



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:34 PM UTC

PDB ID : 6BPO / pdb_00006bpo
Title : The crystal structure of the Ferric-Catecholate import receptor Fiu from K12
E. coli: Closed form (P1)
Authors : Grinter, R.
Deposited on : 2017-11-23
Resolution : 2.90 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

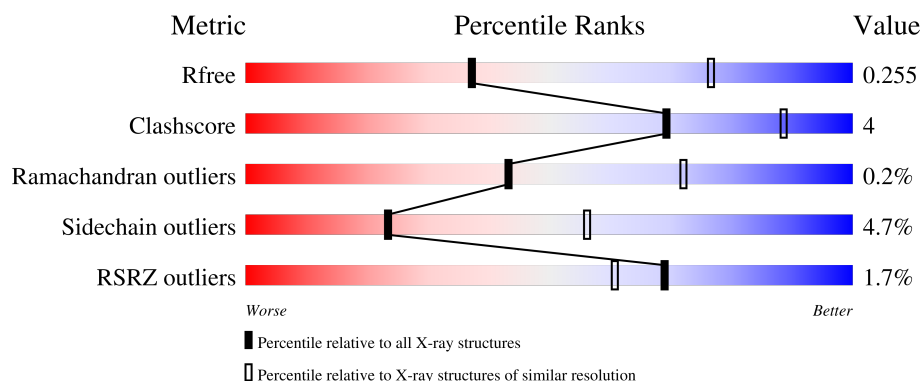
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	727	% 83% 14% .
1	B	727	2% 84% 13% ..
1	C	727	2% 83% 13% ..
1	D	727	% 85% 12% ..

2 Entry composition [i](#)

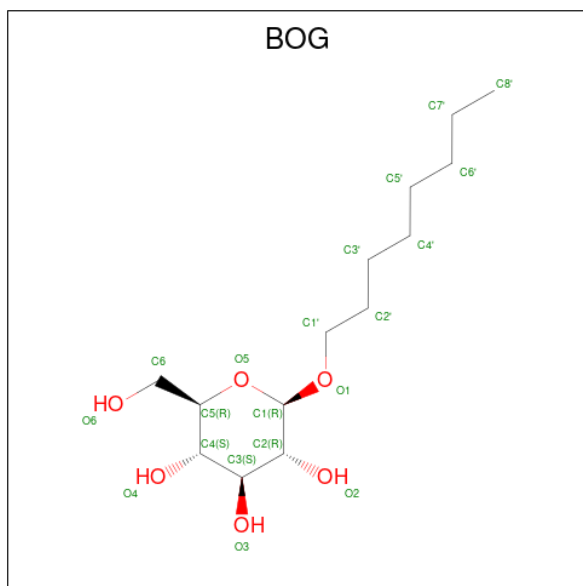
There are 3 unique types of molecules in this entry. The entry contains 22034 atoms, of which 56 are hydrogens and 0 are deuteriums.

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 Catecholate siderophore receptor Fiu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	1	0
			5417	3348	955	1102	12			
1	B	711	Total	C	N	O	S	0	1	0
			5421	3351	957	1101	12			
1	C	711	Total	C	N	O	S	0	2	0
			5427	3354	958	1103	12			
1	D	711	Total	C	N	O	S	0	1	0
			5417	3348	955	1102	12			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			48	14	28	6		
2	B	1	Total	C	H	O	0	0
			48	14	28	6		

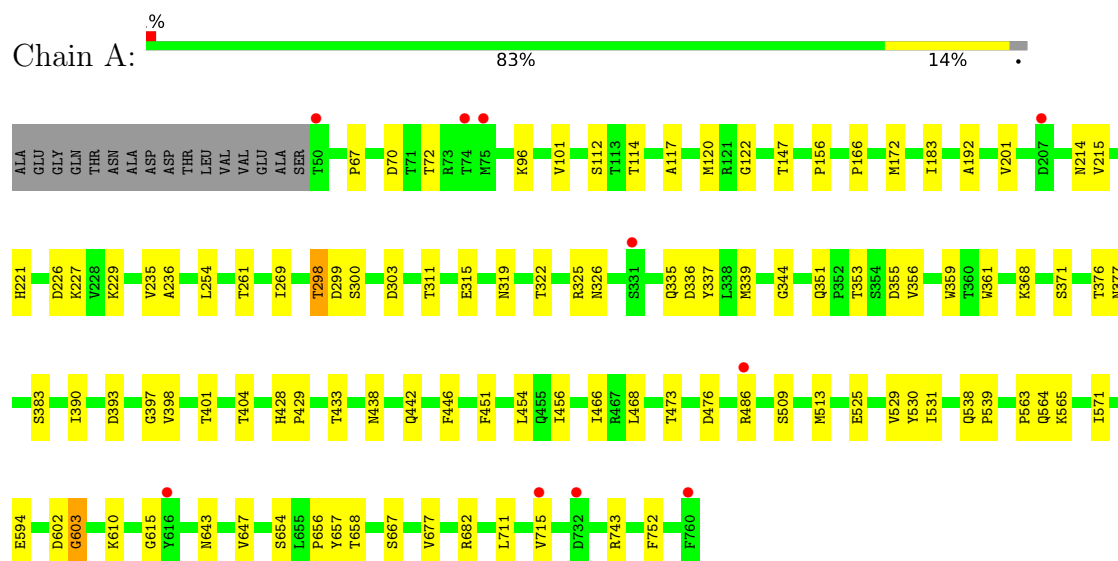
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	58	Total 58	O 58	0	0
3	C	58	Total 58	O 58	0	0
3	D	67	Total 67	O 67	0	0

