



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:41 PM GMT

PDB ID : 3ULU
Title : Structure of quaternary complex of human TLR3ecd with three Fabs (Form1)
Authors : Luo, J.; Gilliland, G.L.; Obmolova, O.; Malia, T.; Teplyakov, A.
Deposited on : 2011-11-11
Resolution : 3.52 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

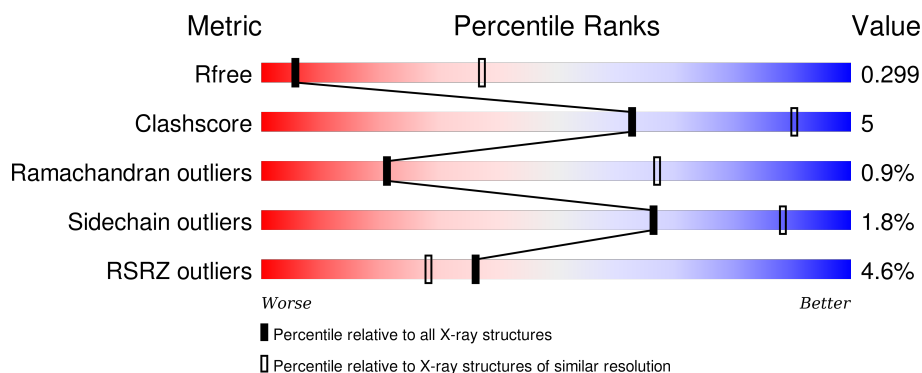
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	694	<div> <div>7%</div> <div>79% 16% 5%</div> </div>
2	L	214	<div> <div>7%</div> <div>85% 14%</div> </div>
3	H	225	<div> <div>12%</div> <div>83% 16%</div> </div>
4	C	213	<div> <div>2%</div> <div>83% 15%</div> </div>
5	D	226	<div> <div>5%</div> <div>76% 23%</div> </div>

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Mol	Chain	Length	Quality of chain
6	E	215	
7	F	223	

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
9	SO4	A	821	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15521 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	659	5284	3380	896	991	17	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	CLONING ARTIFACT	UNP O15455
A	18	ASP	-	CLONING ARTIFACT	UNP O15455
A	19	LEU	-	CLONING ARTIFACT	UNP O15455
A	20	GLY	-	CLONING ARTIFACT	UNP O15455
A	21	SER	-	CLONING ARTIFACT	UNP O15455
A	703	ALA	-	EXPRESSION TAG	UNP O15455
A	704	SER	-	EXPRESSION TAG	UNP O15455
A	705	HIS	-	EXPRESSION TAG	UNP O15455
A	706	HIS	-	EXPRESSION TAG	UNP O15455
A	707	HIS	-	EXPRESSION TAG	UNP O15455
A	708	HIS	-	EXPRESSION TAG	UNP O15455
A	709	HIS	-	EXPRESSION TAG	UNP O15455
A	710	HIS	-	EXPRESSION TAG	UNP O15455

- Molecule 2 is a protein called Fab15 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1633	1020	273	334	6	0	0	0

- Molecule 3 is a protein called Fab15 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	225	1720	1088	286	337	9	0	0	0

- Molecule 4 is a protein called Fab12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	210	Total	C	N	O	S	0	0	0
			1579	987	260	328	4			

- Molecule 5 is a protein called Fab12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	224	Total	C	N	O	S	0	0	0
			1712	1080	294	333	5			

