



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:14 PM UTC

PDB ID : 6MIT / pdb_00006mit
Title : LptBFGC from Enterobacter cloacae
Authors : Owens, T.W.; Kahne, D.; Kruse, A.C.
Deposited on : 2018-09-20
Resolution : 3.20 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

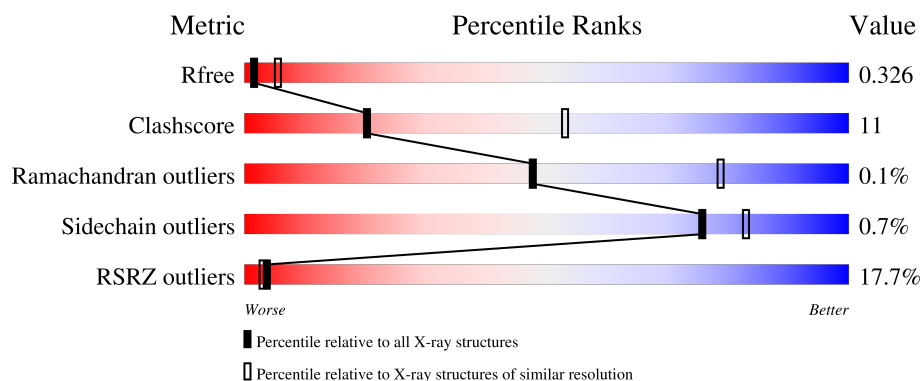
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	241	18% 75% 24%
1	B	241	10% 76% 24%
1	D	241	8% 68% 31%
1	E	241	17% 76% 22% .
2	C	195	21% 66% 24% 10%

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Mol	Chain	Length	Quality of chain
2	H	195	
3	F	366	
3	I	366	
4	G	360	
4	J	360	

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
5	SO4	G	403	-	-	X	-
6	CL	A	303	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19733 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 Lipopolysaccharide export system ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1802	1134	323	341	4			
1	B	240	Total	C	N	O	S	0	0	0
			1792	1128	319	341	4			
1	D	240	Total	C	N	O	S	0	0	0
			1814	1144	326	340	4			
1	E	238	Total	C	N	O	S	0	0	0
			1736	1091	304	337	4			

- Molecule 2 is a protein called Lipopolysaccharide export system protein LptC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	175	Total	C	N	O	S	0	0	0
			1336	846	224	263	3			
2	H	175	Total	C	N	O	S	0	0	0
			1324	839	223	259	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	192	LEU	-	expression tag	UNP A0A0H3CU18
C	193	VAL	-	expression tag	UNP A0A0H3CU18
C	194	PRO	-	expression tag	UNP A0A0H3CU18
C	195	ARG	-	expression tag	UNP A0A0H3CU18
H	192	LEU	-	expression tag	UNP A0A0H3CU18
H	193	VAL	-	expression tag	UNP A0A0H3CU18
H	194	PRO	-	expression tag	UNP A0A0H3CU18
H	195	ARG	-	expression tag	UNP A0A0H3CU18

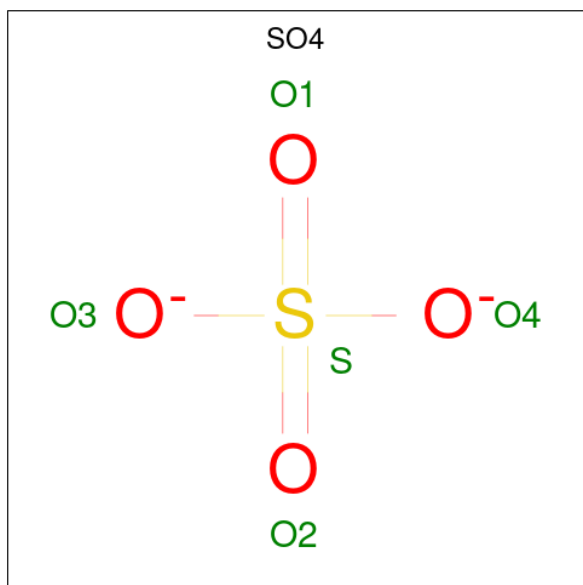
- Molecule 3 is a protein called LPS export ABC transporter permease LptF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	350	Total	C	N	O	S	0	0	0
			2581	1679	425	460	17			
3	I	335	Total	C	N	O	S	0	0	0
			2435	1591	394	434	16			

- Molecule 4 is a protein called Lipopolysaccharide export system permease protein LptG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	355	Total	C	N	O	S	0	0	0
			2619	1708	426	468	17			
4	J	309	Total	C	N	O	S	0	0	0
			2186	1427	355	389	15			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		

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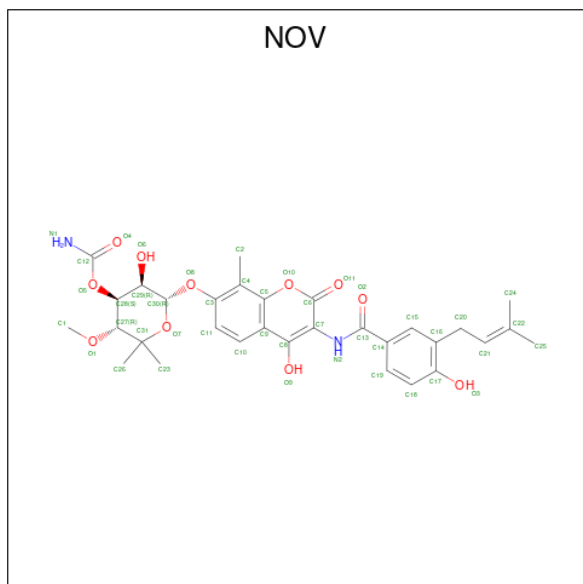
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is NOVOBIOCIN (CCD ID: NOV) (formula: C₃₁H₃₆N₂O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			44	31	2	11		

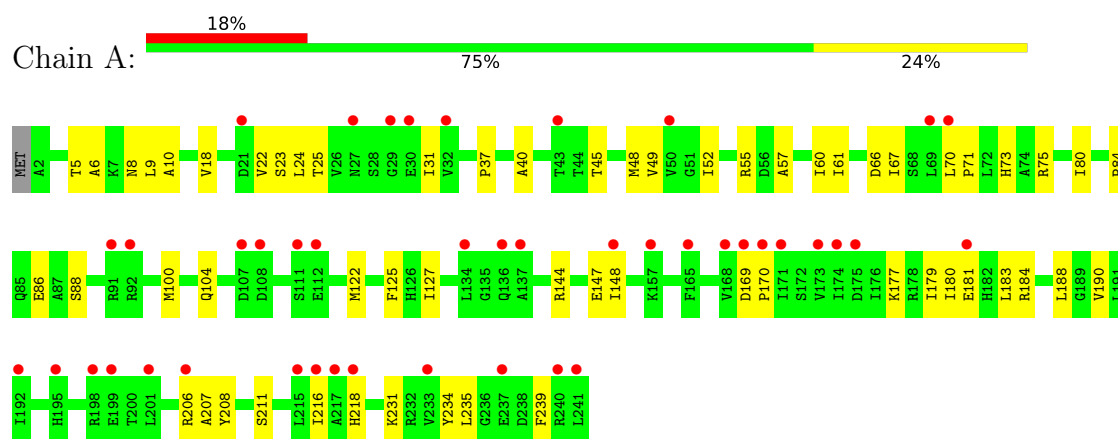
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total 3	O 3	0	0
8	B	2	Total 2	O 2	0	0
8	D	2	Total 2	O 2	0	0
8	E	1	Total 1	O 1	0	0

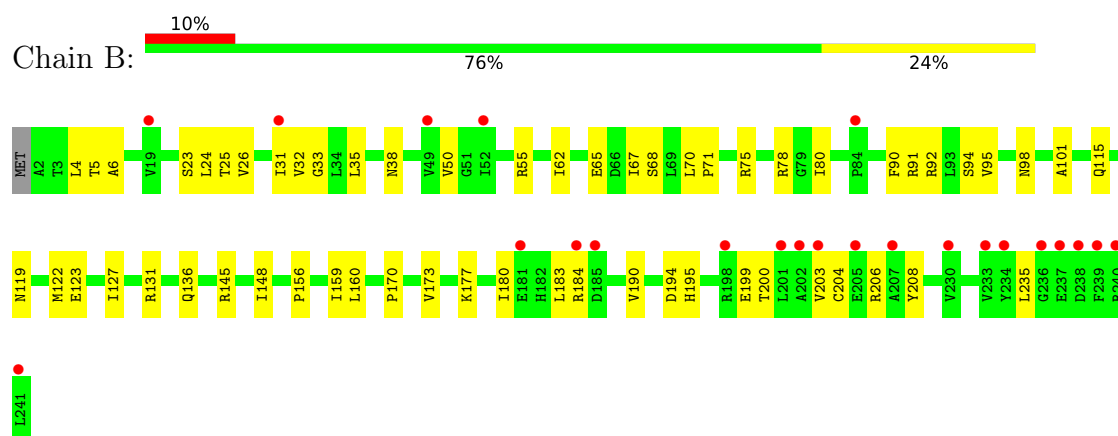
3 Residue-property plots [i](#)

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.

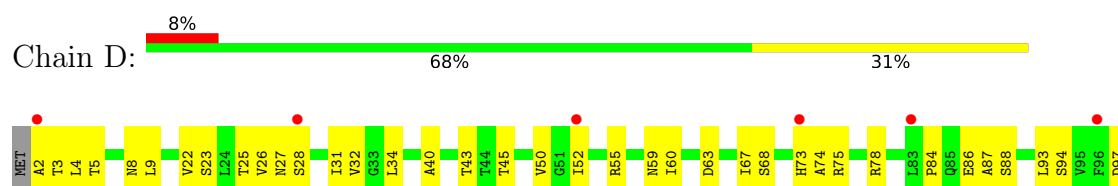
- Molecule 1: Lipopolysaccharide export system ATP-binding protein