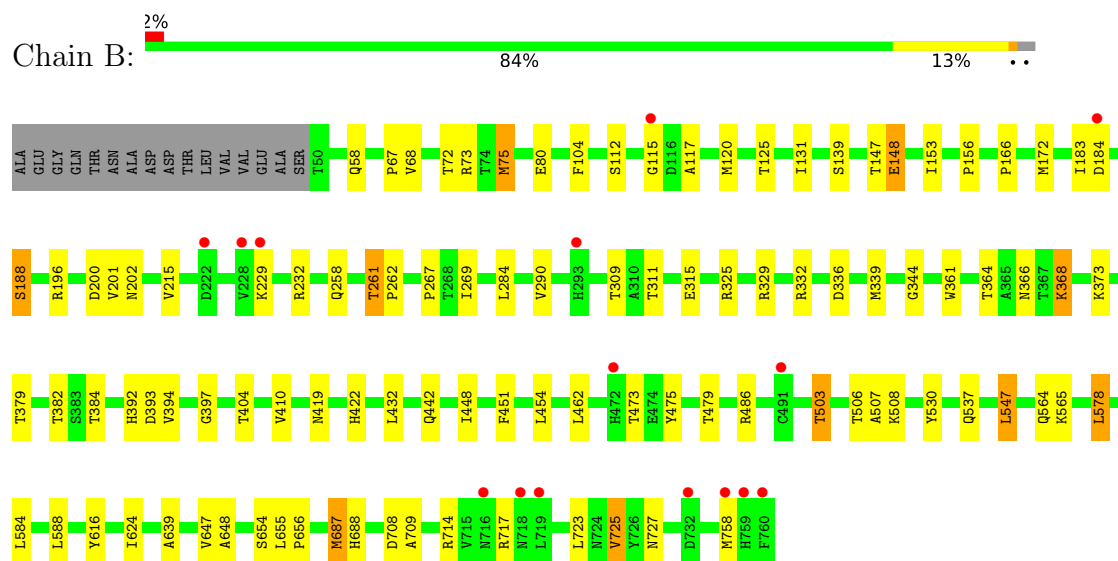
3 Residue-property plots [i](#)

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: Catecholate siderophore receptor Fiu

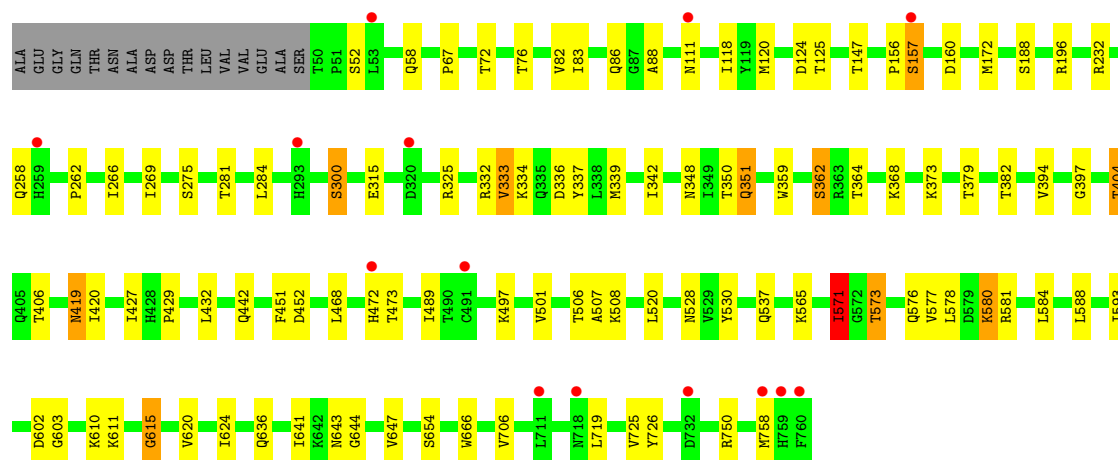


• Molecule 1: Catecholate siderophore receptor Fiu



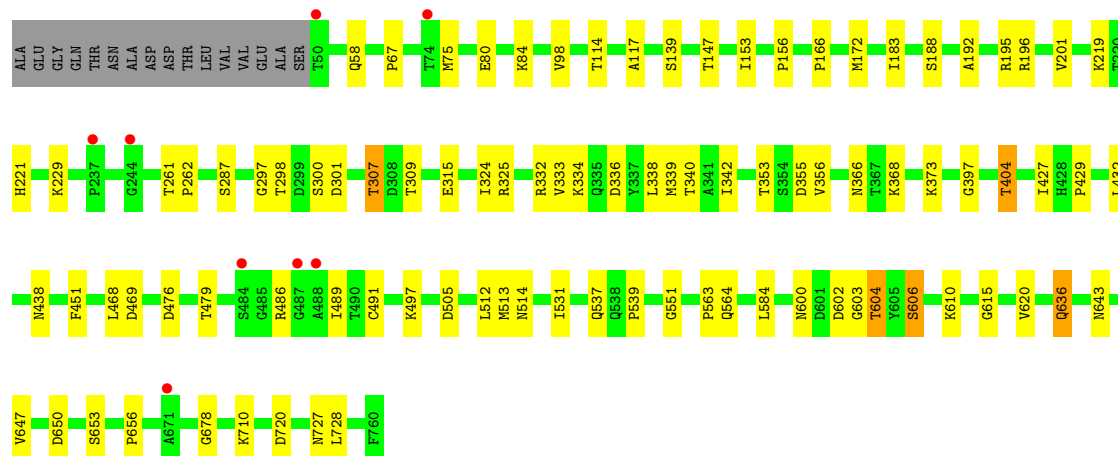
• Molecule 1: Catecholate siderophore receptor Fiu

Chain C:  2% 83% 13% ..