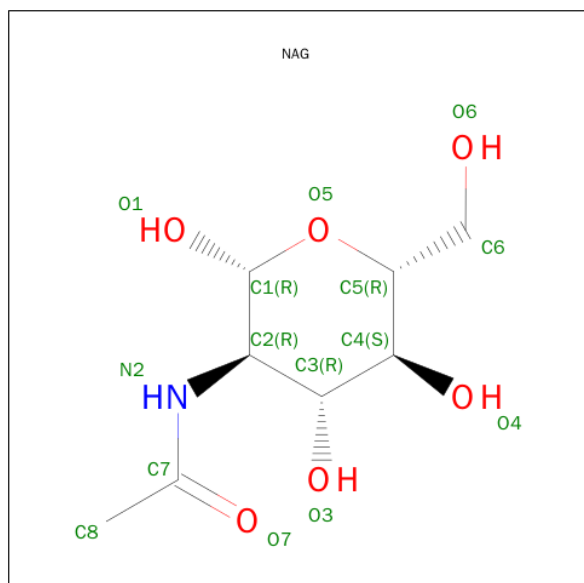
- Molecule 6 is a protein called Fab1068 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	215	Total	C	N	O	S	0	0	0
			1661	1040	279	336	6			

- Molecule 7 is a protein called Fab1068 heavy chain.

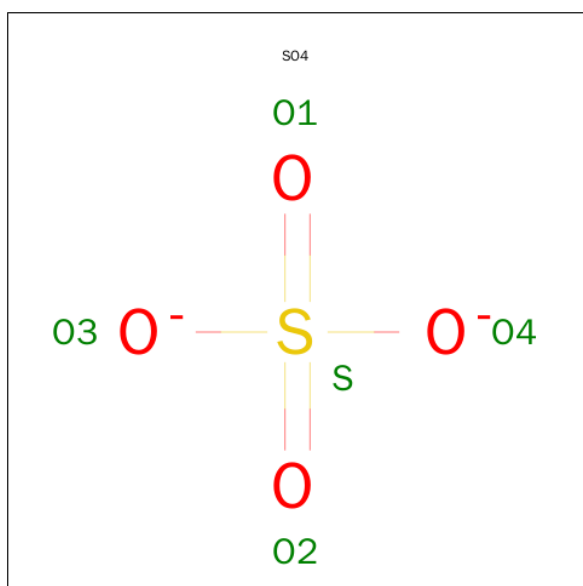
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	217	Total	C	N	O	S	0	0	0
			1656	1050	279	320	7			

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	2	Total	C	N	O	0	0
			28	16	2	10		
10	A	2	Total	C	N	O	0	0
			28	16	2	10		
10	A	2	Total	C	N	O	0	0
			28	16	2	10		
10	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	4	Total	C	N	O	0	0
			50	28	2	20		

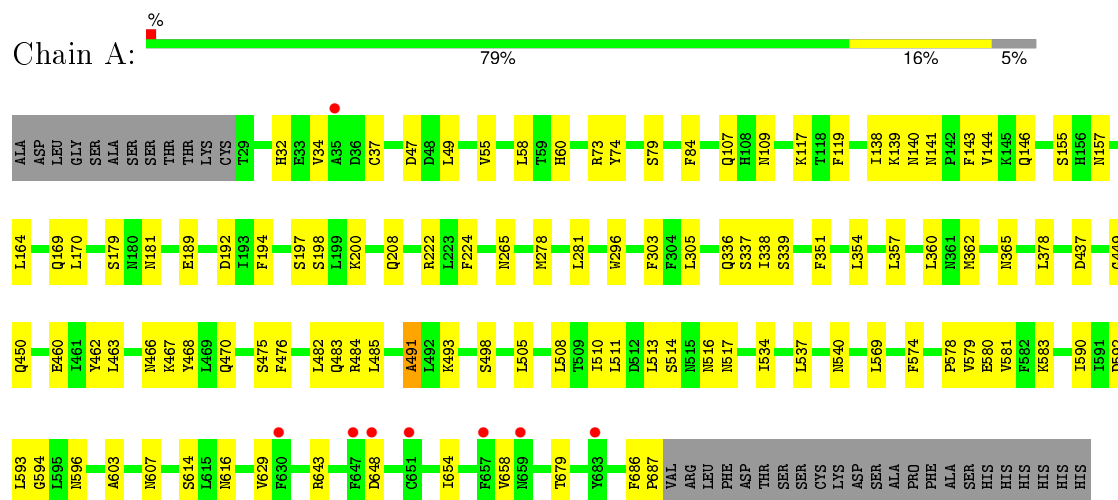
- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	3	Total	C	N	O	0	0
			39	22	2	15		