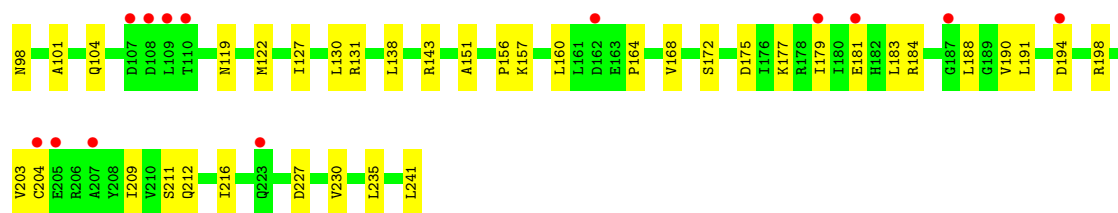


- Molecule 1: Lipopolysaccharide export system ATP-binding protein

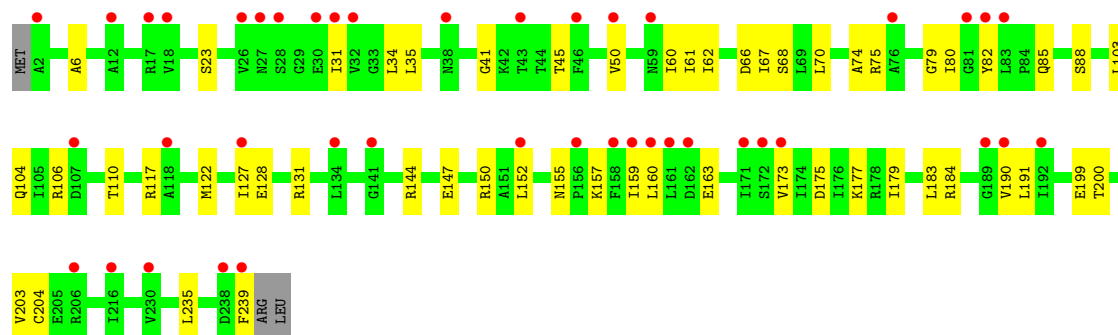
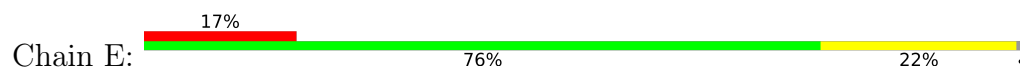


- Molecule 1: Lipopolysaccharide export system ATP-binding protein

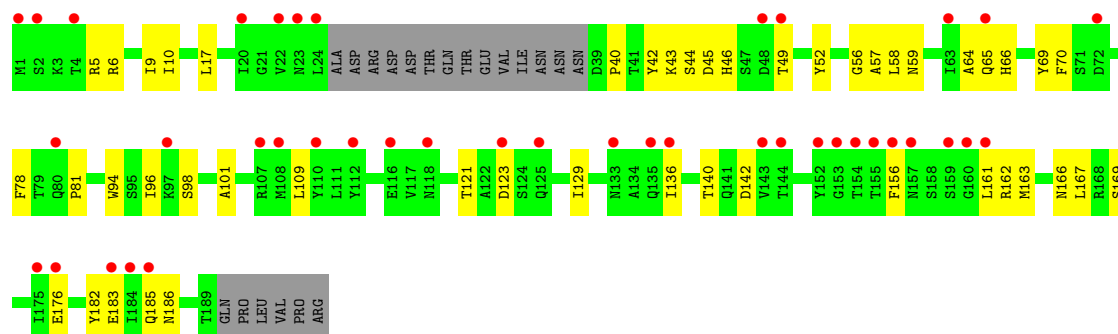




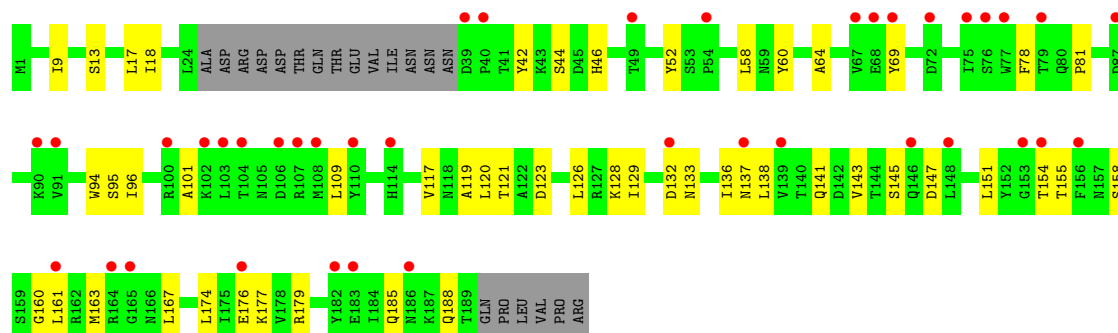
• Molecule 1: Lipopolysaccharide export system ATP-binding protein



• Molecule 2: Lipopolysaccharide export system protein LptC



• Molecule 2: Lipopolysaccharide export system protein LptC



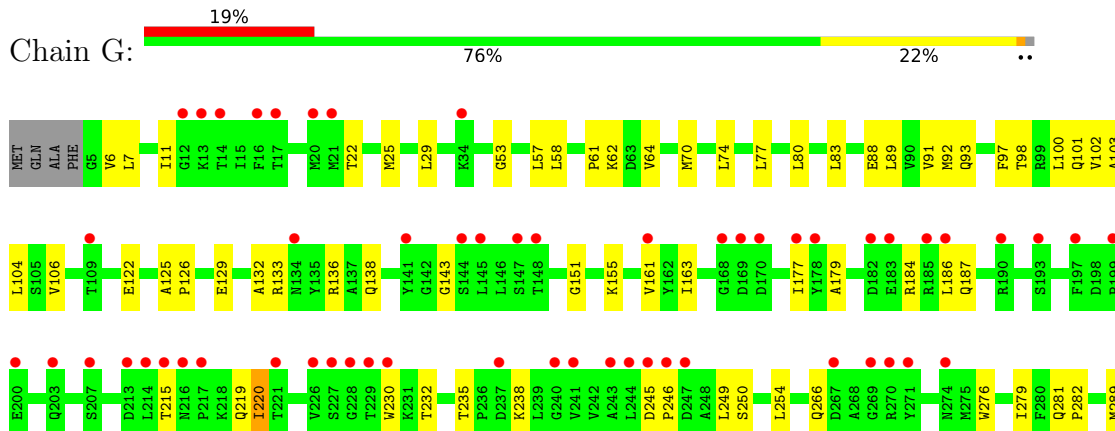
Chain F:



Chain I:

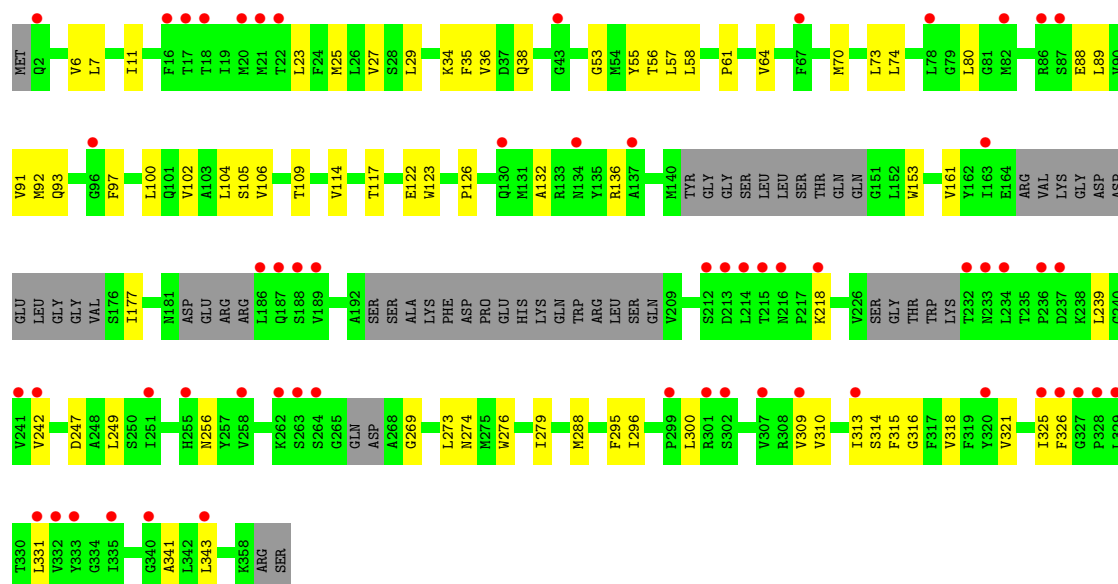


Chain G:





● Molecule 4: Lipopolysaccharide export system permease protein LptG



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	116.43Å 156.98Å 295.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 3.20 49.33 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.33-3.20) 99.3 (49.33-3.20)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.279 , 0.320 0.284 , 0.326	Depositor DCC
R_{free} test set	2000 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	111.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: CL, NOV, SO4

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	0.34	0/1828	0.56	0/2483
1	B	0.34	0/1818	0.56	0/2470
1	D	0.38	0/1840	0.59	0/2496
1	E	0.28	0/1761	0.47	0/2400
2	C	0.45	0/1359	0.64	1/1857 (0.1%)
2	H	0.35	0/1346	0.60	2/1841 (0.1%)
3	F	0.37	0/2627	0.60	0/3586
3	I	0.32	0/2476	0.53	0/3381
4	G	0.31	0/2675	0.54	0/3642
4	J	0.32	0/2224	0.55	0/3026
All	All	0.34	0/19954	0.56	3/27182 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	GLN	CA-C-N	5.23	131.12	121.70
2	H	188	GLN	C-N-CA	5.23	131.12	121.70
2	C	185	GLN	N-CA-C	-5.11	101.89	109.96

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	1802	0	1771	43	0
1	B	1792	0	1743	43	0
1	D	1814	0	1809	53	0
1	E	1736	0	1647	40	0
2	C	1336	0	1269	37	0
2	H	1324	0	1258	37	0
3	F	2581	0	2574	67	0
3	I	2435	0	2409	50	0
4	G	2619	0	2602	63	0
4	J	2186	0	2118	48	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	1	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	15	0	0	2	0
5	J	10	0	0	1	0
6	A	1	0	0	0	0
7	E	44	0	34	2	0
8	A	3	0	0	0	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
8	E	1	0	0	0	0
All	All	19733	0	19234	439	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 11.