• Molecule 1: Catecholate siderophore receptor Fiu

Chain D:  0% 85% 12% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.67Å 133.16Å 135.10Å 101.50° 107.42° 92.88°	Depositor
Resolution (Å)	29.23 – 2.90 29.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.23-2.90) 98.9 (29.23-2.90)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.197 , 0.238 0.215 , 0.255	Depositor DCC
R_{free} test set	5866 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22034	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: BOG

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	0.75	0/5533	1.19	12/7536 (0.2%)
1	B	0.75	1/5538 (0.0%)	1.19	10/7543 (0.1%)
1	C	0.76	0/5544	1.21	22/7551 (0.3%)
1	D	0.73	0/5533	1.20	16/7536 (0.2%)
All	All	0.74	1/22148 (0.0%)	1.20	60/30166 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	687	MET	SD-CE	-5.98	1.64	1.79

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	PHE	CA-CB-CG	8.33	122.13	113.80
1	C	603	GLY	CA-C-N	7.73	132.18	120.82
1	C	603	GLY	C-N-CA	7.73	132.18	120.82
1	A	303	ASP	CA-CB-CG	7.07	119.67	112.60
1	B	624	ILE	N-CA-C	-6.88	104.15	110.82
1	A	615	GLY	N-CA-C	6.88	120.16	110.74
1	B	451	PHE	CA-CB-CG	6.68	120.48	113.80
1	C	644	GLY	N-CA-C	6.67	118.92	111.85
1	D	451	PHE	CA-CB-CG	6.49	120.29	113.80
1	D	603	GLY	CA-C-N	6.28	133.54	121.54
1	D	603	GLY	C-N-CA	6.28	133.54	121.54
1	C	602	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	117	ALA	CA-C-N	6.03	128.65	120.63
1	A	117	ALA	C-N-CA	6.03	128.65	120.63
1	C	419	ASN	CA-CB-CG	6.03	118.63	112.60
1	D	727	ASN	CA-C-N	6.02	128.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	727	ASN	C-N-CA	6.02	128.63	120.38
1	C	333	VAL	N-CA-CB	6.02	119.46	111.64
1	B	708	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	117	ALA	CA-C-N	5.96	129.38	120.69
1	B	117	ALA	C-N-CA	5.96	129.38	120.69
1	A	603	GLY	CA-C-N	5.92	129.53	120.82
1	A	603	GLY	C-N-CA	5.92	129.53	120.82
1	B	261	THR	CB-CA-C	5.90	116.72	110.17
1	D	505	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	281	THR	CA-C-N	5.79	128.31	120.38
1	C	281	THR	C-N-CA	5.79	128.31	120.38
1	A	397	GLY	N-CA-C	5.67	119.02	110.18
1	D	80	GLU	CA-C-N	5.58	128.08	120.54
1	D	80	GLU	C-N-CA	5.58	128.08	120.54
1	A	451	PHE	CA-CB-CG	5.58	119.38	113.80
1	C	571	ILE	CB-CA-C	5.58	116.77	110.41
1	B	727	ASN	CA-C-N	5.50	129.07	120.82
1	B	727	ASN	C-N-CA	5.50	129.07	120.82
1	C	452	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	476	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	117	ALA	CA-C-N	5.47	127.91	120.63
1	D	117	ALA	C-N-CA	5.47	127.91	120.63
1	B	397	GLY	N-CA-C	5.47	118.71	110.18
1	A	226	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	615	GLY	N-CA-C	5.43	117.76	110.43
1	D	397	GLY	N-CA-C	5.42	118.64	110.18
1	D	650	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	98	VAL	CB-CA-C	5.42	115.63	110.16
1	C	624	ILE	N-CA-C	-5.39	105.47	110.53
1	D	551	GLY	N-CA-C	5.35	120.05	113.79
1	C	156	PRO	CA-C-N	5.34	131.73	121.54
1	C	156	PRO	C-N-CA	5.34	131.73	121.54
1	C	124	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	602	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	602	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	397	GLY	N-CA-C	5.19	118.15	110.63
1	B	725	VAL	N-CA-CB	5.17	119.07	111.52
1	C	266	ILE	N-CA-C	5.16	113.57	107.84
1	C	82	VAL	CA-C-N	5.10	127.07	120.70
1	C	82	VAL	C-N-CA	5.10	127.07	120.70
1	D	476	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	319	ASN	CA-CB-CG	5.03	117.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASN	CA-CB-CG	5.02	117.62	112.60
1	C	118	ILE	N-CA-C	5.00	115.55	109.30

There are no chirality outliers.

There are no planarity outliers.

