



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 3P24 / pdb_00003p24
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 ⓘ 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

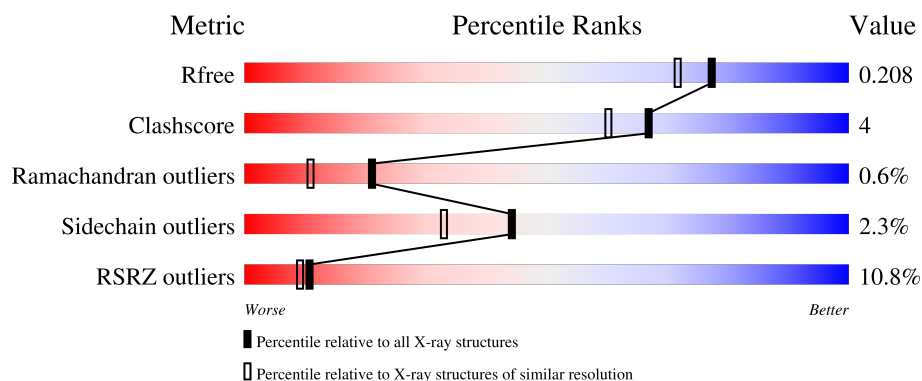
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	397	
1	B	397	
1	C	397	
1	D	397	

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
4	AZI	A	510	-	X	-	-
4	AZI	A	511	-	X	-	-
4	AZI	B	509	-	X	-	-

2 Entry composition [i](#)

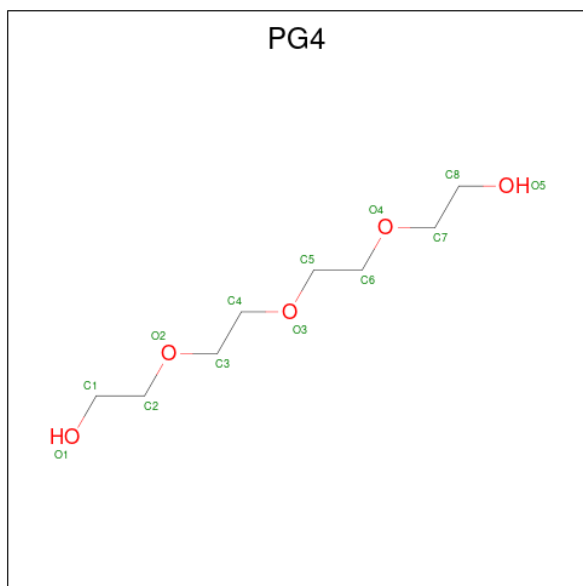
There are 6 unique types of molecules in this entry. The entry contains 12617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



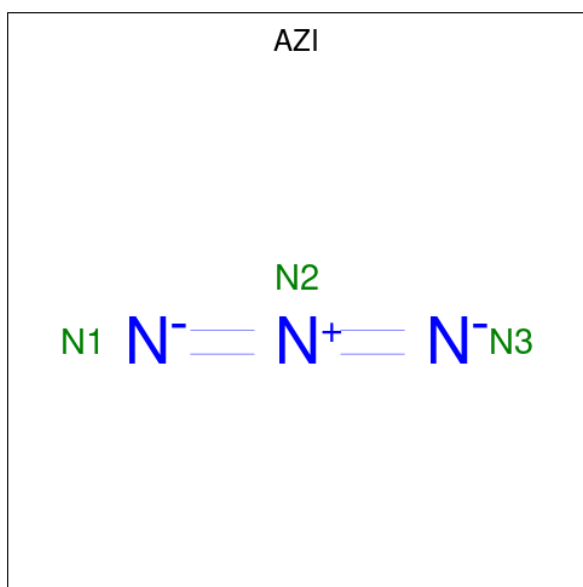
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is AZIDE ION (CCD ID: 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 (CCD ID: 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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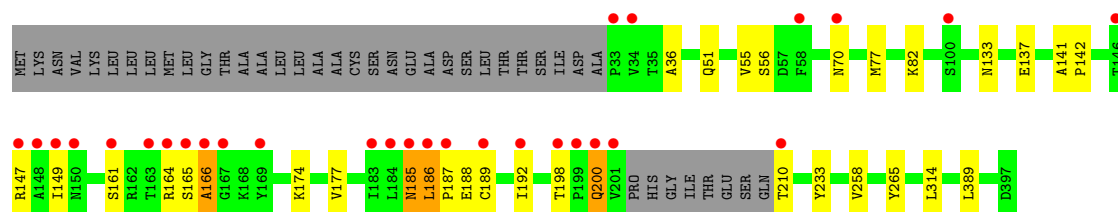
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	290	Total 290	O 290	0	0
6	D	295	Total 295	O 295	0	0

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.

