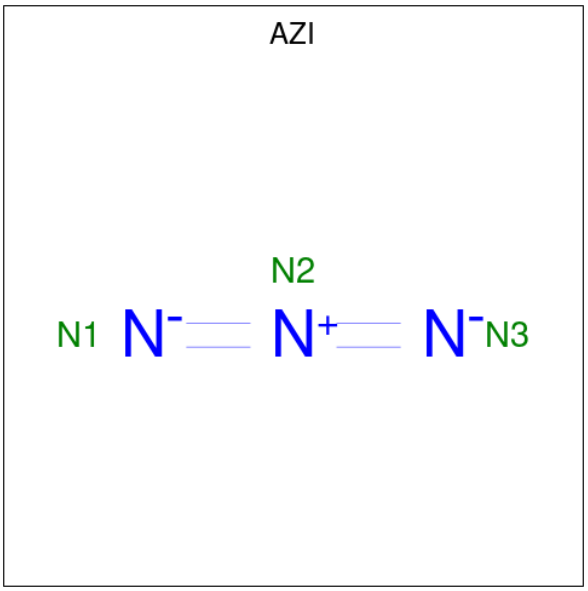
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0
2	D	1	13	8	5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 3 3	0	0
4	A	1	Total N 3 3	0	0
4	B	1	Total N 3 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	341	Total O 341 341	0	0
6	B	221	Total O 221 221	0	0

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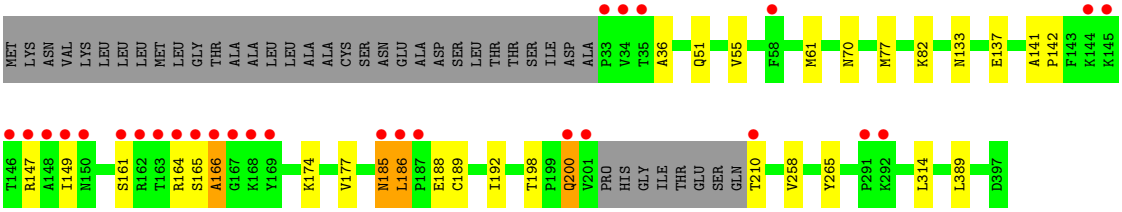
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	290	290	290	0	0
			Total	O		
6	D	295	295	295	0	0

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: BFT-3

Chain A:

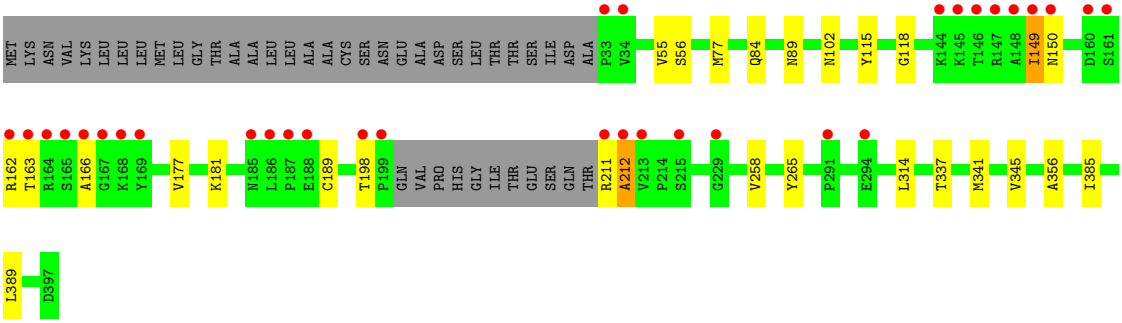


• Molecule 1: BFT-3

Chain B:

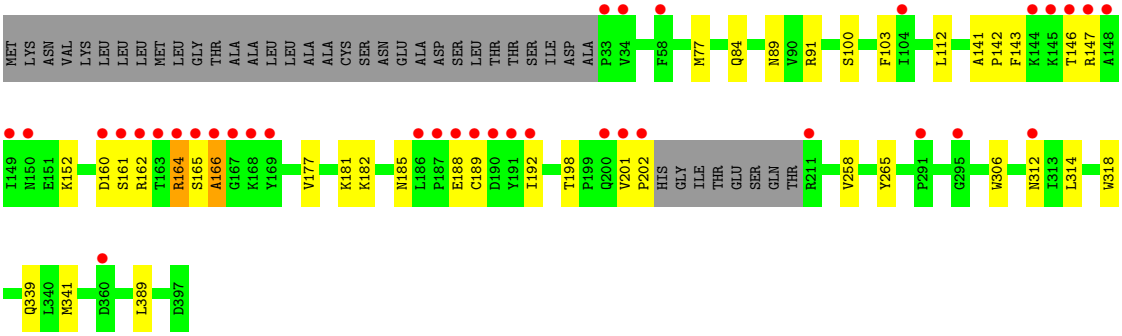
• Molecule 1: BFT-3

Chain C:



• Molecule 1: BFT-3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.74Å 69.14Å 158.91Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 45.16 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-1.80) 98.9 (45.16-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.204 0.177 , 0.208	Depositor DCC
R_{free} test set	781 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12617	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: AZI, ZN, PG4, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.59	0/2924	0.65	0/3959
1	B	0.51	0/2906	0.66	4/3932 (0.1%)
1	C	0.54	0/2935	0.64	0/3972
1	D	0.56	0/2944	0.65	0/3985
All	All	0.55	0/11709	0.65	4/15848 (0.0%)

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	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	B	113	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	B	113	ARG	CD-NE-CZ	6.06	132.08	123.60
1	B	113	ARG	CG-CD-NE	5.81	124.01	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	ILE	Peptide
1	C	149	ILE	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	2852	0	2768	17	0
1	B	2836	0	2758	20	0
1	C	2847	0	2764	17	0
1	D	2860	0	2775	22	0
2	A	13	0	18	0	0
2	D	13	0	18	0	0
3	A	18	0	24	0	0
3	B	6	0	8	2	0
3	D	12	0	16	0	0
4	A	6	0	0	0	0
4	B	3	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	341	0	0	2	0
6	B	221	0	0	0	0
6	C	290	0	0	1	0
6	D	295	0	0	2	0
All	All	12617	0	11149	76	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 3.