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	5417	0	5147	35	0
1	B	5421	0	5149	42	0
1	C	5427	0	5153	39	0
1	D	5417	0	5147	34	0
2	A	20	28	28	0	0
2	B	20	28	28	0	0
3	A	73	0	0	1	0
3	B	58	0	0	2	0
3	C	58	0	0	1	0
3	D	67	0	0	0	0
All	All	21978	56	20652	150	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 (150) 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:D:300:SER:HB2	1:D:429:PRO:HD2	1.71	0.71
1:A:298:THR:HG22	1:A:300:SER:H	1.56	0.70
1:B:147:THR:HG21	1:B:172:MET:HE2	1.75	0.69
1:D:307:THR:HB	1:D:333:VAL:HG22	1.79	0.64
1:C:332:ARG:HD3	1:C:334:LYS:HG3	1.80	0.63
1:D:336:ASP:HA	1:D:368:LYS:O	1.99	0.62
1:D:353:THR:HG22	1:D:355:ASP:H	1.67	0.60
1:C:188:SER:HB2	1:C:196:ARG:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LYS:HB2	1:C:404:THR:HG23	1.83	0.60
1:B:184:ASP:HB2	1:B:200:ASP:HB3	1.84	0.59
1:A:183:ILE:HG23	1:A:201:VAL:HG22	1.85	0.58
1:A:326:ASN:HD21	1:A:377:ASN:HD21	1.50	0.58
1:A:390:ILE:HD12	1:A:456:ILE:HA	1.87	0.57
1:D:156:PRO:HG3	1:D:166:PRO:HA	1.87	0.57
1:B:112:SER:HB2	1:B:366:ASN:HD22	1.71	0.56
1:C:157:SER:HB3	1:C:160:ASP:HB2	1.87	0.56
1:C:52:SER:HA	1:C:581:ARG:HH21	1.71	0.56
1:A:122:GLY:HA2	1:A:658:THR:OG1	2.06	0.56
1:A:96:LYS:HB3	1:A:682:ARG:HD3	1.87	0.55
1:B:336:ASP:HA	1:B:368:LYS:O	2.08	0.54
1:B:229:LYS:H	1:B:261:THR:HB	1.72	0.54
1:D:147:THR:HG21	1:D:172:MET:HE2	1.89	0.54
1:D:262:PRO:HB2	1:D:339:MET:HG2	1.88	0.54
1:A:538:GLN:HE21	1:A:539:PRO:HD2	1.72	0.53
1:D:584:LEU:HD23	1:D:620:VAL:HG12	1.91	0.53
1:D:229:LYS:H	1:D:261:THR:HB	1.73	0.53
1:C:576:GLN:HB3	1:C:580:LYS:HG3	1.90	0.53
1:C:610:LYS:HB2	1:C:643:ASN:HB2	1.90	0.53
1:A:67:PRO:HD2	1:A:70:ASP:HB2	1.91	0.52
1:D:615:GLY:HA3	1:D:636:GLN:O	2.10	0.52
1:D:315:GLU:HG2	1:D:325:ARG:HG2	1.92	0.52
1:D:339:MET:HB2	1:D:366:ASN:HB2	1.91	0.52
1:B:183:ILE:HG12	1:B:201:VAL:HG13	1.92	0.51
1:A:298:THR:HG21	1:A:429:PRO:CD	2.40	0.51
1:B:639:ALA:HB1	1:B:655:LEU:HD12	1.93	0.50
1:A:315:GLU:HG2	1:A:325:ARG:HG2	1.92	0.50
1:D:373:LYS:HB2	1:D:404:THR:HG23	1.93	0.50
1:C:584:LEU:HD23	1:C:620:VAL:HG12	1.93	0.50
1:A:112:SER:HB3	1:A:743:ARG:HH22	1.77	0.50
1:C:419:ASN:HD22	1:C:420:ILE:N	2.10	0.49
1:A:156:PRO:HG3	1:A:166:PRO:HA	1.92	0.49
1:A:336:ASP:HA	1:A:368:LYS:O	2.11	0.49
1:A:398:VAL:HG13	1:A:446:PHE:HE1	1.77	0.49
1:B:262:PRO:HB2	1:B:339:MET:HG3	1.94	0.49
1:B:714:ARG:HH21	1:B:717:ARG:HA	1.77	0.49
1:A:335:GLN:HG3	3:A:902:HOH:O	2.12	0.49
1:B:410:VAL:HG21	1:B:432:LEU:HD22	1.94	0.49
1:C:348:ASN:HB3	1:C:362:SER:HB3	1.94	0.49
1:D:600:ASN:HD21	1:D:606:SER:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:HB	1:B:329:ARG:HH12	1.78	0.49
1:B:339:MET:HB3	1:B:366:ASN:HB2	1.93	0.48
1:C:269:ILE:HD13	1:C:284:LEU:HD22	1.94	0.48
1:A:376:THR:HB	1:A:401:THR:HG23	1.96	0.48
1:B:647:VAL:HG23	1:B:656:PRO:HD3	1.96	0.48
1:C:654:SER:HB2	3:C:840:HOH:O	2.14	0.48
1:C:262:PRO:HB2	1:C:339:MET:HG3	1.96	0.48
1:D:192:ALA:O	1:D:221:HIS:HB2	2.13	0.48
1:D:647:VAL:HG23	1:D:656:PRO:HD3	1.96	0.48
1:A:337:TYR:CE1	1:A:339:MET:HE3	2.50	0.47
1:B:58:GLN:HG3	1:B:67:PRO:HA	1.97	0.47
1:C:577:VAL:HG12	1:C:578:LEU:N	2.30	0.47
1:A:147:THR:HG21	1:A:172:MET:HE2	1.95	0.47
1:A:647:VAL:HG23	1:A:656:PRO:HD3	1.96	0.47
1:D:183:ILE:HG12	1:D:201:VAL:HG12	1.97	0.47
1:A:322:THR:HG23	1:A:383:SER:HB2	1.97	0.47
1:A:344:GLY:HA3	1:A:361:TRP:CE2	2.50	0.47
1:B:68:VAL:HG13	1:B:75:MET:HB3	1.97	0.47
1:C:577:VAL:HG12	1:C:578:LEU:H	1.80	0.47
1:A:214:ASN:HB2	1:A:236:ALA:HB3	1.96	0.46
1:C:641:ILE:HD11	1:C:647:VAL:HG22	1.97	0.46
1:B:120:MET:HB3	1:B:125:THR:HG21	1.97	0.46
1:C:571:ILE:HG23	1:C:588:LEU:HB2	1.97	0.46
1:B:382:THR:HA	1:B:394:VAL:O	2.15	0.46
1:A:539:PRO:HA	1:A:563:PRO:HB3	1.97	0.46
1:C:232:ARG:HB3	1:C:258:GLN:HG2	1.98	0.46