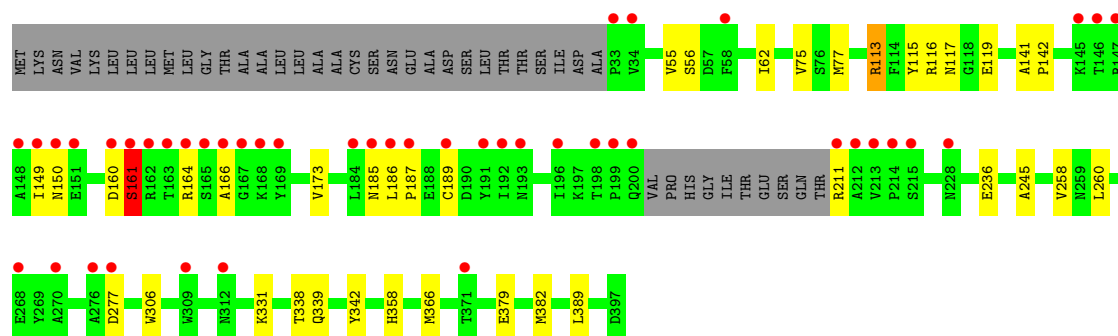
• Molecule 1: BFT-3

Chain A: 



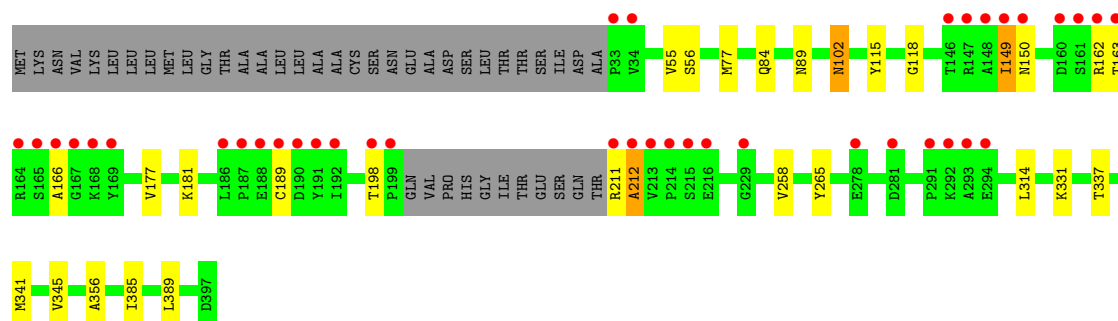
• Molecule 1: BFT-3

Chain B: 

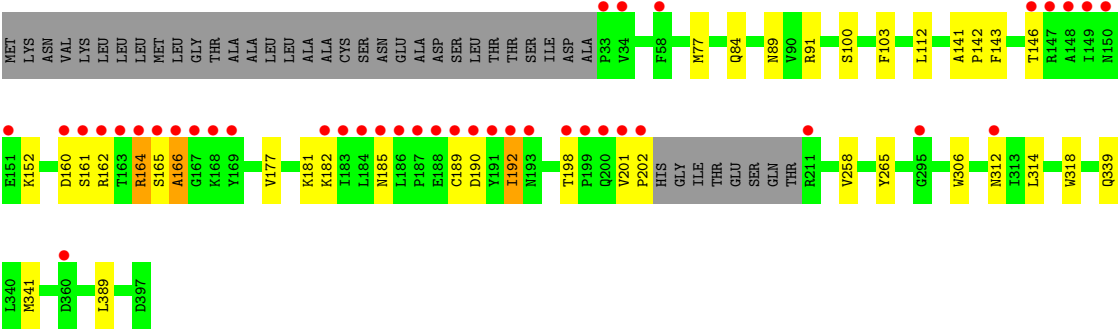
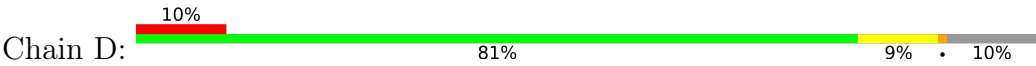


• Molecule 1: BFT-3

Chain C: 



● Molecule 1: BFT-3



4 Data and refinement statistics

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 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-1.80) 98.9 (50.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: GOL, AZI, ZN, PG4