All (439) 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)
4:G:136:ARG:NH1	5:G:403:SO4:O3	2.06	0.88
2:H:58:LEU:HD23	4:J:218:LYS:HB3	1.52	0.87
3:F:30:LYS:HG3	3:F:59:MET:HE2	1.59	0.85
1:B:94:SER:O	1:B:98:ASN:ND2	2.13	0.81
2:H:9:ILE:HD13	3:I:300:LEU:HD23	1.63	0.79
1:D:181:GLU:OE1	1:D:184:ARG:NH2	2.19	0.75
2:H:42:TYR:HB3	2:H:69:TYR:HB3	1.68	0.75
3:I:295:ARG:HB3	3:I:299:MET:HE3	1.69	0.74
4:J:23:LEU:O	4:J:27:VAL:HG23	1.87	0.74
1:B:31:ILE:HG12	1:B:184:ARG:HD3	1.69	0.73
1:E:152:LEU:HD21	1:E:183:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:HIS:HA	2:C:64:ALA:O	1.88	0.73
1:D:2:ALA:N	1:D:63:ASP:OD1	2.23	0.71
1:D:67:ILE:HD12	1:D:75:ARG:HG3	1.72	0.71
2:H:129:ILE:HD13	2:H:163:MET:HE1	1.73	0.70
4:J:122:GLU:HG3	4:J:123:TRP:CD1	2.27	0.70
4:G:138:GLN:HA	4:G:143:GLY:H	1.58	0.69
2:H:78:PHE:HB2	2:H:101:ALA:HB3	1.74	0.69
1:B:91:ARG:HB3	1:B:136:GLN:HB3	1.75	0.69
4:G:161:VAL:HG12	4:G:177:ILE:HG12	1.73	0.69
1:E:150:ARG:HH22	3:I:87:VAL:HG13	1.58	0.69
4:G:249:LEU:HD21	4:G:254:LEU:HD13	1.75	0.68
2:C:45:ASP:HA	2:C:66:HIS:HA	1.75	0.68
4:G:11:ILE:HD13	4:G:102:VAL:HG13	1.75	0.68
3:I:93:LEU:HD21	3:I:97:VAL:HG21	1.76	0.68
3:F:158:VAL:HG23	3:F:177:LEU:HD21	1.76	0.67
1:D:73:HIS:NE2	5:J:402:SO4:O3	2.26	0.67
1:A:144:ARG:NH1	1:A:147:GLU:OE1	2.28	0.66
2:C:140:THR:O	2:C:166:ASN:ND2	2.28	0.66
2:C:42:TYR:CD1	2:C:69:TYR:HB3	2.31	0.66
4:G:133:ARG:NH1	5:G:403:SO4:O1	2.29	0.66
3:I:282:ILE:HG22	3:I:342:ALA:HB2	1.77	0.65
4:J:74:LEU:HD11	4:J:309:VAL:HG23	1.77	0.65
4:G:61:PRO:HB2	4:G:125:ALA:HA	1.78	0.65
1:B:95:VAL:HG11	1:B:127:ILE:HG21	1.79	0.64
1:B:50:VAL:HG22	1:B:160:LEU:HD12	1.78	0.64
4:J:35:PHE:HB2	4:J:56:THR:HG21	1.80	0.64
4:G:80:LEU:HB2	4:G:296:ILE:HD13	1.80	0.64
3:I:172:VAL:HG11	3:I:207:LEU:HD11	1.79	0.64
1:D:104:GLN:HE22	4:J:6:VAL:HG23	1.63	0.64
1:D:88:SER:HB2	4:J:91:VAL:HG21	1.80	0.63
1:A:6:ALA:HB3	1:A:24:LEU:HD23	1.79	0.63
2:C:52:TYR:CD2	4:G:220:ILE:HD11	2.34	0.63
3:I:275:THR:HG21	3:I:310:PHE:CE1	2.34	0.63
1:A:25:THR:O	1:A:206:ARG:NH1	2.31	0.63
1:B:206:ARG:NH2	1:B:208:TYR:OH	2.32	0.63
4:G:70:MET:HE2	4:G:320:TYR:HB2	1.82	0.62
4:G:98:THR:HG23	4:G:101:GLN:H	1.65	0.62
1:B:70:LEU:CD1	1:B:75:ARG:HG2	2.30	0.62
1:D:55:ARG:HE	1:D:68:SER:HB3	1.65	0.62
1:E:177:LYS:HG2	1:E:203:VAL:HB	1.80	0.61
1:D:94:SER:O	1:D:98:ASN:ND2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:70:MET:HG3	4:J:316:GLY:HA3	1.82	0.61
2:H:133:ASN:ND2	2:H:147:ASP:OD2	2.34	0.61
1:E:85:GLN:HB2	1:E:163:GLU:HB2	1.82	0.61
2:H:145:SER:HB3	2:H:163:MET:HG2	1.83	0.60
1:A:100:MET:O	1:A:104:GLN:HG3	2.00	0.60
1:A:231:LYS:HD2	1:A:235:LEU:HD23	1.83	0.60
4:G:62:LYS:HD2	4:G:129:GLU:OE1	2.00	0.60
1:D:177:LYS:HG2	1:D:203:VAL:HG11	1.82	0.60
3:I:212:ARG:NH2	3:I:214:GLU:OE2	2.34	0.60
1:A:67:ILE:HD12	1:A:75:ARG:HG3	1.83	0.60
1:E:122:MET:HE1	1:E:131:ARG:HG2	1.83	0.60
4:J:38:GLN:OE1	4:J:136:ARG:NH1	2.34	0.60
1:D:8:ASN:H	1:D:23:SER:HG	1.50	0.60
2:C:78:PHE:HB2	2:C:101:ALA:HB3	1.83	0.59
3:F:145:ALA:HB1	3:F:169:PHE:CE1	2.37	0.59
1:A:181:GLU:OE1	1:A:184:ARG:NH2	2.34	0.59
4:G:329:LEU:HD13	4:G:332:VAL:HG21	1.84	0.59
2:C:121:THR:HG22	2:C:123:ASP:H	1.68	0.59
2:C:42:TYR:HD1	2:C:69:TYR:HB3	1.68	0.59
1:E:50:VAL:HG22	1:E:160:LEU:HD12	1.85	0.59
4:J:269:GLY:HA3	4:J:331:LEU:HD11	1.84	0.59
3:F:60:ALA:HA	3:F:63:ILE:HG12	1.84	0.58
1:B:65:GLU:O	1:B:67:ILE:HG13	2.03	0.58
3:F:213:PHE:HD1	3:F:224:ILE:HD12	1.67	0.58
1:E:35:LEU:HD21	1:E:200:THR:HG21	1.84	0.58
2:H:126:LEU:HD21	2:H:129:ILE:HD11	1.84	0.58
2:H:13:SER:O	2:H:17:LEU:HG	2.03	0.58
3:I:249:MET:HB3	3:I:253:THR:HB	1.85	0.58
2:H:60:TYR:CZ	2:H:138:LEU:HD11	2.38	0.58
2:H:95:SER:HB2	2:H:120:LEU:HD11	1.86	0.57
2:C:81:PRO:HG2	2:C:98:SER:HB3	1.86	0.57
1:B:31:ILE:HD11	1:B:184:ARG:HB2	1.85	0.57
1:B:55:ARG:HE	1:B:68:SER:HB3	1.69	0.57
3:I:89:HIS:HA	3:I:93:LEU:O	2.03	0.57
1:B:123:GLU:OE1	1:D:212:GLN:NE2	2.38	0.57
1:A:208:TYR:HD2	1:A:216:ILE:HD12	1.70	0.57
4:G:100:LEU:O	4:G:104:LEU:HG	2.04	0.57
4:J:161:VAL:HG13	4:J:177:ILE:HG13	1.86	0.57
3:I:44:PRO:HD2	3:I:47:LEU:HD23	1.86	0.57
3:F:278:MET:SD	3:F:338:TYR:HB3	2.45	0.56
1:D:60:ILE:H	1:D:68:SER:HG	1.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:80:LEU:HB3	4:J:296:ILE:HG21	1.87	0.56
1:E:122:MET:HE2	1:E:128:GLU:HA	1.86	0.56
1:D:87:ALA:HB2	1:D:143:ARG:HH11	1.71	0.56
1:D:60:ILE:N	1:D:68:SER:OG	2.27	0.56
1:D:211:SER:HB3	1:D:216:ILE:HD11	1.86	0.56
4:J:58:LEU:HB2	4:J:132:ALA:HB2	1.87	0.56
2:C:42:TYR:HB3	2:C:69:TYR:HB3	1.87	0.56
2:C:9:ILE:HD13	3:F:300:LEU:HD23	1.85	0.56
1:E:150:ARG:HH22	3:I:87:VAL:CG1	2.18	0.56
2:H:154:THR:HG22	2:H:155:THR:HG23	1.88	0.56
3:F:42:GLU:HA	3:F:139:PRO:HB3	1.88	0.56
2:C:81:PRO:HG3	2:C:101:ALA:HB2	1.87	0.55
1:A:88:SER:HB2	4:G:91:VAL:CG2	2.37	0.55
2:H:185:GLN:N	2:H:185:GLN:OE1	2.40	0.55
1:D:5:THR:HG22	1:D:25:THR:HG23	1.88	0.55
1:D:9:LEU:HB2	1:D:22:VAL:O	2.07	0.55
4:J:80:LEU:HB2	4:J:296:ILE:HG13	1.89	0.55
3:F:230:TYR:OH	3:F:232:ALA:HB2	2.06	0.55
3:F:174:LEU:HB2	3:F:188:VAL:HG22	1.88	0.55
3:F:72:LEU:HD11	3:F:105:LEU:HD13	1.90	0.54
3:I:60:ALA:HA	3:I:63:ILE:HG12	1.88	0.54
2:H:161:LEU:HB3	2:H:176:GLU:HB2	1.89	0.54
3:I:152:ALA:HB1	3:I:155:GLY:HA2	1.89	0.54
4:G:295:PHE:HB3	4:G:300:LEU:HD12	1.88	0.54
2:H:81:PRO:HG3	2:H:101:ALA:HB2	1.89	0.54
4:J:239:LEU:HD11	4:J:256:ASN:HB2	1.90	0.54
2:C:56:GLY:HA2	4:G:220:ILE:HB	1.89	0.54
3:F:341:LEU:O	3:F:345:LEU:HG	2.07	0.54
1:E:67:ILE:HA	1:E:70:LEU:HD13	1.88	0.54
2:H:141:GLN:HG2	2:H:167:LEU:HB2	1.90	0.54
4:J:25:MET:O	4:J:29:LEU:HG	2.07	0.54
2:C:5:ARG:NH2	3:F:301:PRO:HG3	2.22	0.54
1:A:88:SER:HB2	4:G:91:VAL:HG21	1.91	0.53
1:B:6:ALA:O	1:B:23:SER:HA	2.09	0.53
4:G:88:GLU:O	4:G:92:MET:HG3	2.08	0.53
4:G:300:LEU:HD22	4:G:303:VAL:HG21	1.91	0.53
3:F:44:PRO:HG2	3:F:46:ASN:OD1	2.09	0.53
3:I:61:GLN:HB3	3:I:272:LEU:HD21	1.89	0.53
3:I:341:LEU:O	3:I:345:LEU:HG	2.07	0.53
4:J:326:PHE:CE2	4:J:343:LEU:HD22	2.43	0.53
1:B:90:PHE:HE1	3:F:88:MET:HE3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:HG3	1:D:127:ILE:HG13	1.90	0.53
1:A:55:ARG:HH21	1:A:57:ALA:HA	1.73	0.53
1:A:169:ASP:OD1	1:B:38:ASN:ND2	2.41	0.53
3:I:259:THR:HG23	3:I:262:ALA:H	1.74	0.53
4:J:273:LEU:HD12	4:J:341:ALA:HB2	1.90	0.53
4:G:276:TRP:CE3	4:G:279:ILE:HD11	2.44	0.53
2:H:160:GLY:HA2	2:H:177:LYS:O	2.09	0.53
1:A:177:LYS:HA	1:A:180:ILE:HG22	1.90	0.53
3:F:74:MET:SD	3:F:299:MET:HE1	2.49	0.53
3:I:325:LEU:HD11	3:I:330:TRP:CD1	2.44	0.53
3:F:230:TYR:CD1	3:F:231:GLN:N	2.77	0.53
4:G:7:LEU:HD22	4:G:92:MET:HE2	1.91	0.53
3:I:250:ASP:OD1	3:I:251:MET:N	2.42	0.53
4:J:315:PHE:HA	4:J:318:VAL:HG22	1.92	0.52
1:B:75:ARG:HB3	1:B:80:ILE:HD12	1.91	0.52
1:B:145:ARG:HD3	7:E:302:NOV:O3	2.08	0.52
4:J:88:GLU:O	4:J:92:MET:HG3	2.10	0.52
2:C:161:LEU:HB2	2:C:176:GLU:HB2	1.90	0.52
3:F:63:ILE:O	3:F:67:SER:N	2.27	0.52
4:G:138:GLN:HA	4:G:143:GLY:N	2.24	0.52
1:D:50:VAL:HG22	1:D:160:LEU:HD12	1.92	0.52
1:E:61:ILE:HG22	1:E:66:ASP:HA	1.91	0.52
4:G:186:LEU:HD13	4:G:215:THR:HG22	1.92	0.52
3:I:11:THR:HG22	3:I:75:THR:HB	1.92	0.52
1:B:156:PRO:HG2	1:B:159:ILE:HD11	1.91	0.52
1:B:177:LYS:HG2	1:B:203:VAL:HG21	1.91	0.52
4:J:55:TYR:HD1	4:J:132:ALA:HB1	1.75	0.52
4:G:80:LEU:HD23	4:G:83:LEU:HD12	1.92	0.51
2:C:101:ALA:HB1	2:C:109:LEU:HD11	1.92	0.51
3:F:189:VAL:HG13	4:G:184:ARG:HD3	1.91	0.51
2:C:182:TYR:CB	2:C:186:ASN:HA	2.41	0.51
3:F:160:PHE:HE1	4:G:266:GLN:HG3	1.76	0.51
3:F:230:TYR:CZ	3:F:232:ALA:HB2	2.46	0.51
1:A:9:LEU:HD21	1:A:60:ILE:HD11	1.93	0.51
1:E:34:LEU:HD21	1:E:45:THR:HG23	1.92	0.51
3:I:212:ARG:HB3	3:I:225:THR:OG1	2.11	0.51
4:J:7:LEU:HD21	4:J:92:MET:SD	2.51	0.51
4:J:89:LEU:O	4:J:93:GLN:HG3	2.10	0.51
3:F:279:MET:HE2	3:F:306:TYR:HD2	1.76	0.51
1:E:104:GLN:OE1	3:I:2:ILE:N	2.34	0.51
7:E:302:NOV:O6	7:E:302:NOV:N1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:326:ASP:OD2	3:F:329:VAL:HG23	2.11	0.51
1:D:31:ILE:HB	1:D:204:CYS:HA	1.92	0.51
2:H:17:LEU:HD11	4:J:29:LEU:HD22	1.92	0.51
1:D:43:THR:N	5:D:301:SO4:O2	2.43	0.50
1:E:75:ARG:HB3	1:E:80:ILE:HD12	1.92	0.50
3:I:253:THR:O	3:I:257:THR:OG1	2.28	0.50
1:A:61:ILE:HD13	1:A:66:ASP:HA	1.94	0.50
2:H:121:THR:HG22	2:H:123:ASP:H	1.77	0.50
2:H:60:TYR:HE2	2:H:138:LEU:HD21	1.76	0.50
1:B:101:ALA:HB1	3:F:3:ILE:HG13	1.93	0.50
1:E:160:LEU:HD22	1:E:191:LEU:HD23	1.94	0.50
1:E:31:ILE:HD11	1:E:184:ARG:HB2	1.94	0.50
2:C:166:ASN:OD1	2:C:169:SER:N	2.40	0.50
4:G:97:PHE:CZ	4:G:101:GLN:HB3	2.46	0.50
4:G:122:GLU:OE1	4:G:250:SER:OG	2.29	0.50
3:F:160:PHE:CE2	4:G:155:LYS:HE3	2.47	0.49
1:A:104:GLN:NE2	4:G:6:VAL:HG23	2.26	0.49
1:A:235:LEU:HD11	1:A:239:PHE:CG	2.46	0.49
3:I:3:ILE:HD13	3:I:93:LEU:HD22	1.94	0.49
3:I:116:ASN:HA	3:I:120:ALA:HB3	1.95	0.49
1:A:170:PRO:HG2	1:B:235:LEU:HD23	1.94	0.49
1:E:160:LEU:HD22	1:E:191:LEU:HB3	1.93	0.49
1:D:2:ALA:HB1	1:D:28:SER:OG	2.13	0.49
1:D:34:LEU:HD21	1:D:45:THR:HG23	1.93	0.49
1:D:119:ASN:OD1	1:D:131:ARG:NH1	2.45	0.49
3:F:351:VAL:HB	3:F:352:PRO:HD3	1.95	0.49
1:D:101:ALA:HB1	4:J:7:LEU:HB2	1.95	0.49
2:H:52:TYR:HA	2:H:58:LEU:HA	1.95	0.49
4:J:276:TRP:CE3	4:J:279:ILE:HD11	2.47	0.49
1:B:92:ARG:HB2	3:F:6:TYR:HE1	1.78	0.49
1:E:60:ILE:HB	1:E:68:SER:HA	1.93	0.49
1:A:75:ARG:O	1:A:80:ILE:HB	2.13	0.48
3:F:117:VAL:HG11	3:F:269:ARG:HB3	1.95	0.48
2:C:109:LEU:HB3	2:C:136:ILE:HG23	1.94	0.48
3:F:117:VAL:CG1	3:F:269:ARG:HB3	2.44	0.48
3:F:348:TRP:HA	3:F:353:VAL:HG11	1.94	0.48
4:G:61:PRO:HA	4:G:64:VAL:HG12	1.94	0.48
1:B:122:MET:HE1	1:B:131:ARG:HG3	1.95	0.48
3:F:174:LEU:HB2	3:F:188:VAL:CG2	2.43	0.48
1:D:4:LEU:HB3	1:D:26:VAL:CG1	2.44	0.48
4:J:61:PRO:HA	4:J:64:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:212:ARG:HB3	3:F:225:THR:HB	1.95	0.48
2:C:40:PRO:HB3	2:C:70:PHE:HE1	1.78	0.48
3:I:348:TRP:HA	3:I:353:VAL:HG11	1.95	0.48
1:A:73:HIS:HA	4:G:93:GLN:O	2.14	0.48
3:F:14:SER:O	3:F:18:ILE:HG13	2.12	0.48
1:E:82:TYR:HB3	3:I:90:ALA:HB1	1.95	0.48
4:J:53:GLY:O	4:J:57:LEU:HG	2.14	0.48
3:I:64:LEU:HB2	3:I:65:PRO:HD3	1.96	0.48
3:I:347:LEU:O	3:I:350:THR:OG1	2.32	0.48
1:B:173:VAL:HG11	1:B:199:GLU:HG3	1.96	0.47