1:D:58:GLN:HG3	1:D:67:PRO:HA	1.97	0.46
1:A:192:ALA:O	1:A:221:HIS:HB2	2.16	0.46
1:B:588:LEU:HD23	1:B:616:TYR:HB3	1.97	0.46
1:B:75:MET:HG3	1:B:153:ILE:HG12	1.97	0.45
1:B:419:ASN:HB3	1:B:422:HIS:O	2.16	0.45
1:C:315:GLU:HG2	1:C:325:ARG:HG2	1.98	0.45
1:D:298:THR:HG22	1:D:301:ASP:OD1	2.17	0.45
1:A:298:THR:CG2	1:A:429:PRO:CD	2.95	0.45
1:C:120:MET:HB3	1:C:125:THR:HG21	1.99	0.45
1:C:336:ASP:HA	1:C:368:LYS:O	2.17	0.45
1:B:479:THR:HG23	3:B:908:HOH:O	2.16	0.45
1:C:489:ILE:HD11	1:C:501:VAL:HB	1.98	0.45
1:B:373:LYS:HB2	1:B:404:THR:HG22	1.99	0.45
1:C:472[B]:HIS:HE1	1:C:507:ALA:HB1	1.80	0.45
1:B:112:SER:HB2	1:B:366:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG22	1:A:120:MET:HG3	2.00	0.44
1:C:726:TYR:O	1:C:750:ARG:HA	2.17	0.44
1:C:442:GLN:O	1:C:473:THR:HA	2.18	0.44
1:D:514:ASN:ND2	1:D:537:GLN:HE21	2.16	0.44
1:D:491:CYS:SG	1:D:497:LYS:HA	2.57	0.44
1:B:475:TYR:HB3	1:B:547:LEU:HB2	1.99	0.44
1:B:503:THR:HB	3:B:908:HOH:O	2.17	0.44
1:B:648:ALA:HB1	1:B:688:HIS:CD2	2.53	0.44
1:D:195:ARG:HH21	1:D:219:LYS:HG2	1.83	0.44
1:B:344:GLY:HA3	1:B:361:TRP:CE2	2.52	0.44
1:B:442:GLN:O	1:B:473:THR:HA	2.17	0.44
1:C:72:THR:HG22	1:C:530:TYR:HB2	2.00	0.44
1:D:469:ASP:HB2	1:D:512:LEU:HB2	1.99	0.44
1:B:73:ARG:HE	1:B:153:ILE:HG21	1.81	0.44
1:B:232:ARG:HB3	1:B:258:GLN:HG2	2.00	0.44
1:D:539:PRO:HA	1:D:563:PRO:HB3	1.99	0.44
1:B:269:ILE:HD13	1:B:284:LEU:HD22	1.99	0.43
1:C:577:VAL:HG12	1:C:578:LEU:HG	2.00	0.43
1:D:75:MET:HE2	1:D:153:ILE:HG12	1.99	0.43
1:A:442:GLN:O	1:A:473:THR:HA	2.18	0.43
1:D:300:SER:CB	1:D:429:PRO:HD2	2.43	0.43
1:A:229:LYS:H	1:A:261:THR:HB	1.83	0.43
1:A:610:LYS:HB2	1:A:643:ASN:HB2	1.99	0.43
1:C:615:GLY:HA3	1:C:636:GLN:O	2.18	0.43
1:A:299:ASP:HB3	1:A:428:HIS:CE1	2.53	0.43
1:C:528:ASN:O	1:C:573:THR:HG22	2.18	0.43
1:D:338:LEU:HB2	1:D:432:LEU:HD21	2.00	0.43
1:D:188:SER:HB2	1:D:196:ARG:HB3	2.01	0.43
1:A:72:THR:HG22	1:A:530:TYR:HB2	2.01	0.43
1:C:58:GLN:HG3	1:C:67:PRO:HA	2.00	0.43
1:C:86:GLN:HE21	1:C:666:TRP:CG	2.36	0.43
1:B:267:PRO:HD2	1:B:290:VAL:HG21	2.01	0.42
1:B:315:GLU:HG2	1:B:325:ARG:HG2	2.01	0.42
1:B:537:GLN:HG2	1:B:565:LYS:HG2	2.00	0.42
1:C:382:THR:HA	1:C:394:VAL:O	2.19	0.42
1:D:298:THR:HG23	1:D:300:SER:H	1.83	0.42
1:B:72:THR:HG22	1:B:530:TYR:HB2	2.01	0.42
1:D:610:LYS:HB2	1:D:643:ASN:HB2	2.01	0.42
1:B:384:THR:HA	1:B:392:HIS:O	2.19	0.42
1:B:473:THR:O	1:B:507:ALA:HA	2.20	0.42
1:D:332:ARG:HG2	1:D:373:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:ALA:HB3	1:B:725:VAL:HG22	2.02	0.42
1:A:565:LYS:HB2	1:A:594:GLU:HG3	2.01	0.42
1:C:593:ILE:HB	1:C:611:LYS:HB2	2.01	0.42
1:D:678:GLY:HA3	1:D:710:LYS:HB3	2.01	0.42
1:B:156:PRO:HG3	1:B:166:PRO:HA	2.02	0.41
1:C:351:GLN:HB3	1:C:359:TRP:NE1	2.36	0.41
1:B:104:PHE:CG	1:B:687:MET:HE1	2.56	0.41
1:C:147:THR:HG21	1:C:172:MET:HE2	2.01	0.41
1:C:537:GLN:HG2	1:C:565:LYS:HG2	2.01	0.41
1:B:80:GLU:HB2	1:B:148:GLU:O	2.20	0.41
1:A:269:ILE:H	1:A:269:ILE:HG13	1.77	0.41
1:A:353:THR:C	1:A:355:ASP:H	2.29	0.41
1:D:332:ARG:HD3	1:D:334:LYS:HG3	2.03	0.41
1:A:351:GLN:HG2	1:A:359:TRP:CE2	2.56	0.40
1:C:337:TYR:CE1	1:C:368:LYS:HD2	2.56	0.40
1:B:188:SER:HB2	1:B:196:ARG:HB3	2.02	0.40
1:C:83:ILE:HG23	1:C:88:ALA:O	2.22	0.40
1:C:300:SER:HB2	1:C:429:PRO:HD2	2.03	0.40
1:D:297:GLY:HA2	1:D:340:THR:HB	2.04	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	710/727 (98%)	680 (96%)	28 (4%)	2 (0%)	36	65
1	B	710/727 (98%)	680 (96%)	28 (4%)	2 (0%)	36	65
1	C	711/727 (98%)	683 (96%)	27 (4%)	1 (0%)	48	77
1	D	710/727 (98%)	679 (96%)	30 (4%)	1 (0%)	48	77
All	All	2841/2908 (98%)	2722 (96%)	113 (4%)	6 (0%)	43	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	GLY
1	D	604	THR
1	C	157	SER
1	A	227	LYS
1	A	603	GLY
1	B	578	LEU