All (76) 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:177:VAL:HG13	1:C:341:MET:HE2	1.26	1.10
1:B:160:ASP:HB3	1:B:166:ALA:HB2	1.31	1.08
1:D:177:VAL:HG13	1:D:341:MET:HE1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:CYS:HB2	1:D:314:LEU:HD21	1.70	0.74
1:B:258:VAL:HG11	1:B:389:LEU:HD22	1.71	0.70
1:A:82:LYS:NZ	6:A:543:HOH:O	2.25	0.68
1:C:258[B]:VAL:HG11	1:C:389:LEU:HD22	1.78	0.66
1:C:84:GLN:HE21	1:C:89:ASN:HD22	1.45	0.65
1:C:177:VAL:CG1	1:C:341:MET:HE2	2.16	0.62
1:B:160:ASP:OD1	1:B:161:SER:N	2.34	0.61
1:D:189:CYS:CB	1:D:314:LEU:HD21	2.32	0.60
1:B:160:ASP:HB3	1:B:166:ALA:CB	2.21	0.59
1:D:177:VAL:HG21	6:D:1387:HOH:O	2.04	0.57
1:C:198:THR:HG21	6:C:905:HOH:O	2.05	0.56
1:D:84:GLN:HE21	1:D:89:ASN:HD22	1.53	0.56
1:D:103:PHE:CE1	1:D:112:LEU:HD13	2.40	0.56
1:D:162:ARG:NH1	6:D:1326:HOH:O	2.38	0.56
1:B:186:LEU:HD21	1:B:342:TYR:CE2	2.41	0.56
1:A:186:LEU:HD13	1:A:186:LEU:O	2.06	0.56
1:B:306:TRP:O	1:B:339:GLN:HG3	2.05	0.56
1:C:258[A]:VAL:HG21	1:C:389:LEU:HD22	1.88	0.55
1:C:56:SER:C	1:C:77:MET:HE3	2.27	0.55
1:A:133:ASN:O	1:A:137:GLU:HG3	2.06	0.54
1:D:189:CYS:HA	1:D:312:ASN:HB3	1.88	0.54
1:A:165:SER:O	1:A:166:ALA:HB3	2.07	0.54
1:B:116:ARG:HH21	3:B:506:GOL:H11	1.73	0.54
1:D:160:ASP:OD2	1:D:161:SER:N	2.40	0.53
1:A:141:ALA:HB3	1:A:142:PRO:HD3	1.91	0.53
1:D:258:VAL:HG11	1:D:389:LEU:HD22	1.92	0.52
1:A:258[A]:VAL:HG21	1:A:389:LEU:HD22	1.92	0.51
1:D:165:SER:O	1:D:166:ALA:HB3	2.11	0.51
1:B:117:ASN:OD1	3:B:506:GOL:H12	2.10	0.50
1:D:198:THR:HG23	1:D:318:TRP:CZ3	2.47	0.50
1:D:143:PHE:HA	1:D:146:THR:HG22	1.93	0.49
1:A:200:GLN:HE21	1:A:200:GLN:HA	1.78	0.48
1:A:165:SER:O	1:A:166:ALA:CB	2.62	0.48
1:C:211:ARG:O	1:C:212:ALA:HB2	2.14	0.48
1:D:182:LYS:O	1:D:185:ASN:ND2	2.47	0.48
1:B:62:ILE:HD12	1:B:75:VAL:HG21	1.95	0.47
1:A:174:LYS:HD2	1:A:174:LYS:C	2.35	0.47
1:C:181:LYS:HE2	1:C:341:MET:O	2.15	0.46
1:B:55:VAL:O	1:B:77:MET:CE	2.63	0.46
1:D:306:TRP:O	1:D:339:GLN:HG3	2.16	0.46
1:A:55:VAL:O	1:A:77:MET:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ARG:O	1:D:164:ARG:HG3	2.16	0.45
1:A:185:ASN:O	1:A:185:ASN:CG	2.54	0.44
1:C:84:GLN:HE21	1:C:89:ASN:ND2	2.11	0.44
1:A:55:VAL:O	1:A:77:MET:CE	2.66	0.44
1:A:177:VAL:HG21	6:A:606:HOH:O	2.17	0.44
1:C:356:ALA:HB2	1:C:385:ILE:HD11	2.00	0.44
1:C:115[A]:TYR:CE2	1:C:118:GLY:HA2	2.52	0.44
1:D:165:SER:O	1:D:166:ALA:CB	2.66	0.43
1:B:115:TYR:HA	1:B:119:GLU:O	2.18	0.43
1:B:77:MET:HB3	4:B:509:AZI:N2	2.33	0.43
1:C:163:THR:HB	1:C:166:ALA:HB3	2.00	0.43
1:D:181:LYS:HE2	1:D:341:MET:O	2.19	0.43
1:B:55:VAL:O	1:B:77:MET:HE2	2.18	0.43
1:B:141:ALA:HB3	1:B:142:PRO:HD3	2.01	0.43
1:B:56:SER:C	1:B:77:MET:HE3	2.39	0.43
1:C:55:VAL:O	1:C:77:MET:HE2	2.19	0.43
1:A:186:LEU:HD22	1:A:188:GLU:HA	2.02	0.42
1:D:77[B]:MET:HE2	1:D:91:ARG:HD2	2.01	0.42
1:A:186:LEU:CD2	1:A:188:GLU:HA	2.50	0.42
1:B:185:ASN:N	1:B:185:ASN:HD22	2.18	0.42
1:B:358:HIS:HA	1:B:366:MET:O	2.20	0.42
1:C:337:THR:HG22	1:C:345:VAL:HG11	2.01	0.42
1:B:186:LEU:HD23	1:B:187:PRO:O	2.19	0.42
1:A:189:CYS:HB2	1:A:314:LEU:HD21	2.02	0.41
1:C:189:CYS:HB2	1:C:314:LEU:HD21	2.02	0.41
1:D:201:VAL:HG12	1:D:202:PRO:HD2	2.03	0.41
1:B:245:ALA:HA	1:B:260:LEU:HD12	2.03	0.41
1:D:141:ALA:HB3	1:D:142:PRO:HD3	2.03	0.41
1:A:36:ALA:HB1	1:A:51:GLN:OE1	2.21	0.40
1:C:115[A]:TYR:CZ	1:C:118:GLY:HA2	2.54	0.40
1:D:201:VAL:CG1	1:D:202:PRO:HD2	2.51	0.40
1:B:236:GLU:HB3	1:B:338:THR:O	2.22	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	356/397 (90%)	349 (98%)	5 (1%)	2 (1%)	25	12
1	B	354/397 (89%)	343 (97%)	9 (2%)	2 (1%)	25	12
1	C	357/397 (90%)	349 (98%)	6 (2%)	2 (1%)	25	12
1	D	359/397 (90%)	343 (96%)	14 (4%)	2 (1%)	25	12
All	All	1426/1588 (90%)	1384 (97%)	34 (2%)	8 (1%)	25	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ALA
1	D	166	ALA
1	C	149	ILE
1	B	189	CYS
1	C	212	ALA
1	A	192	ILE
1	B	161	SER
1	D	192	ILE

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	310/339 (91%)	297 (96%)	13 (4%)	30	15
1	B	308/339 (91%)	301 (98%)	7 (2%)	50	37
1	C	311/339 (92%)	306 (98%)	5 (2%)	62	54
1	D	313/339 (92%)	305 (97%)	8 (3%)	46	32
All	All	1242/1356 (92%)	1209 (97%)	33 (3%)	49	31