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	0.68	0/2924	0.76	1/3959 (0.0%)
1	B	0.59	0/2906	0.78	3/3932 (0.1%)
1	C	0.62	0/2935	0.76	0/3972
1	D	0.66	0/2944	0.77	1/3985 (0.0%)
All	All	0.64	0/11709	0.77	5/15848 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASN	N-CA-C	-6.83	102.19	111.55
1	D	190	ASP	N-CA-C	6.20	116.26	108.45
1	B	113	ARG	CD-NE-CZ	5.48	132.08	124.40
1	B	113	ARG	CG-CD-NE	5.46	124.01	112.00
1	A	233	TYR	CB-CA-C	5.25	115.66	109.47

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

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	19	0
1	B	2836	0	2758	20	0
1	C	2847	0	2764	20	0
1	D	2860	0	2775	25	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	84	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 4.

All (84) 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:160:ASP:HB3	1:B:166:ALA:HB2	1.31	1.08
1:C:177:VAL:HG13	1:C:341:MET:HE2	1.43	0.99
1:B:55:VAL:O	1:B:77:MET:HE2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:O	1:A:77:MET:HE2	1.87	0.74
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:C:177:VAL:HG13	1:C:341:MET:CE	2.21	0.69
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:55:VAL:O	1:C:77:MET:HE2	1.98	0.63
1:C:341:MET:HE2	1:C:341:MET:HA	1.81	0.62
1:D:177:VAL:HG13	1:D:341:MET:HE2	1.83	0.61
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:C:56:SER:C	1:C:77:MET:HE3	2.26	0.60
1:B:160:ASP:HB3	1:B:166:ALA:CB	2.21	0.59
1:D:77[B]:MET:HE1	1:D:91:ARG:CG	2.33	0.59
1:B:56:SER:C	1:B:77:MET:HE3	2.28	0.58
1:D:341:MET:HE2	1:D:341:MET:HA	1.85	0.58
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:D:77[B]:MET:HE1	1:D:91:ARG:HG2	1.89	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:A:174:LYS:HD2	1:A:174:LYS:C	2.35	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:A:56:SER:C	1:A:77:MET:HE3	2.37	0.50
1:D:143:PHE:HA	1:D:146:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:O	1:A:185:ASN:CG	2.54	0.49
1:C:177:VAL:HA	1:C:341:MET:HE1	1.94	0.48
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:C:181:LYS:HE2	1:C:341:MET:O	2.15	0.46
1:D:306:TRP:O	1:D:339:GLN:HG3	2.16	0.46
1:D:164:ARG:O	1:D:164:ARG:HG3	2.16	0.45
1:C:84:GLN:HE21	1:C:89:ASN:ND2	2.11	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:77[B]:MET:HE1	1:D:91:ARG:HB3	2.00	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:141:ALA:HB3	1:B:142:PRO:HD3	2.01	0.43
1:A:186:LEU:HD22	1:A:187:PRO:C	2.45	0.42
1:A:186:LEU:HD22	1:A:188:GLU:HA	2.02	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:B:379:GLU:HA	1:B:382:MET:HE2	2.02	0.41
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:C:102:ASN:HD22	1:C:102:ASN:C	2.29	0.40
1:A:55:VAL:O	1:A:77:MET:CE	2.66	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

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	356/397 (90%)	349 (98%)	5 (1%)	2 (1%)	21	11
1	B	354/397 (89%)	343 (97%)	9 (2%)	2 (1%)	21	11
1	C	357/397 (90%)	349 (98%)	6 (2%)	2 (1%)	21	11
1	D	359/397 (90%)	343 (96%)	14 (4%)	2 (1%)	21	11
All	All	1426/1588 (90%)	1384 (97%)	34 (2%)	8 (1%)	21	11

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

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%)	298 (96%)	12 (4%)	28	16
1	B	308/339 (91%)	301 (98%)	7 (2%)	44	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	311/339 (92%)	305 (98%)	6 (2%)	50	41
1	D	313/339 (92%)	306 (98%)	7 (2%)	45	34
All	All	1242/1356 (92%)	1210 (97%)	32 (3%)	44	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	211	ARG
1	B	277	ASP
1	B	331	LYS
1	C	102	ASN
1	C	150	ASN
1	C	162	ARG
1	C	265[A]	TYR
1	C	265[B]	TYR
1	C	331	LYS
1	D	100[A]	SER
1	D	100[B]	SER
1	D	152	LYS
1	D	164	ARG
1	D	192	ILE
1	D	265[A]	TYR
1	D	265[B]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	102	ASN
1	A	200	GLN
1	A	357	ASN
1	B	67	ASN
1	B	185	ASN
1	B	200	GLN
1	C	89	ASN
1	C	133	ASN
1	C	259	ASN
1	D	89	ASN
1	D	185	ASN
1	D	200	GLN