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	580/591 (98%)	550 (95%)	30 (5%)	21	52
1	B	580/591 (98%)	553 (95%)	27 (5%)	23	56
1	C	581/591 (98%)	555 (96%)	26 (4%)	24	58
1	D	580/591 (98%)	555 (96%)	25 (4%)	26	60
All	All	2321/2364 (98%)	2213 (95%)	108 (5%)	23	56

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	215	VAL
1	A	235	VAL
1	A	254	LEU
1	A	298	THR
1	A	311	THR
1	A	356	VAL
1	A	371	SER
1	A	393	ASP
1	A	404	THR
1	A	433	THR
1	A	438	ASN
1	A	454	LEU
1	A	466	ILE

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Mol	Chain	Res	Type
1	A	468	LEU
1	A	486	ARG
1	A	509	SER
1	A	513	MET
1	A	525	GLU
1	A	529	VAL
1	A	531	ILE
1	A	564	GLN
1	A	571	ILE
1	A	654	SER
1	A	657	TYR
1	A	667	SER
1	A	677	VAL
1	A	711	LEU
1	A	715	VAL
1	A	752	PHE
1	B	75	MET
1	B	139	SER
1	B	148	GLU
1	B	188	SER
1	B	202	ASN
1	B	215	VAL
1	B	309	THR
1	B	311	THR
1	B	332	ARG
1	B	364	THR
1	B	368	LYS
1	B	379	THR
1	B	393	ASP
1	B	448	ILE
1	B	454	LEU
1	B	462	LEU
1	B	486	ARG
1	B	503	THR
1	B	506	THR
1	B	508	LYS
1	B	547	LEU
1	B	564	GLN
1	B	578	LEU
1	B	584	LEU
1	B	654	SER
1	B	723	LEU

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Mol	Chain	Res	Type
1	B	758	MET
1	C	76	THR
1	C	275	SER
1	C	300	SER
1	C	333	VAL
1	C	342	ILE
1	C	350	THR
1	C	351	GLN
1	C	362	SER
1	C	364	THR
1	C	379	THR
1	C	404	THR
1	C	406	THR
1	C	427	ILE
1	C	432	LEU
1	C	468	LEU
1	C	497	LYS
1	C	506	THR
1	C	508	LYS
1	C	520	LEU
1	C	571	ILE
1	C	573	THR
1	C	580	LYS
1	C	706	VAL
1	C	719	LEU
1	C	725	VAL
1	C	758	MET
1	D	84	LYS
1	D	114	THR
1	D	139	SER
1	D	287	SER
1	D	307	THR
1	D	309	THR
1	D	324	ILE
1	D	342	ILE
1	D	356	VAL
1	D	404	THR
1	D	427	ILE
1	D	438	ASN
1	D	468	LEU
1	D	479	THR
1	D	486	ARG

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Mol	Chain	Res	Type
1	D	489	ILE
1	D	513	MET
1	D	531	ILE
1	D	564	GLN
1	D	604	THR
1	D	606	SER
1	D	636	GLN
1	D	653	SER
1	D	720	ASP
1	D	728	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	146	ASN
1	A	176	GLN
1	A	214	ASN
1	A	252	ASN
1	A	286	HIS
1	A	321	ASN
1	A	326	ASN
1	A	366	ASN
1	A	428	HIS
1	A	511	ASN
1	A	538	GLN
1	A	564	GLN
1	A	643	ASN
1	A	722	GLN
1	B	109	ASN
1	B	146	ASN
1	B	176	GLN
1	B	179	ASN
1	B	214	ASN
1	B	252	ASN
1	B	258	GLN
1	B	260	ASN
1	B	326	ASN
1	B	366	ASN
1	B	377	ASN
1	B	428	HIS
1	B	511	ASN

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Mol	Chain	Res	Type
1	B	514	ASN
1	B	526	ASN
1	B	537	GLN
1	B	564	GLN
1	B	600	ASN
1	B	722	GLN
1	C	81	GLN
1	C	90	ASN
1	C	111	ASN
1	C	176	GLN
1	C	252	ASN
1	C	260	ASN
1	C	286	HIS
1	C	293	HIS
1	C	321	ASN
1	C	351	GLN
1	C	366	ASN
1	C	405	GLN
1	C	407	ASN
1	C	419	ASN
1	C	455	GLN
1	C	463	ASN
1	C	470	ASN
1	C	532	ASN
1	C	661	HIS
1	C	718	ASN
1	D	146	ASN
1	D	176	GLN
1	D	214	ASN
1	D	252	ASN
1	D	321	ASN
1	D	366	ASN
1	D	405	GLN
1	D	407	ASN
1	D	428	HIS
1	D	442	GLN
1	D	470	ASN
1	D	511	ASN
1	D	526	ASN
1	D	537	GLN
1	D	567	ASN
1	D	600	ASN