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MET
1	A	70	ASN
1	A	147	ARG
1	A	149	ILE
1	A	161	SER
1	A	164	ARG
1	A	185	ASN
1	A	186	LEU
1	A	198	THR
1	A	200	GLN
1	A	210	THR
1	A	265[A]	TYR
1	A	265[B]	TYR
1	B	113	ARG
1	B	161	SER
1	B	164	ARG
1	B	173	VAL
1	B	185	ASN
1	B	211	ARG
1	B	277	ASP
1	C	102	ASN
1	C	150	ASN
1	C	162	ARG
1	C	265[A]	TYR
1	C	265[B]	TYR
1	D	100[A]	SER
1	D	100[B]	SER
1	D	147	ARG
1	D	152	LYS
1	D	164	ARG
1	D	188	GLU
1	D	265[A]	TYR
1	D	265[B]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	200	GLN
1	B	67	ASN
1	B	84	GLN
1	B	89	ASN
1	B	185	ASN

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Mol	Chain	Res	Type
1	B	200	GLN
1	C	89	ASN
1	C	102	ASN
1	D	89	ASN
1	D	185	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	GOL	D	508	-	5,5,5	0.36	0	5,5,5	0.30	0
3	GOL	A	505	-	5,5,5	0.40	0	5,5,5	0.48	0
2	PG4	A	502	-	12,12,12	0.52	0	11,11,11	0.24	0
4	AZI	A	511	-	0,2,2	-	-	0,1,1	-	-
3	GOL	B	506	-	5,5,5	0.44	0	5,5,5	0.54	0
4	AZI	B	509	-	0,2,2	-	-	0,1,1	-	-
3	GOL	A	503	-	5,5,5	0.50	0	5,5,5	0.69	0
3	GOL	D	507	-	5,5,5	0.40	0	5,5,5	0.13	0
2	PG4	D	501	-	12,12,12	0.52	0	11,11,11	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.39	0
4	AZI	A	510	-	0,2,2	-	-	0,1,1	-	-