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](#)

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	$\# Z > 2$
4	AZI	A	510	-	2,2,2	3.12	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AZI	B	509	-	2,2,2	2.98	2 (100%)	0,1,1	-	-
3	GOL	D	507	-	5,5,5	0.41	0	5,5,5	0.15	0
3	GOL	A	505	-	5,5,5	0.41	0	5,5,5	0.49	0
4	AZI	A	511	-	2,2,2	2.98	2 (100%)	0,1,1	-	-
3	GOL	B	506	-	5,5,5	0.45	0	5,5,5	0.58	0
2	PG4	D	501	-	12,12,12	0.52	0	11,11,11	0.16	0
3	GOL	A	503	-	5,5,5	0.51	0	5,5,5	0.75	0
3	GOL	D	508	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	A	504	-	5,5,5	0.39	0	5,5,5	0.40	0
2	PG4	A	502	-	12,12,12	0.52	0	11,11,11	0.24	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	GOL	D	507	-	-	1/4/4/4	-
3	GOL	A	505	-	-	3/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
2	PG4	D	501	-	-	2/10/10/10	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	D	508	-	-	0/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
2	PG4	A	502	-	-	2/10/10/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	AZI	N1-N2	-3.15	1.16	1.23
4	B	509	AZI	N1-N2	-3.14	1.16	1.23
4	A	510	AZI	N3-N2	-3.10	1.16	1.23
4	A	511	AZI	N1-N2	-3.00	1.17	1.23
4	A	511	AZI	N3-N2	-2.96	1.17	1.23
4	B	509	AZI	N3-N2	-2.82	1.17	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (16) 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
3	D	507	GOL	O2-C2-C3-O3
2	A	502	PG4	C8-C7-O4-C6
2	D	501	PG4	O1-C1-C2-O2
2	D	501	PG4	C8-C7-O4-C6
2	A	502	PG4	O4-C7-C8-O5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	509	AZI	1	0
3	B	506	GOL	2	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	357/397 (89%)	0.24	29 (8%) 18 16	10, 25, 63, 80	3 (0%)
1	B	355/397 (89%)	0.64	45 (12%) 8 6	14, 34, 72, 90	3 (0%)
1	C	354/397 (89%)	0.33	39 (11%) 10 9	10, 28, 64, 83	7 (1%)
1	D	357/397 (89%)	0.42	40 (11%) 10 8	10, 28, 70, 86	6 (1%)
All	All	1423/1588 (89%)	0.41	153 (10%) 11 9	10, 29, 68, 90	19 (1%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	ALA	10.0
1	C	149	ILE	7.5
1	B	149	ILE	7.0
1	D	192	ILE	6.9
1	D	189	CYS	6.8
1	C	166	ALA	5.9
1	B	166	ALA	5.9
1	B	167	GLY	5.9
1	B	186	LEU	5.8
1	C	33	PRO	5.7
1	A	166	ALA	5.6
1	D	34	VAL	5.5
1	D	33	PRO	5.4
1	A	165	SER	5.4
1	B	165	SER	5.3
1	D	148	ALA	5.3
1	D	163	THR	5.3
1	A	149	ILE	5.2
1	A	146	THR	5.1
1	B	187	PRO	5.1
1	C	212	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	167	GLY	4.8
1	C	150	ASN	4.7
1	D	187	PRO	4.7
1	C	198	THR	4.7
1	B	189	CYS	4.7
1	A	200	GLN	4.6
1	B	33	PRO	4.6
1	C	199	PRO	4.6
1	B	169	TYR	4.6
1	D	149	ILE	4.6
1	A	186	LEU	4.6
1	B	148	ALA	4.5
1	B	212	ALA	4.5
1	D	201	VAL	4.4
1	D	160	ASP	4.4
1	C	215	SER	4.3
1	B	199	PRO	4.3
1	D	165	SER	4.2
1	C	213	VAL	4.2