3:I:146:GLN:O	3:I:167:SER:HA	2.14	0.47
4:J:11:ILE:HD13	4:J:102:VAL:HG13	1.95	0.47
3:F:145:ALA:HB1	3:F:169:PHE:HE1	1.80	0.47
4:J:239:LEU:HA	4:J:242:VAL:HG22	1.96	0.47
1:E:67:ILE:HG13	1:E:70:LEU:HD22	1.95	0.47
1:A:8:ASN:H	1:A:23:SER:HG	1.57	0.47
3:F:12:LEU:HD23	3:F:12:LEU:HA	1.66	0.47
1:D:31:ILE:HD11	1:D:184:ARG:HB2	1.96	0.47
3:I:275:THR:HG21	3:I:310:PHE:HE1	1.77	0.47
1:B:70:LEU:HD12	1:B:70:LEU:C	2.40	0.47
2:C:58:LEU:HD12	2:C:59:ASN:H	1.79	0.47
4:G:25:MET:O	4:G:29:LEU:HG	2.15	0.47
4:J:295:PHE:HB3	4:J:300:LEU:HD23	1.96	0.47
2:C:58:LEU:HD12	2:C:59:ASN:N	2.30	0.47
3:F:176:GLN:O	3:F:177:LEU:HD23	2.15	0.47
3:F:282:ILE:O	3:F:285:PRO:HD2	2.15	0.47
1:D:50:VAL:O	1:D:75:ARG:HD2	2.14	0.46
1:B:31:ILE:HD12	1:B:190:VAL:HB	1.97	0.46
2:C:46:HIS:H	2:C:65:GLN:C	2.24	0.46
3:F:79:LEU:HD22	3:F:84:GLU:OE1	2.15	0.46
1:E:235:LEU:HD22	1:E:239:PHE:HZ	1.80	0.46
3:I:199:LYS:HA	3:I:199:LYS:HD3	1.67	0.46
1:E:122:MET:HE1	1:E:131:ARG:CG	2.44	0.46
1:D:168:VAL:HG13	1:D:172:SER:HB2	1.98	0.46
1:E:70:LEU:HD23	1:E:74:ALA:HB1	1.97	0.46
4:J:7:LEU:HD22	4:J:97:PHE:CZ	2.51	0.46
4:J:321:VAL:O	4:J:325:ILE:HG12	2.15	0.46
1:D:164:PRO:HD2	1:D:194:ASP:HB2	1.98	0.46
3:I:79:LEU:HD22	3:I:84:GLU:OE1	2.15	0.46
2:C:156:PHE:HB3	2:C:182:TYR:CE1	2.50	0.46
3:F:148:GLN:O	3:F:161:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LEU:HD13	1:D:138:LEU:HD22	1.96	0.46
1:E:6:ALA:O	1:E:23:SER:HA	2.16	0.46
1:A:148:ILE:HD13	1:A:179:ILE:HG21	1.98	0.46
1:D:9:LEU:HD11	1:D:60:ILE:HD11	1.98	0.46
2:H:46:HIS:HA	2:H:64:ALA:O	2.16	0.46
4:J:55:TYR:CD1	4:J:132:ALA:HB1	2.51	0.46
4:G:22:THR:HG21	4:G:74:LEU:HB3	1.97	0.46
1:E:144:ARG:NH1	1:E:147:GLU:OE1	2.49	0.46
2:H:94:TRP:CD1	2:H:167:LEU:HB3	2.50	0.46
3:F:347:LEU:HB3	3:F:353:VAL:HG21	1.98	0.45
1:E:41:GLY:O	1:E:45:THR:HG22	2.16	0.45
1:E:62:ILE:HD11	1:E:80:ILE:HD11	1.98	0.45
3:I:179:THR:HG22	3:I:185:PRO:HD3	1.97	0.45
1:A:67:ILE:HD12	1:A:75:ARG:CG	2.46	0.45
1:D:227:ASP:HB3	1:D:230:VAL:HG12	1.98	0.45
3:I:88:MET:HB3	3:I:93:LEU:HD23	1.98	0.45
1:E:173:VAL:HG11	1:E:199:GLU:HG3	1.99	0.45
4:J:309:VAL:O	4:J:313:ILE:HG22	2.16	0.45
3:F:73:LEU:HD13	3:F:299:MET:HB3	1.98	0.45
4:G:336:PRO:HB2	4:G:339:ILE:HG12	1.99	0.45
1:A:235:LEU:HD11	1:A:239:PHE:CD1	2.52	0.45
1:D:84:PRO:HB2	1:D:86:GLU:OE2	2.17	0.45
3:I:351:VAL:HB	3:I:352:PRO:HD3	1.98	0.45
4:J:34:LYS:O	4:J:38:GLN:HG2	2.16	0.45
2:C:6:ARG:O	2:C:10:ILE:HG12	2.16	0.45
4:G:77:LEU:HA	4:G:296:ILE:HD11	1.98	0.45
3:I:278:MET:HE3	3:I:278:MET:HA	1.98	0.45
1:A:122:MET:HE2	1:A:122:MET:HB3	1.81	0.45
1:D:78:ARG:O	1:D:157:LYS:NZ	2.45	0.45
2:H:117:VAL:O	2:H:128:LYS:HA	2.17	0.45
2:C:129:ILE:HD13	2:C:163:MET:HE1	1.99	0.45
4:G:151:GLY:HA2	4:G:163:ILE:O	2.17	0.45
4:J:100:LEU:O	4:J:104:LEU:HG	2.17	0.45
4:G:58:LEU:HB2	4:G:132:ALA:HB2	2.00	0.44
1:D:9:LEU:HD21	1:D:60:ILE:HD11	1.99	0.44
1:E:88:SER:O	1:E:150:ARG:NH1	2.47	0.44
3:I:93:LEU:HD11	3:I:97:VAL:HG11	1.98	0.44
3:I:275:THR:O	3:I:279:MET:HG2	2.18	0.44
3:F:220:ARG:HB3	4:G:220:ILE:HG21	2.00	0.44
1:D:86:GLU:H	1:D:86:GLU:CD	2.25	0.44
3:F:230:TYR:CD1	3:F:230:TYR:C	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:102:VAL:O	4:G:106:VAL:HG23	2.17	0.44
3:I:176:GLN:O	4:J:153:TRP:NE1	2.46	0.44
1:A:9:LEU:HB2	1:A:22:VAL:O	2.17	0.44
1:B:170:PRO:HA	1:B:173:VAL:HB	2.00	0.44
4:J:105:SER:O	4:J:109:THR:HG22	2.17	0.44
4:J:295:PHE:O	4:J:300:LEU:HB2	2.18	0.44
1:B:67:ILE:HG22	1:B:67:ILE:O	2.17	0.44
3:F:164:VAL:HG12	3:F:166:GLY:H	1.81	0.44
3:F:205:VAL:HG21	3:F:234:ILE:HD12	1.99	0.44
1:D:183:LEU:O	1:D:188:LEU:HB2	2.18	0.44
1:A:207:ALA:O	1:A:218:HIS:HA	2.18	0.44
1:D:198:ARG:HG3	1:D:241:LEU:HA	1.99	0.44
1:D:198:ARG:NE	1:D:241:LEU:OXT	2.49	0.44
1:E:159:ILE:HG23	1:E:190:VAL:HG13	1.99	0.44
1:A:24:LEU:HB2	1:A:208:TYR:CD1	2.52	0.44
1:A:84:PRO:HB2	1:A:86:GLU:OE2	2.17	0.44
2:C:43:LYS:HB2	3:F:231:GLN:HB3	2.00	0.44
1:E:175:ASP:O	1:E:179:ILE:HG13	2.17	0.44
4:G:89:LEU:O	4:G:93:GLN:HG3	2.18	0.44
3:I:56:ILE:HG13	3:I:57:PRO:HD3	2.00	0.44
1:A:40:ALA:HB1	1:A:211:SER:HA	1.99	0.43
1:E:106:ARG:NH2	1:E:155:ASN:HB2	2.33	0.43
3:I:104:ILE:O	3:I:108:PHE:HD1	2.01	0.43
3:F:88:MET:HB3	3:F:93:LEU:HD22	2.00	0.43
1:D:209:ILE:HD13	1:D:230:VAL:HG21	2.00	0.43
1:E:103:LEU:HD21	1:E:117:ARG:HB3	2.00	0.43
2:H:18:ILE:HG13	4:J:36:VAL:HG21	2.00	0.43
2:H:132:ASP:N	2:H:132:ASP:OD1	2.51	0.43
4:J:310:VAL:HA	4:J:313:ILE:HG22	1.98	0.43
1:B:35:LEU:HD21	1:B:200:THR:HG21	2.00	0.43
4:G:7:LEU:HD12	4:G:97:PHE:CG	2.53	0.43
2:C:49:THR:HG22	3:F:225:THR:HG23	2.01	0.43
3:F:268:TRP:CE2	3:F:272:LEU:HD22	2.53	0.43
1:D:175:ASP:O	1:D:179:ILE:HG13	2.19	0.43
2:H:94:TRP:CZ3	2:H:119:ALA:HB2	2.53	0.43
4:J:114:VAL:HA	4:J:117:THR:HG22	1.99	0.43
1:A:49:VAL:HG22	1:A:60:ILE:HD12	1.99	0.43
1:B:4:LEU:HB3	1:B:26:VAL:HG23	2.00	0.43
2:C:42:TYR:CZ	3:F:212:ARG:NH1	2.86	0.43
1:D:74:ALA:O	1:D:78:ARG:HG2	2.18	0.43
2:H:96:ILE:HG12	2:H:117:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:177:LEU:HD22	4:G:151:GLY:O	2.19	0.43
4:G:235:THR:O	4:G:238:LYS:N	2.51	0.43
4:G:315:PHE:HA	4:G:318:VAL:HG22	2.00	0.43
2:H:137:ASN:O	2:H:141:GLN:N	2.51	0.43
4:J:102:VAL:O	4:J:106:VAL:HG23	2.19	0.43
1:A:67:ILE:HG22	1:A:70:LEU:HD12	1.99	0.43
2:C:96:ILE:HD11	2:C:167:LEU:HD11	2.00	0.43
4:G:103:ALA:HA	4:G:293:LEU:HD21	2.01	0.43
3:I:4:ILE:HD12	3:I:4:ILE:HG23	1.75	0.43
1:D:32:VAL:O	1:D:191:LEU:HD12	2.19	0.43
1:A:24:LEU:HD23	1:A:24:LEU:H	1.83	0.43
1:A:88:SER:O	4:G:91:VAL:HG21	2.19	0.43
1:B:115:GLN:O	1:B:119:ASN:ND2	2.42	0.43
3:F:147:GLY:O	3:F:161:ILE:HD12	2.19	0.43
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.85	0.42
4:G:281:GLN:N	4:G:282:PRO:HD2	2.34	0.42
1:A:31:ILE:HG23	1:A:190:VAL:HG23	2.01	0.42
2:C:44:SER:HA	3:F:229:ASN:O	2.19	0.42
1:E:200:THR:O	1:E:204:CYS:N	2.51	0.42
1:B:26:VAL:HG12	1:B:32:VAL:HG21	2.02	0.42
3:F:114:ALA:HB2	3:F:273:VAL:HG11	2.02	0.42
4:G:179:ALA:O	4:G:187:GLN:HA	2.18	0.42
3:I:265:GLU:O	3:I:269:ARG:HG3	2.19	0.42
1:B:194:ASP:OD1	1:B:195:HIS:N	2.48	0.42
1:D:4:LEU:HB3	1:D:26:VAL:HG13	2.00	0.42
1:D:160:LEU:HD22	1:D:191:LEU:HB3	2.02	0.42
1:A:37:PRO:HG3	1:A:234:TYR:HD1	1.85	0.42
1:B:71:PRO:HD3	3:F:351:VAL:HG22	2.01	0.42
2:C:136:ILE:HA	2:C:142:ASP:O	2.18	0.42
1:E:127:ILE:HG22	1:E:127:ILE:O	2.19	0.42
1:B:67:ILE:HG12	1:B:78:ARG:HH11	1.85	0.42
4:G:161:VAL:HG11	4:G:230:TRP:CZ2	2.55	0.42
1:D:59:ASN:HA	1:D:68:SER:OG	2.20	0.42
1:E:128:GLU:O	1:E:131:ARG:HG3	2.19	0.42
3:F:11:THR:HG22	3:F:75:THR:HB	2.02	0.42
4:G:318:VAL:HG23	4:G:348:PHE:HZ	1.84	0.42
1:B:5:THR:HG23	1:B:25:THR:HG22	2.02	0.42
3:F:348:TRP:HA	3:F:353:VAL:CG1	2.49	0.42
1:A:10:ALA:HB3	1:A:57:ALA:HB3	2.02	0.42
1:B:33:GLY:N	1:B:204:CYS:SG	2.93	0.42
1:B:70:LEU:HD12	1:B:70:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:TYR:CD2	3:F:288:VAL:HG13	2.55	0.42
1:D:87:ALA:HB2	1:D:143:ARG:NH1	2.35	0.42
4:J:314:SER:O	4:J:318:VAL:HG13	2.20	0.42
1:D:151:ALA:O	1:D:156:PRO:HD3	2.20	0.41
2:C:56:GLY:CA	4:G:220:ILE:HB	2.49	0.41
3:F:64:LEU:HB2	3:F:65:PRO:HD3	2.01	0.41
1:E:235:LEU:HD22	1:E:239:PHE:CZ	2.55	0.41
3:I:73:LEU:HG	3:I:299:MET:HG2	2.02	0.41
3:I:108:PHE:O	3:I:112:VAL:HG23	2.20	0.41
3:F:107:LEU:HA	3:F:277:PHE:CZ	2.55	0.41
1:D:230:VAL:HG22	1:D:235:LEU:HG	2.02	0.41
3:I:57:PRO:O	3:I:61:GLN:HG3	2.21	0.41
4:J:247:ASP:O	4:J:274:ASN:ND2	2.52	0.41
1:B:24:LEU:HD11	1:B:208:TYR:CD2	2.55	0.41
2:C:162:ARG:NE	2:C:176:GLU:OE2	2.54	0.41
3:F:275:THR:HG21	3:F:310:PHE:CE1	2.55	0.41
3:F:279:MET:HE2	3:F:306:TYR:CD2	2.55	0.41
3:I:267:HIS:NE2	3:I:328:MET:HB2	2.35	0.41
4:G:53:GLY:O	4:G:57:LEU:HG	2.21	0.41
1:E:79:GLY:O	1:E:157:LYS:N	2.53	0.41
2:H:96:ILE:HG23	2:H:117:VAL:HG22	2.01	0.41
1:A:45:THR:HA	1:A:48:MET:HE2	2.03	0.41
1:B:24:LEU:HA	1:B:24:LEU:HD12	1.71	0.41
2:C:57:ALA:N	4:G:219:GLN:O	2.53	0.41
1:A:183:LEU:O	1:A:188:LEU:HB2	2.21	0.41
4:J:126:PRO:HB3	4:J:249:LEU:HA	2.01	0.41
3:F:61:GLN:HB3	3:F:272:LEU:HD21	2.03	0.41
2:H:60:TYR:CE2	2:H:138:LEU:HD11	2.56	0.41
1:A:5:THR:HB	1:A:25:THR:HG23	2.02	0.41
1:B:62:ILE:HD11	1:B:80:ILE:HD11	2.02	0.41
2:C:17:LEU:HD11	4:G:29:LEU:HD22	2.02	0.41
1:D:40:ALA:HB1	1:D:211:SER:HA	2.02	0.41
2:H:151:LEU:HG	2:H:174:LEU:HD21	2.03	0.41
4:J:73:LEU:HB2	4:J:288:MET:HB3	2.02	0.41
1:B:148:ILE:HD11	1:B:183:LEU:HD22	2.02	0.41
3:F:285:PRO:HG2	3:F:345:LEU:HD13	2.03	0.41
4:G:245:ASP:N	4:G:246:PRO:HD3	2.36	0.41
1:D:93:LEU:HD22	1:D:97:ASP:HB3	2.03	0.41
1:E:103:LEU:HD12	1:E:106:ARG:HD3	2.01	0.41
1:B:55:ARG:NE	1:B:68:SER:HB3	2.34	0.40
4:G:126:PRO:HB3	4:G:249:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:SER:O	1:E:75:ARG:NH2	2.54	0.40
2:H:136:ILE:HG12	2:H:143:VAL:HG22	2.02	0.40
1:B:180:ILE:HG23	1:B:180:ILE:HD12	1.81	0.40
3:F:63:ILE:HD13	3:F:63:ILE:HG21	1.77	0.40
2:H:101:ALA:HB1	2:H:109:LEU:HD11	2.03	0.40
4:G:230:TRP:NE1	4:G:232:THR:HB	2.36	0.40
4:G:298:GLY:O	4:G:301:ARG:HG3	2.21	0.40
1:D:3:THR:HG22	1:D:27:ASN:OD1	2.22	0.40
1:A:125:PHE:O	1:A:127:ILE:HG23	2.21	0.40
2:C:94:TRP:CD2	2:C:167:LEU:HD22	2.57	0.40
3:F:220:ARG:O	4:G:220:ILE:HD12	2.21	0.40
4:G:289:MET:HE2	4:G:289:MET:HB3	1.88	0.40
2:H:44:SER:HA	3:I:229:ASN:O	2.21	0.40
3:I:222:PHE:HD1	3:I:222:PHE:HA	1.78	0.40
1:A:104:GLN:HE22	4:G:6:VAL:HG23	1.86	0.40
3:F:84:GLU:O	3:F:87:VAL:HG12	2.21	0.40
2:H:60:TYR:CE2	2:H:138:LEU:HD21	2.55	0.40
2:H:158:SER:HA	2:H:179:ARG:O	2.21	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	238/241 (99%)	221 (93%)	16 (7%)	1 (0%)	30	62
1	B	238/241 (99%)	221 (93%)	17 (7%)	0	100	100
1	D	238/241 (99%)	219 (92%)	19 (8%)	0	100	100
1	E	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
2	C	171/195 (88%)	160 (94%)	11 (6%)	0	100	100
2	H	171/195 (88%)	159 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	346/366 (94%)	328 (95%)	17 (5%)	1 (0%)	36	68
3	I	327/366 (89%)	313 (96%)	14 (4%)	0	100	100
4	G	353/360 (98%)	338 (96%)	15 (4%)	0	100	100
4	J	295/360 (82%)	284 (96%)	11 (4%)	0	100	100
All	All	2613/2806 (93%)	2468 (94%)	143 (6%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	139	PRO
1	A	71	PRO