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	GOL	D	508	-	-	0/4/4/4	-
3	GOL	A	505	-	-	3/4/4/4	-
2	PG4	A	502	-	-	2/10/10/10	-
3	GOL	B	506	-	-	2/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	D	507	-	-	2/4/4/4	-
2	PG4	D	501	-	-	2/10/10/10	-
3	GOL	A	504	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	A	504	GOL	C1-C2-C3-O3
3	A	505	GOL	O1-C1-C2-C3
3	B	506	GOL	C1-C2-C3-O3
3	A	505	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	504	GOL	O2-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	B	506	GOL	O2-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
2	A	502	PG4	C8-C7-O4-C6
3	D	507	GOL	O2-C2-C3-O3
2	D	501	PG4	C8-C7-O4-C6
2	D	501	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	502	PG4	O4-C7-C8-O5
3	D	507	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	506	GOL	2	0
4	B	509	AZI	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	357/397 (89%)	0.37	28 (7%)	13	10	14, 25, 63, 80	0
1	B	355/397 (89%)	0.44	37 (10%)	6	5	16, 34, 72, 90	0
1	C	354/397 (89%)	0.30	32 (9%)	9	7	14, 28, 64, 83	0
1	D	357/397 (89%)	0.49	36 (10%)	7	5	14, 28, 70, 86	0
All	All	1423/1588 (89%)	0.40	133 (9%)	8	6	14, 29, 68, 90	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	ALA	13.0
1	B	166	ALA	11.8
1	D	163	THR	10.4
1	C	166	ALA	9.7
1	D	33	PRO	9.6
1	C	149	ILE	9.4
1	A	165	SER	9.2
1	B	186	LEU	9.0
1	A	166	ALA	9.0
1	B	149	ILE	8.9
1	C	162	ARG	8.7
1	B	162	ARG	8.6
1	D	201	VAL	8.4
1	B	165	SER	8.4
1	A	149	ILE	8.0
1	A	164	ARG	8.0
1	D	34	VAL	7.9
1	B	167	GLY	7.8
1	B	163	THR	7.7
1	D	162	ARG	7.6
1	C	33	PRO	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	210	THR	7.5
1	D	165	SER	7.3
1	B	164	ARG	7.2
1	A	163	THR	7.0
1	A	34	VAL	7.0
1	C	164	ARG	6.9
1	A	201	VAL	6.6
1	D	149	ILE	6.5
1	C	161	SER	6.4
1	C	165	SER	6.3
1	B	34	VAL	6.3
1	C	163	THR	6.2
1	C	150	ASN	6.1
1	D	150	ASN	6.0
1	C	199	PRO	6.0
1	A	161	SER	5.9
1	D	187	PRO	5.9
1	B	169	TYR	5.7
1	B	33	PRO	5.7
1	C	211	ARG	5.7
1	B	200	GLN	5.6
1	D	161	SER	5.6
1	D	146	THR	5.5
1	C	147	ARG	5.4
1	B	211	ARG	5.3
1	C	167	GLY	5.3
1	B	147	ARG	5.3
1	A	33	PRO	5.3
1	D	167	GLY	5.3
1	B	161	SER	5.3
1	C	212	ALA	5.2
1	A	148	ALA	5.1
1	C	186	LEU	5.1
1	C	145	LYS	5.0
1	B	189	CYS	4.9
1	B	188	GLU	4.9
1	D	147	ARG	4.9
1	A	167	GLY	4.8
1	D	202	PRO	4.7
1	A	200	GLN	4.6
1	B	212	ALA	4.6
1	D	168	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	164	ARG	4.5
1	A	185	ASN	4.4
1	A	186	LEU	4.4
1	D	192	ILE	4.2
1	A	291	PRO	4.2
1	A	146	THR	4.2
1	B	148	ALA	4.2
1	C	215	SER	4.2
1	C	169	TYR	4.2
1	C	34	VAL	4.1
1	D	148	ALA	4.1
1	D	58	PHE	4.1
1	B	150	ASN	4.0
1	D	291	PRO	3.9
1	A	168	LYS	3.8
1	B	145	LYS	3.8
1	C	146	THR	3.8
1	A	162	ARG	3.7
1	D	200	GLN	3.7
1	D	189	CYS	3.7
1	C	291	PRO	3.6
1	B	146	THR	3.6
1	A	169	TYR	3.5
1	C	148	ALA	3.5
1	C	168	LYS	3.5
1	B	168	LYS	3.5
1	D	169	TYR	3.3
1	A	147	ARG	3.1
1	B	190	ASP	3.0
1	D	160	ASP	3.0
1	C	213	VAL	2.9
1	C	144	LYS	2.9
1	B	144	LYS	2.9
1	B	199	PRO	2.9
1	A	58	PHE	2.9
1	C	229	GLY	2.8
1	D	211	ARG	2.8
1	B	185	ASN	2.8
1	C	198	THR	2.8
1	B	187	PRO	2.8
1	A	144	LYS	2.8
1	C	188	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	294	GLU	2.7
1	C	185	ASN	2.7
1	A	150	ASN	2.6
1	D	188	GLU	2.6
1	B	228	ASN	2.5
1	A	35	THR	2.5
1	C	187	PRO	2.4
1	D	186	LEU	2.4
1	A	145	LYS	2.4
1	B	312	ASN	2.4
1	D	144	LYS	2.4
1	B	213	VAL	2.3
1	B	291	PRO	2.3
1	B	229	GLY	2.3
1	D	295	GLY	2.3
1	B	311	ASN	2.3
1	B	160	ASP	2.3
1	C	294	GLU	2.2
1	A	187	PRO	2.1
1	D	145	LYS	2.1
1	D	190	ASP	2.1
1	A	292	LYS	2.1
1	D	312	ASN	2.1
1	D	191	TYR	2.0
1	B	215	SER	2.0
1	D	104	ILE	2.0
1	D	360	ASP	2.0
1	C	160	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	505	6/6	0.57	0.27	59,61,61,61	0
3	GOL	A	503	6/6	0.77	0.23	46,48,48,50	0
3	GOL	D	507	6/6	0.83	0.17	67,68,68,68	0
3	GOL	B	506	6/6	0.84	0.19	56,56,56,57	0
4	AZI	A	510	3/3	0.84	0.14	44,44,48,48	0
3	GOL	D	508	6/6	0.85	0.13	57,58,59,59	0
3	GOL	A	504	6/6	0.85	0.13	65,65,66,67	0
4	AZI	A	511	3/3	0.86	0.20	48,48,48,50	0
2	PG4	D	501	13/13	0.88	0.20	45,48,55,56	0
2	PG4	A	502	13/13	0.89	0.17	43,45,53,54	0
4	AZI	B	509	3/3	0.91	0.15	40,40,46,47	0
5	ZN	A	999	1/1	1.00	0.08	19,19,19,19	0
5	ZN	B	999	1/1	1.00	0.04	34,34,34,34	0
5	ZN	C	999	1/1	1.00	0.07	25,25,25,25	0
5	ZN	D	999	1/1	1.00	0.07	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.