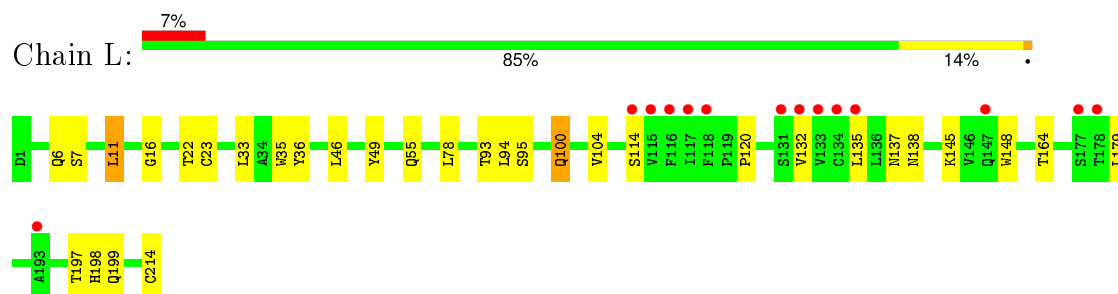
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

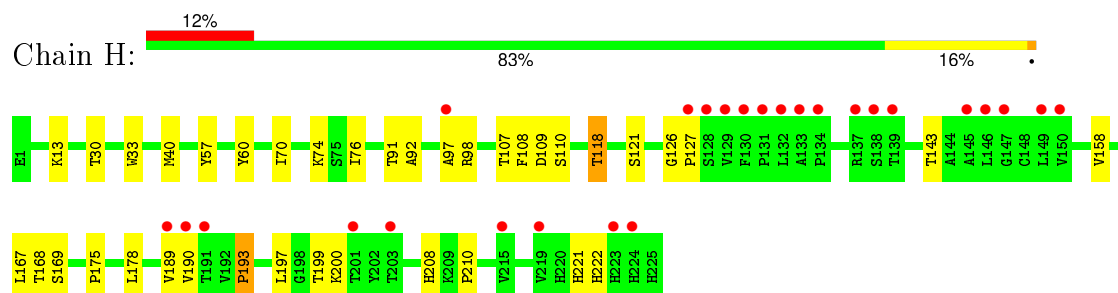
• Molecule 1: Toll-like receptor 3



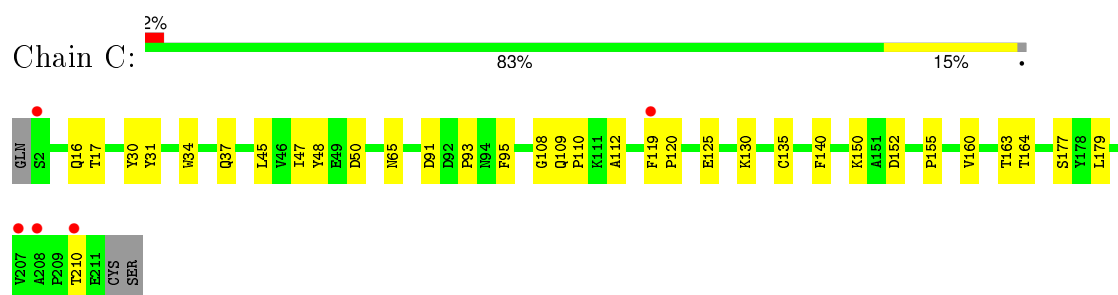
• Molecule 2: Fab15 light chain



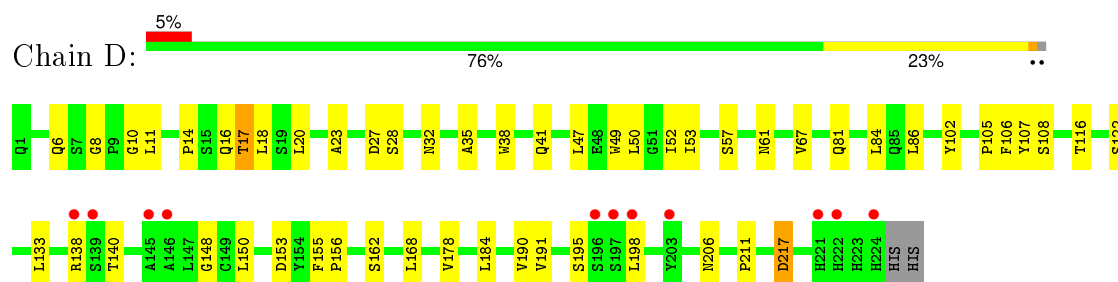
• Molecule 3: Fab15 heavy chain



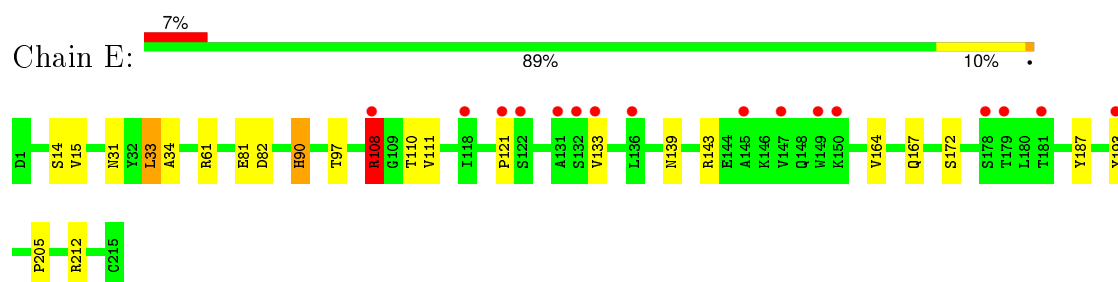
• Molecule 4: Fab12 light chain



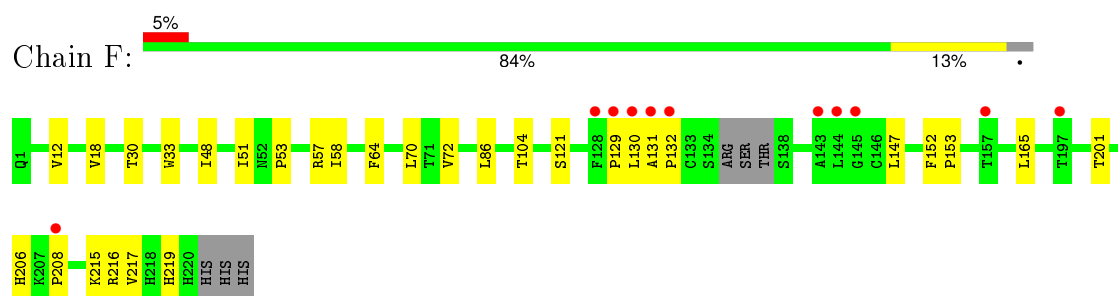
- Molecule 5: Fab12 heavy chain



- Molecule 6: Fab1068 light chain



- Molecule 7: Fab1068 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.90 Å 142.08 Å 125.04 Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	45.08 – 3.52 46.23 – 3.52	Depositor EDS
% Data completeness (in resolution range)	75.9 (45.08-3.52) 76.0 (46.23-3.52)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.48 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1009)	Depositor
R, R_{free}	0.268 , 0.309 0.251 , 0.299	Depositor DCC
R_{free} test set	1732 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34547 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	15521	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BMA, NAG, MAN

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	0.21	0/5396	0.37	0/7326
2	L	0.21	0/1666	0.38	0/2259
3	H	0.21	0/1770	0.39	0/2412
4	C	0.21	0/1620	0.41	0/2217
5	D	0.21	0/1759	0.40	0/2405
6	E	0.22	0/1699	0.41	0/2304
7	F	0.21	0/1699	0.41	0/2320
All	All	0.21	0/15609	0.39	0/21243

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5284	0	5286	67	0
2	L	1633	0	1591	17	0
3	H	1720	0	1646	21	0
4	C	1579	0	1501	16	0
5	D	1712	0	1671	32	0
6	E	1661	0	1598	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	1656	0	1626	13	0
8	A	70	0	65	1	0
9	A	5	0	0	0	0
10	A	112	0	100	0	0
11	A	50	0	43	0	0
12	A	39	0	34	0	0
All	All	15521	0	15161	161	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 5.