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	183/202 (91%)	181 (99%)	2 (1%)	65	79
1	B	179/202 (89%)	179 (100%)	0	100	100
1	D	187/202 (93%)	185 (99%)	2 (1%)	65	79
1	E	170/202 (84%)	169 (99%)	1 (1%)	78	84
2	C	141/179 (79%)	140 (99%)	1 (1%)	76	83
2	H	138/179 (77%)	138 (100%)	0	100	100
3	F	261/307 (85%)	258 (99%)	3 (1%)	65	79
3	I	242/307 (79%)	239 (99%)	3 (1%)	63	79
4	G	266/300 (89%)	264 (99%)	2 (1%)	73	82
4	J	209/300 (70%)	209 (100%)	0	100	100
All	All	1976/2380 (83%)	1962 (99%)	14 (1%)	76	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	52	ILE
2	C	183	GLU
3	F	4	ILE
3	F	117	VAL
3	F	345	LEU
4	G	220	ILE
4	G	296	ILE
1	D	52	ILE
1	D	190	VAL
1	E	110	THR
3	I	1	MET
3	I	48	VAL
3	I	345	LEU

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	126	HIS
1	B	214	ASN
2	C	118	ASN
2	C	171	ASN
3	F	15	GLN
1	D	182	HIS
1	D	218	HIS
1	D	223	GLN
1	E	119	ASN
1	E	229	HIS
3	I	290	ASN
4	J	101	GLN
4	J	256	ASN