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Mol	Chain	Res	Type
1	D	636	GLN
1	D	649	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	BOG	B	801	-	20,20,20	0.21	0	25,25,25	0.23	0
2	BOG	A	801	-	20,20,20	0.16	0	25,25,25	0.20	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
2	BOG	B	801	-	-	4/11/31/31	0/1/1/1
2	BOG	A	801	-	-	4/11/31/31	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

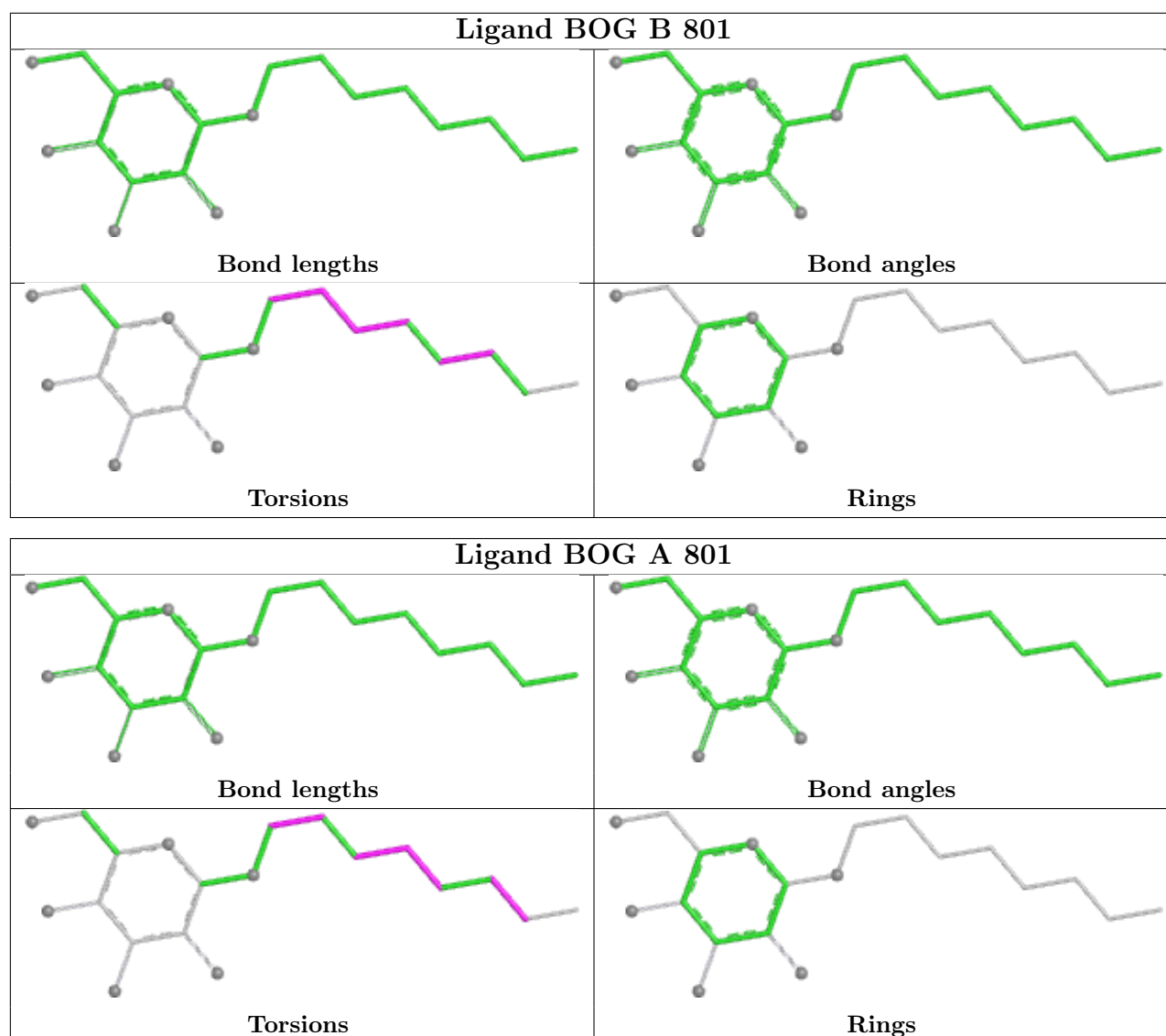
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	BOG	O1-C1'-C2'-C3'
2	B	801	BOG	C2'-C3'-C4'-C5'
2	B	801	BOG	C1'-C2'-C3'-C4'
2	A	801	BOG	O1-C1'-C2'-C3'
2	A	801	BOG	C5'-C6'-C7'-C8'
2	A	801	BOG	C3'-C4'-C5'-C6'
2	B	801	BOG	C4'-C5'-C6'-C7'
2	A	801	BOG	C2'-C3'-C4'-C5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	711/727 (97%)	0.09	10 (1%) 73 65	33, 54, 82, 125	1 (0%)
1	B	711/727 (97%)	0.06	15 (2%) 63 54	21, 52, 77, 122	1 (0%)
1	C	711/727 (97%)	0.05	14 (1%) 65 56	21, 52, 78, 117	2 (0%)
1	D	711/727 (97%)	0.06	8 (1%) 78 71	29, 53, 80, 113	1 (0%)
All	All	2844/2908 (97%)	0.07	47 (1%) 69 61	21, 53, 79, 125	5 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472[A]	HIS	10.7
1	C	472[A]	HIS	4.7
1	B	760	PHE	4.5
1	C	760	PHE	4.1
1	C	157	SER	4.0
1	B	758	MET	3.9
1	D	487	GLY	3.7
1	D	50	THR	3.6
1	B	759	HIS	3.5
1	A	760	PHE	3.5
1	A	616	TYR	3.5
1	C	732	ASP	3.1
1	B	718	ASN	3.0
1	B	229	LYS	2.9
1	B	716	ASN	2.9
1	A	732	ASP	2.9
1	B	293	HIS	2.9
1	C	759	HIS	2.9
1	C	491	CYS	2.7
1	C	293	HIS	2.6
1	B	184	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	228	VAL	2.6
1	D	237	PRO	2.6
1	D	74	THR	2.6
1	C	718	ASN	2.6
1	A	715	VAL	2.6
1	A	486	ARG	2.5
1	A	50	THR	2.5
1	D	484	SER	2.5
1	B	115	GLY	2.5
1	D	671	ALA	2.4
1	D	488	ALA	2.4
1	B	719	LEU	2.4
1	D	244	GLY	2.4
1	B	491	CYS	2.4
1	A	75	MET	2.4
1	C	758	MET	2.3
1	C	711	LEU	2.3
1	A	207	ASP	2.2
1	A	74	THR	2.2
1	C	320	ASP	2.2
1	B	222	ASP	2.1
1	B	732	ASP	2.1
1	C	53	LEU	2.1
1	A	331	SER	2.1
1	C	259	HIS	2.0
1	C	111	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](#)