1	A	198	THR	4.2
1	C	162	ARG	4.1
1	A	148	ALA	4.1
1	D	202	PRO	4.1
1	A	201	VAL	4.1
1	D	146	THR	4.1
1	A	169	TYR	4.0
1	A	210	THR	4.0
1	A	184	LEU	4.0
1	D	162	ARG	3.9
1	A	58	PHE	3.9
1	D	147	ARG	3.9
1	A	199	PRO	3.9
1	A	161	SER	3.8
1	C	148	ALA	3.8
1	D	58	PHE	3.8
1	C	211	ARG	3.8
1	C	163	THR	3.7
1	B	163	THR	3.7
1	B	200	GLN	3.7
1	D	150	ASN	3.7
1	D	169	TYR	3.6
1	D	167	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	163	THR	3.6
1	D	184	LEU	3.6
1	A	185	ASN	3.5
1	D	312	ASN	3.5
1	D	161	SER	3.5
1	C	169	TYR	3.5
1	A	33	PRO	3.5
1	D	191	TYR	3.4
1	B	192	ILE	3.4
1	B	161	SER	3.4
1	D	199	PRO	3.4
1	C	164	ARG	3.4
1	D	186	LEU	3.4
1	C	187	PRO	3.3
1	C	189	CYS	3.3
1	B	160	ASP	3.3
1	D	168	LYS	3.2
1	B	198	THR	3.2
1	B	215	SER	3.2
1	C	161	SER	3.2
1	C	191	TYR	3.2
1	C	192	ILE	3.2
1	A	147	ARG	3.2
1	A	34	VAL	3.2
1	A	183	ILE	3.1
1	D	190	ASP	3.1
1	C	186	LEU	3.1
1	B	150	ASN	3.1
1	B	191	TYR	3.1
1	A	192	ILE	3.0
1	D	164	ARG	3.0
1	B	211	ARG	3.0
1	B	162	ARG	3.0
1	C	34	VAL	3.0
1	A	167	GLY	3.0
1	A	189	CYS	2.9
1	D	198	THR	2.8
1	D	188	GLU	2.8
1	C	165	SER	2.8
1	C	291	PRO	2.7
1	D	183	ILE	2.7
1	C	216	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	168	LYS	2.6
1	B	164	ARG	2.6
1	C	160	ASP	2.6
1	C	292	LYS	2.6
1	C	278	GLU	2.6
1	C	293	ALA	2.6
1	C	281	ASP	2.5
1	A	150	ASN	2.5
1	A	187	PRO	2.5
1	B	228	ASN	2.5
1	D	200	GLN	2.4
1	C	190	ASP	2.4
1	B	146	THR	2.4
1	B	184	LEU	2.4
1	B	268	GLU	2.4
1	A	164	ARG	2.3
1	A	100	SER	2.3
1	B	34	VAL	2.3
1	B	309	TRP	2.3
1	B	145	LYS	2.3
1	C	294	GLU	2.3
1	B	58	PHE	2.2
1	C	214	PRO	2.2
1	D	295	GLY	2.2
1	B	277	ASP	2.2
1	B	151	GLU	2.2
1	C	188	GLU	2.2
1	C	229	GLY	2.2
1	B	270	ALA	2.2
1	D	185	ASN	2.2
1	B	213	VAL	2.2
1	D	193	ASN	2.1
1	C	147	ARG	2.1
1	D	182	LYS	2.1
1	D	360	ASP	2.1
1	B	371	THR	2.1
1	B	147	ARG	2.1
1	B	168	LYS	2.1
1	B	214	PRO	2.1
1	C	146	THR	2.0
1	A	70	ASN	2.0
1	B	276	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	211	ARG	2.0
1	D	151	GLU	2.0
1	B	196	ILE	2.0
1	B	185	ASN	2.0
1	B	193	ASN	2.0
1	B	312	ASN	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
3	GOL	A	505	6/6	0.68	0.23	59,61,61,61	0
3	GOL	D	507	6/6	0.74	0.19	67,68,68,68	0
3	GOL	A	503	6/6	0.77	0.23	46,48,48,50	0
3	GOL	B	506	6/6	0.81	0.19	56,56,56,57	0
3	GOL	A	504	6/6	0.83	0.18	65,65,66,67	0
2	PG4	D	501	13/13	0.86	0.14	45,48,55,56	0
2	PG4	A	502	13/13	0.87	0.15	43,45,53,54	0
3	GOL	D	508	6/6	0.90	0.16	57,58,59,59	0
4	AZI	A	510	3/3	0.90	0.13	44,44,48,48	0
4	AZI	B	509	3/3	0.90	0.15	40,40,46,47	0
4	AZI	A	511	3/3	0.92	0.15	48,48,48,50	0
5	ZN	A	999	1/1	1.00	0.01	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	0.01	25,25,25,25	0
5	ZN	D	999	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.