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
5	SO4	F	401	-	4,4,4	0.30	0	6,6,6	0.43	0
5	SO4	B	301	-	4,4,4	0.20	0	6,6,6	0.26	0
5	SO4	A	302	-	4,4,4	0.30	0	6,6,6	0.56	0
5	SO4	G	403	-	4,4,4	0.26	0	6,6,6	0.23	0
5	SO4	J	401	-	4,4,4	0.21	0	6,6,6	0.62	0
5	SO4	J	402	-	4,4,4	0.32	0	6,6,6	0.35	0
5	SO4	G	401	-	4,4,4	0.29	0	6,6,6	0.46	0
7	NOV	E	302	-	47,47,47	1.68	7 (14%)	65,70,70	1.48	10 (15%)
5	SO4	A	301	-	4,4,4	0.29	0	6,6,6	0.20	0
5	SO4	D	301	-	4,4,4	0.25	0	6,6,6	0.63	0
5	SO4	G	402	-	4,4,4	0.41	0	6,6,6	0.87	0
5	SO4	E	301	-	4,4,4	0.30	0	6,6,6	0.32	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
7	NOV	E	302	-	-	8/23/46/46	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	302	NOV	O7-C31	-6.30	1.38	1.46
7	E	302	NOV	C28-C27	3.59	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	302	NOV	C12-N1	3.53	1.40	1.33
7	E	302	NOV	O7-C30	-3.39	1.36	1.42
7	E	302	NOV	C9-C8	-3.25	1.40	1.45
7	E	302	NOV	C31-C27	2.70	1.57	1.53
7	E	302	NOV	C29-C28	2.06	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	302	NOV	C2-C4-C3	3.10	125.19	120.67
7	E	302	NOV	C5-O10-C6	-2.96	119.14	122.64
7	E	302	NOV	C6-C7-N2	2.95	118.50	112.61
7	E	302	NOV	O7-C30-C29	-2.92	104.55	110.42
7	E	302	NOV	O10-C5-C9	2.86	124.38	121.25
7	E	302	NOV	C20-C21-C22	-2.56	123.11	127.52
7	E	302	NOV	C19-C18-C17	-2.51	117.99	120.50
7	E	302	NOV	C28-O5-C12	2.37	120.47	117.03
7	E	302	NOV	C30-C29-C28	-2.23	106.23	110.11
7	E	302	NOV	O5-C12-N1	2.15	114.25	110.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

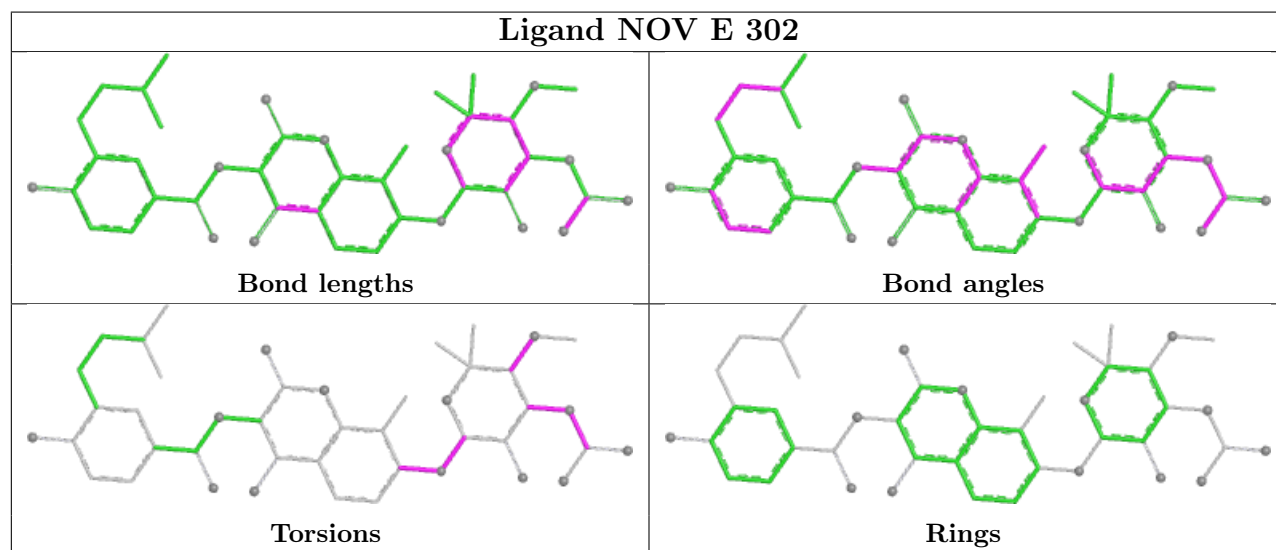
Mol	Chain	Res	Type	Atoms
7	E	302	NOV	N1-C12-O5-C28
7	E	302	NOV	O4-C12-O5-C28
7	E	302	NOV	C27-C28-O5-C12
7	E	302	NOV	O7-C30-O8-C3
7	E	302	NOV	C4-C3-O8-C30
7	E	302	NOV	C28-C27-O1-C1
7	E	302	NOV	C11-C3-O8-C30
7	E	302	NOV	C31-C27-O1-C1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	403	SO4	2	0
5	J	402	SO4	1	0
7	E	302	NOV	2	0
5	D	301	SO4	1	0