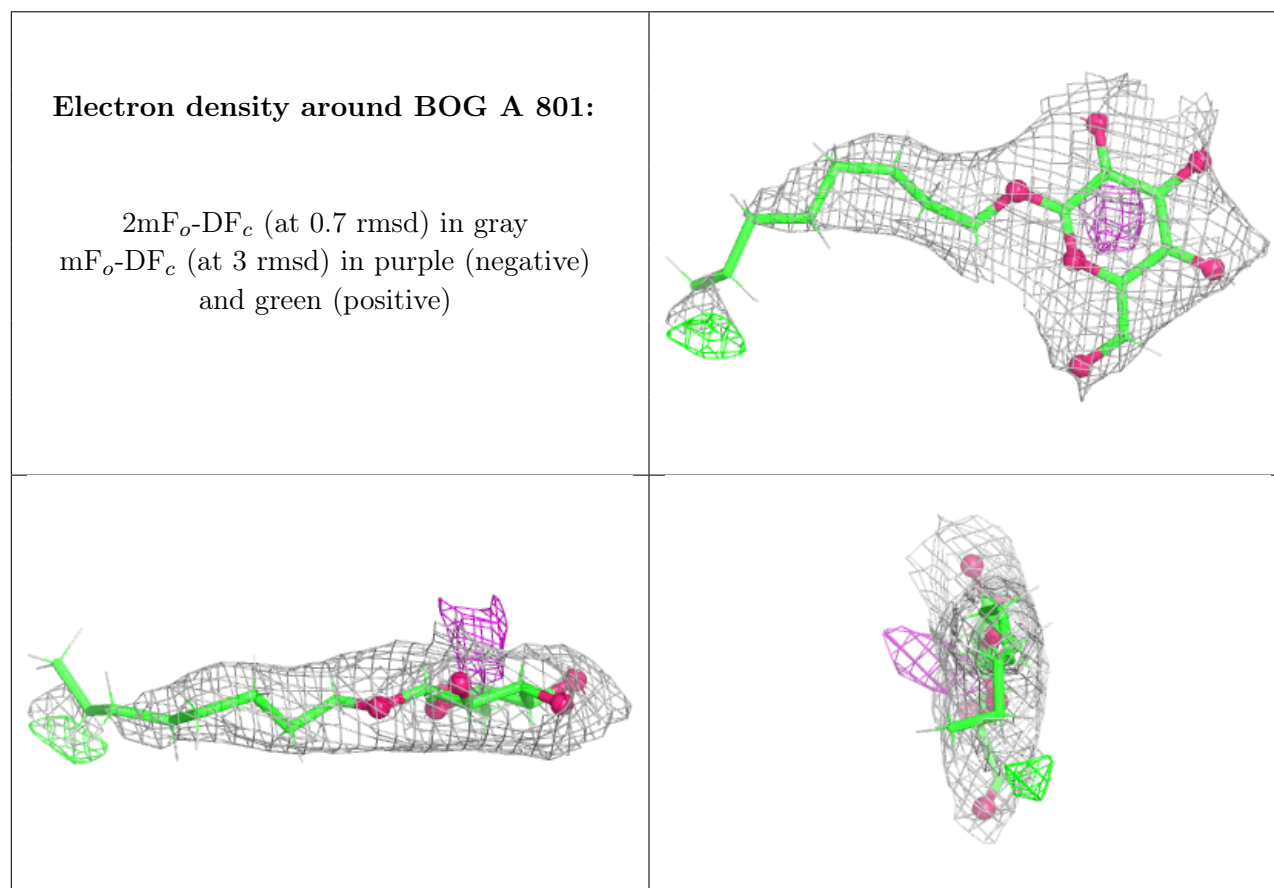
There are no oligosaccharides in this entry.

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.

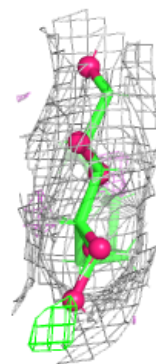
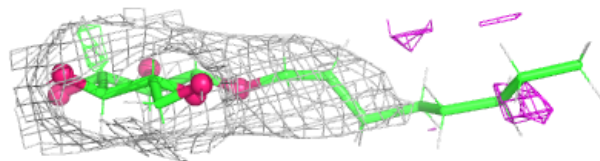
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BOG	A	801	20/20	0.77	0.14	98,101,103,103	0
2	BOG	B	801	20/20	0.85	0.16	91,95,107,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around BOG B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.