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	240/241 (99%)	0.95	43 (17%) 3 3	99, 132, 164, 180	0
1	B	240/241 (99%)	0.68	23 (9%) 13 9	93, 139, 173, 202	0
1	D	240/241 (99%)	0.56	19 (7%) 18 12	86, 120, 148, 170	0
1	E	238/241 (98%)	1.04	42 (17%) 4 3	106, 144, 181, 195	0
2	C	175/195 (89%)	1.20	41 (23%) 2 2	88, 130, 159, 173	0
2	H	175/195 (89%)	1.26	39 (22%) 2 2	95, 142, 189, 203	0
3	F	350/366 (95%)	1.31	82 (23%) 2 2	78, 123, 177, 211	0
3	I	335/366 (91%)	0.95	54 (16%) 4 3	93, 134, 195, 229	0
4	G	355/360 (98%)	1.11	67 (18%) 3 2	89, 131, 175, 203	0
4	J	309/360 (85%)	0.92	59 (19%) 3 2	94, 154, 199, 225	0
All	All	2657/2806 (94%)	1.00	469 (17%) 4 3	78, 134, 186, 229	0

All (469) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	138	ASN	13.1
4	G	215	THR	11.9
3	F	134	GLU	11.7
1	D	107	ASP	11.3
4	G	183	GLU	10.9
4	G	213	ASP	10.6
1	B	241	LEU	10.4
4	G	185	ARG	10.1
4	G	245	ASP	9.0
4	G	302	SER	8.7
4	G	147	SER	8.5
2	C	1	MET	8.0
3	I	150	GLN	7.9

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Mol	Chain	Res	Type	RSRZ
3	F	151	GLN	7.8
4	G	244	LEU	7.6
4	G	216	ASN	7.6
3	F	13	LYS	7.5
3	I	221	ASP	7.4
4	G	270	ARG	7.2
1	B	202	ALA	7.1
1	E	18	VAL	6.9
3	F	135	ALA	6.9
3	F	319	ASN	6.8
1	B	185	ASP	6.8
1	A	170	PRO	6.7
4	J	130	GLN	6.6
1	A	174	ILE	6.6
2	C	4	THR	6.6
4	G	21	MET	6.4
4	G	182	ASP	6.4
4	J	301	ARG	6.3
2	H	77	TRP	6.3
4	G	241	VAL	6.3
4	G	13	LYS	6.1
2	H	68	GLU	6.1
2	H	103	LEU	6.1
2	H	40	PRO	6.0
4	G	237	ASP	6.0
4	J	302	SER	6.0
1	E	12	ALA	6.0
1	E	172	SER	5.9
1	A	240	ARG	5.9
3	I	151	GLN	5.9
3	F	137	ALA	5.8
2	C	183	GLU	5.8
4	G	169	ASP	5.8
3	I	149	PHE	5.8
4	G	217	PRO	5.8
2	C	152	TYR	5.7
2	C	160	GLY	5.6
2	C	153	GLY	5.6
3	F	133	ALA	5.6
2	H	76	SER	5.6
3	F	181	GLY	5.5
2	H	75	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
3	I	103	MET	5.4
4	G	240	GLY	5.4
3	I	340	LEU	5.4
1	E	46	PHE	5.4
4	G	247	ASP	5.4
4	G	17	THR	5.3
1	A	169	ASP	5.3
1	E	190	VAL	5.2
4	G	170	ASP	5.2
3	I	182	ASN	5.2
3	F	12	LEU	5.2
1	B	238	ASP	5.2
1	A	241	LEU	5.2
4	J	187	GLN	5.2
4	G	168	GLY	5.2
3	I	219	LEU	5.1
1	B	240	ARG	5.1
1	E	32	VAL	5.1
3	I	216	THR	5.0
4	G	271	TYR	5.0
3	F	150	GLN	5.0
2	H	156	PHE	5.0
3	F	149	PHE	5.0
4	J	215	THR	5.0
1	E	82	TYR	4.9
1	A	218	HIS	4.9
3	F	228	GLN	4.9
2	H	154	THR	4.8
4	G	355	LEU	4.8
4	G	305	MET	4.8
1	B	201	LEU	4.8
3	F	353	VAL	4.8
2	C	159	SER	4.8
2	C	157	ASN	4.7
3	F	356	ILE	4.7
2	H	106	ASP	4.7
3	F	16	LEU	4.7
3	I	256	ASN	4.7
4	G	246	PRO	4.6
4	G	214	LEU	4.6
4	J	214	LEU	4.6
3	F	14	SER	4.6

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Mol	Chain	Res	Type	RSRZ
3	F	46	ASN	4.6
1	B	239	PHE	4.6
3	F	17	ALA	4.6
3	F	47	LEU	4.5
3	I	232	ALA	4.5
4	G	221	THR	4.5
3	F	148	GLN	4.5
4	G	12	GLY	4.4
2	C	23	ASN	4.4
4	G	16	PHE	4.4
3	I	53	GLY	4.4
2	C	24	LEU	4.4
2	H	100	ARG	4.4
3	I	345	LEU	4.4
1	A	168	VAL	4.3
2	H	54	PRO	4.3
4	J	20	MET	4.3
3	F	289	VAL	4.3
1	E	17	ARG	4.2
3	F	82	GLU	4.2
4	J	18	THR	4.2
3	F	5	ARG	4.2
3	F	132	LEU	4.2
2	C	175	ILE	4.1
2	H	183	GLU	4.1
2	C	156	PHE	4.1
1	E	159	ILE	4.1
4	G	301	ARG	4.1
1	E	30	GLU	4.1
3	I	28	CYS	4.0
4	G	199	PRO	4.0
3	F	349	ASP	4.0
3	I	159	LEU	4.0
3	F	10	GLU	4.0
3	F	97	VAL	4.0
1	E	189	GLY	4.0
3	F	257	THR	4.0
3	I	153	THR	4.0
4	G	186	LEU	4.0
4	G	357	LEU	4.0
1	B	205	GLU	3.9
3	F	249	MET	3.9

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Mol	Chain	Res	Type	RSRZ
3	I	181	GLY	3.9
2	C	176	GLU	3.9
4	J	17	THR	3.9
3	F	318	SER	3.9
3	I	90	ALA	3.9
4	G	227	SER	3.9
3	F	321	ALA	3.9
2	C	63	ILE	3.8
1	E	160	LEU	3.8
4	G	356	LEU	3.8
3	F	6	TYR	3.8
4	J	96	GLY	3.8
2	H	132	ASP	3.8
4	G	299	PRO	3.8
2	C	185	GLN	3.8
4	G	243	ALA	3.8
1	D	108	ASP	3.8
3	F	252	ARG	3.8
4	J	331	LEU	3.8
3	I	29	GLN	3.7
1	E	26	VAL	3.7
1	B	234	TYR	3.7
1	A	108	ASP	3.7
1	E	161	LEU	3.7
2	C	22	VAL	3.7
3	F	186	SER	3.7
3	I	135	ALA	3.7
4	G	332	VAL	3.7
3	F	2	ILE	3.7
4	J	329	LEU	3.7
2	H	67	VAL	3.7
1	A	198	ARG	3.6
3	F	176	GLN	3.6
1	A	21	ASP	3.6
3	F	153	THR	3.6
3	F	147	GLY	3.6
3	F	130	GLU	3.6
3	F	80	TYR	3.6
2	C	123	ASP	3.6
4	J	21	MET	3.6
3	F	191	ASP	3.6
1	B	181	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
4	J	263	SER	3.5
1	D	73	HIS	3.5
4	G	229	THR	3.5
2	C	48	ASP	3.5
3	F	155	GLY	3.5
4	J	212	SER	3.5
2	C	2	SER	3.5
3	I	49	LEU	3.5
2	C	116	GLU	3.4
3	F	262	ALA	3.4
3	F	242	ASP	3.4
1	D	83	LEU	3.4
1	A	107	ASP	3.4
1	A	112	GLU	3.4
4	J	43	GLY	3.4
1	E	2	ALA	3.4
1	A	199	GLU	3.4
3	F	131	VAL	3.4
3	I	158	VAL	3.4
1	A	91	ARG	3.3
3	F	256	ASN	3.3
3	F	8	VAL	3.3
3	F	185	PRO	3.3
1	E	43	THR	3.3
2	H	104	THR	3.3
3	F	178	ARG	3.3
1	B	198	ARG	3.3
2	H	39	ASP	3.3
2	C	49	THR	3.3
4	G	14	THR	3.3
3	I	218	MET	3.3
4	G	20	MET	3.3
3	I	56	ILE	3.2
1	E	83	LEU	3.2
2	C	161	LEU	3.2
3	F	234	ILE	3.2
1	B	207	ALA	3.2
1	D	205	GLU	3.2
4	J	255	HIS	3.2
4	J	82	MET	3.2
4	G	228	GLY	3.2
1	D	52	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	108	MET	3.2
4	G	269	GLY	3.1
2	H	182	TYR	3.1
1	B	31	ILE	3.1
3	I	346	ASN	3.1
4	G	190	ARG	3.1
3	I	217	ALA	3.1
4	J	299	PRO	3.1
1	E	59	ASN	3.1
4	J	335	ILE	3.1
4	J	327	GLY	3.1
1	D	187	GLY	3.1
2	H	49	THR	3.1
1	A	134	LEU	3.0
1	D	207	ALA	3.0
3	I	289	VAL	3.0
3	F	84	GLU	3.0
3	F	255	TRP	3.0
3	I	42	GLU	3.0
3	I	96	ALA	3.0
2	C	20	ILE	3.0
4	J	16	PHE	3.0
1	B	184	ARG	3.0
3	I	347	LEU	3.0
1	A	29	GLY	3.0
1	E	158	PHE	3.0
4	G	226	VAL	2.9
1	E	134	LEU	2.9
2	C	118	ASN	2.9
4	J	232	THR	2.9
4	G	203	GLN	2.9
1	B	230	VAL	2.9
2	C	125	GLN	2.9
1	E	107	ASP	2.9
2	C	154	THR	2.9
4	J	328	PRO	2.9
1	E	152	LEU	2.9
4	G	267	ASP	2.9
1	A	137	ALA	2.9
1	A	237	GLU	2.9
4	G	200	GLU	2.9
3	F	209	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLN	2.8
4	G	207	SER	2.8
3	F	260	ASP	2.8
3	F	139	PRO	2.8
4	G	134	ASN	2.8
1	E	81	GLY	2.8
1	A	171	ILE	2.8
3	I	243	PRO	2.8
1	A	92	ARG	2.8
3	F	136	LYS	2.8
3	F	235	GLY	2.8
2	C	135	GLN	2.8
1	E	118	ALA	2.8
4	G	193	SER	2.8
4	J	234	LEU	2.8
4	J	325	ILE	2.8
1	A	195	HIS	2.8
2	H	107	ARG	2.8
2	H	102	LYS	2.8
1	A	69	LEU	2.8
4	G	148	THR	2.8
1	E	31	ILE	2.8
3	I	24	LEU	2.8
2	H	153	GLY	2.7
4	J	237	ASP	2.7
1	B	233	VAL	2.7
1	D	223	GLN	2.7
2	H	72	ASP	2.7
1	E	206	ARG	2.7
4	J	2	GLN	2.7
1	D	179	ILE	2.7
3	I	244	THR	2.7
4	G	144	SER	2.7
3	I	252	ARG	2.7
4	J	216	ASN	2.7
2	C	184	ILE	2.7
1	D	110	THR	2.7
1	D	2	ALA	2.7
4	J	258	VAL	2.7
4	J	22	THR	2.7
4	J	241	VAL	2.7
3	I	165	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
4	J	233	ASN	2.7
3	I	349	ASP	2.6
1	E	27	ASN	2.6
3	F	324	LYS	2.6
1	E	76	ALA	2.6
2	H	79	THR	2.6
2	H	91	VAL	2.6
1	E	216	ILE	2.6
2	C	80	GLN	2.6
2	H	148	LEU	2.6
3	I	281	LEU	2.6
1	A	206	ARG	2.6
4	G	109	THR	2.6
1	A	201	LEU	2.6
1	D	109	LEU	2.6
4	J	86	ARG	2.6
1	E	156	PRO	2.5
2	H	146	GLN	2.5
4	J	340	GLY	2.5
1	E	173	VAL	2.5
2	H	176	GLU	2.5
3	F	152	ALA	2.5
1	A	165	PHE	2.5
1	D	96	PHE	2.5
3	F	9	ARG	2.5
3	F	347	LEU	2.5
4	J	343	LEU	2.5
3	F	320	GLY	2.5
3	I	92	GLY	2.5
1	E	230	VAL	2.5
4	J	242	VAL	2.5
4	J	213	ASP	2.5
4	J	236	PRO	2.5
4	J	78	LEU	2.5
1	E	141	GLY	2.5
3	F	96	ALA	2.5
1	A	175	ASP	2.5
2	C	107	ARG	2.5
2	H	90	LYS	2.5
2	C	65	GLN	2.5
1	A	30	GLU	2.4
1	E	239	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	222	PHE	2.4
2	C	97	LYS	2.4
4	J	333	TYR	2.4
1	A	233	VAL	2.4
4	J	320	TYR	2.4
4	J	332	VAL	2.4
3	I	316	ILE	2.4
3	I	339	ILE	2.4
4	J	87	SER	2.4
1	D	204	CYS	2.4
2	C	136	ILE	2.4
4	G	358	LYS	2.4
4	J	189	VAL	2.4
2	C	133	ASN	2.4
1	A	217	ALA	2.4
4	J	67	PHE	2.4
2	C	144	THR	2.3
3	I	166	GLY	2.3
3	F	3	ILE	2.3
3	F	4	ILE	2.3
3	I	152	ALA	2.3
3	F	171	ASP	2.3
3	F	177	LEU	2.3
4	G	331	LEU	2.3
2	H	139	VAL	2.3
1	B	84	PRO	2.3
2	C	155	THR	2.3
3	F	30	LYS	2.3
1	E	127	ILE	2.3
4	J	163	ILE	2.3
2	H	114	HIS	2.3
2	C	108	MET	2.3
3	F	182	ASN	2.3
4	J	186	LEU	2.3
3	F	146	GLN	2.3
4	J	326	PHE	2.3
1	A	32	VAL	2.3
1	A	70	LEU	2.3
1	E	192	ILE	2.3
2	H	161	LEU	2.3
2	H	110	TYR	2.3
4	J	262	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLU	2.3
4	J	307	VAL	2.3
3	I	26	PHE	2.3
1	A	27	ASN	2.3
1	A	148	ILE	2.2
4	J	137	ALA	2.2
4	G	145	LEU	2.2
3	F	179	THR	2.2
3	I	180	LYS	2.2
4	G	178	TYR	2.2
4	J	264	SER	2.2
1	B	49	VAL	2.2
1	B	203	VAL	2.2
2	H	186	ASN	2.2
3	F	208	ASN	2.2
1	D	181	GLU	2.2
1	E	162	ASP	2.2
3	F	339	ILE	2.2
3	I	174	LEU	2.2
4	G	197	PHE	2.2
4	J	218	LYS	2.2
2	C	112	TYR	2.2
1	A	173	VAL	2.2
1	E	38	ASN	2.2
3	F	159	LEU	2.2
3	F	81	THR	2.2
3	I	257	THR	2.2
4	J	251	ILE	2.2
3	I	155	GLY	2.2
2	H	164	ARG	2.2
1	E	238	ASP	2.2
2	H	69	TYR	2.1
1	B	52	ILE	2.1
4	G	177	ILE	2.1
3	I	146	GLN	2.1
2	H	165	GLY	2.1
1	D	162	ASP	2.1
1	A	43	THR	2.1
1	A	216	ILE	2.1
4	G	141	TYR	2.1
3	I	71	GLY	2.1
4	J	134	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	194	ASP	2.1
2	C	72	ASP	2.1
4	G	230	TRP	2.1
4	G	320	TYR	2.1
1	A	181	GLU	2.1
1	A	111	SER	2.1
2	H	137	ASN	2.1
1	E	50	VAL	2.1
3	F	258	ASP	2.1
3	I	78	LYS	2.1
4	G	34	LYS	2.1
1	A	192	ILE	2.1
1	B	236	GLY	2.1
1	E	28	SER	2.1
4	J	309	VAL	2.1
1	E	171	ILE	2.1
3	I	154	ASP	2.1
3	I	344	GLY	2.1
3	F	26	PHE	2.1
3	F	352	PRO	2.1
1	B	19	VAL	2.0
4	G	161	VAL	2.0
1	D	28	SER	2.0
4	J	188	SER	2.0
3	F	170	ASN	2.0
4	G	274	ASN	2.0
4	J	313	ILE	2.0
3	F	108	PHE	2.0
1	A	157	LYS	2.0
1	A	50	VAL	2.0
2	C	143	VAL	2.0
1	A	215	LEU	2.0
2	C	110	TYR	2.0
3	I	81	THR	2.0
2	H	87	ASP	2.0
3	F	199	LYS	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 [i](#)

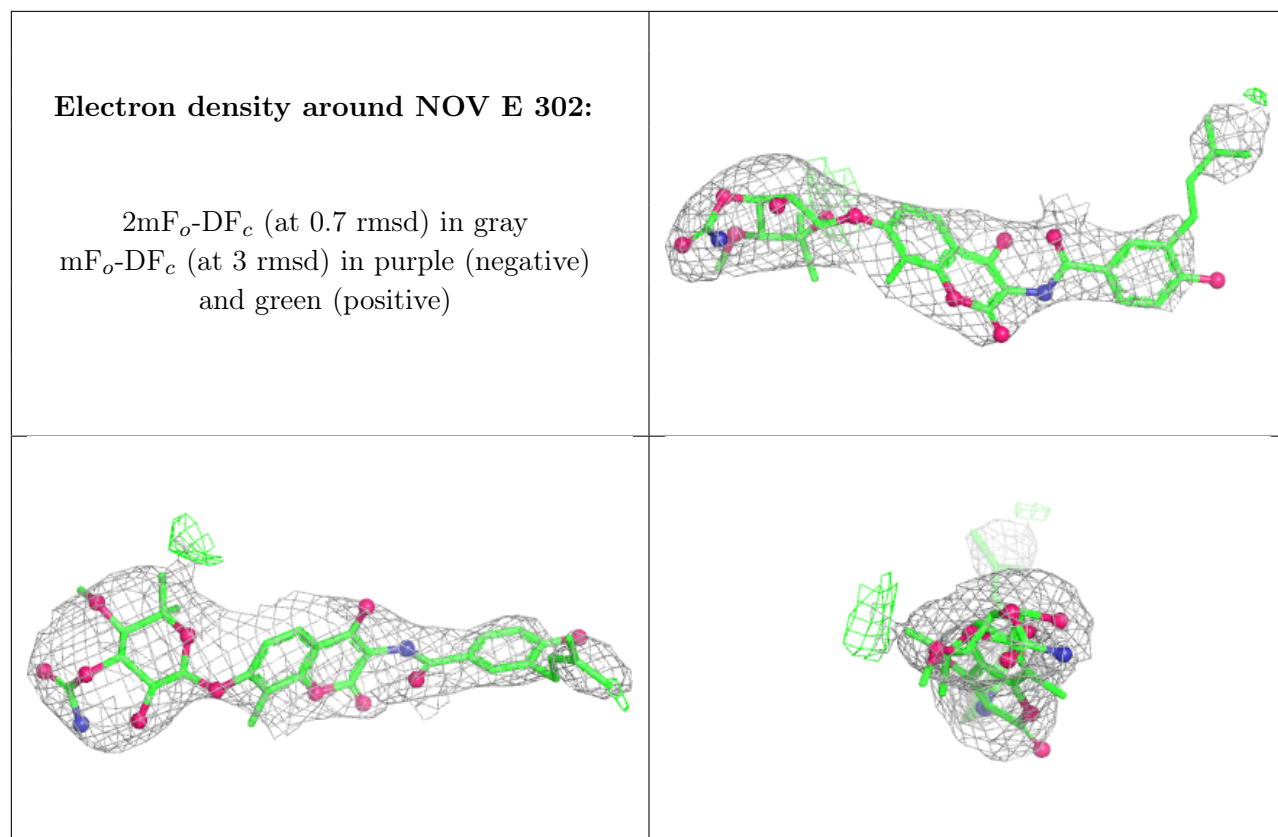
There are no oligosaccharides in this entry.

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
6	CL	A	303	1/1	0.17	0.55	195,195,195,195	0
7	NOV	E	302	44/44	0.69	0.24	102,152,167,171	0
5	SO4	G	403	5/5	0.75	0.09	151,156,173,177	0
5	SO4	A	301	5/5	0.81	0.09	152,153,159,175	0
5	SO4	G	402	5/5	0.84	0.17	81,90,116,131	0
5	SO4	J	402	5/5	0.85	0.26	109,136,140,141	0
5	SO4	F	401	5/5	0.86	0.10	107,115,139,139	0
5	SO4	E	301	5/5	0.88	0.07	142,159,167,168	0
5	SO4	A	302	5/5	0.88	0.09	117,136,145,146	0
5	SO4	G	401	5/5	0.90	0.11	128,130,146,153	0
5	SO4	B	301	5/5	0.93	0.05	144,149,163,166	0
5	SO4	J	401	5/5	0.95	0.06	105,108,118,141	0
5	SO4	D	301	5/5	0.97	0.05	114,118,127,133	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.