All (161) 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:A:579:VAL:HG13	1:A:580:GLU:HG2	1.68	0.76
3:H:167:LEU:HD21	3:H:190:VAL:HG21	1.72	0.72
5:D:35:ALA:HB3	5:D:102:TYR:HB2	1.73	0.71
1:A:463:LEU:O	1:A:466:ASN:ND2	2.25	0.69
4:C:34:TRP:HB2	4:C:47:ILE:HB	1.75	0.68
5:D:53:ILE:HG22	5:D:61:ASN:HB3	1.76	0.68
1:A:450:GLN:NE2	6:E:31:ASN:OD1	2.25	0.68
1:A:119:PHE:O	1:A:146:GLN:NE2	2.27	0.66
1:A:141:ASN:HB3	1:A:144:VAL:HB	1.77	0.66
2:L:145:LYS:HB3	2:L:197:THR:HB	1.77	0.66
1:A:580:GLU:HB3	1:A:583:LYS:HD3	1.78	0.66
1:A:470:GLN:HA	1:A:493:LYS:HB2	1.77	0.65
4:C:150:LYS:HA	4:C:155:PRO:HA	1.79	0.65
6:E:121:PRO:HD3	6:E:133:VAL:HG22	1.80	0.64
6:E:187:TYR:O	6:E:193:TYR:OH	2.14	0.63
1:A:517:ASN:HA	1:A:540:ASN:HA	1.80	0.62
1:A:354:LEU:HD22	1:A:357:LEU:HD22	1.83	0.61
4:C:163:THR:HG22	5:D:178:VAL:HB	1.84	0.60
1:A:198:SER:HA	1:A:222:ARG:HB2	1.82	0.60
1:A:592:ASP:OD1	1:A:616:ASN:ND2	2.35	0.59
6:E:61:ARG:NE	6:E:82:ASP:OD2	2.34	0.58
1:A:357:LEU:HD21	1:A:360:LEU:HD13	1.86	0.58
3:H:30:THR:HG21	3:H:74:LYS:HE3	1.85	0.58
1:A:354:LEU:HB3	1:A:357:LEU:HB2	1.86	0.57
4:C:45:LEU:HD21	4:C:48:TYR:HB3	1.86	0.56
3:H:91:THR:HG23	3:H:118:THR:HA	1.87	0.56
1:A:265:ASN:O	1:A:296:TRP:NE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:206:HIS:CD2	7:F:208:PRO:HD2	2.41	0.55
1:A:336:GLN:HG2	1:A:338:ILE:H	1.72	0.55
2:L:135:LEU:HD22	3:H:189:VAL:HG11	1.89	0.55
1:A:491:ALA:HB2	2:L:94:LEU:HD21	1.89	0.54
1:A:508:LEU:HD21	1:A:511:LEU:HD13	1.88	0.54
2:L:6:GLN:N	2:L:100:GLN:OE1	2.38	0.54
2:L:164:THR:HG22	3:H:175:PRO:HD3	1.89	0.54
1:A:594:GLY:O	1:A:596:ASN:ND2	2.40	0.54
1:A:144:VAL:HG21	5:D:105:PRO:HB3	1.90	0.54
1:A:578:PRO:HB2	1:A:581:VAL:HG13	1.91	0.53
1:A:140:ASN:ND2	4:C:91:ASP:O	2.37	0.53
3:H:143:THR:HA	3:H:193:PRO:HA	1.91	0.53
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.45	0.52
1:A:437:ASP:HA	1:A:462:TYR:HB2	1.92	0.52
1:A:476:PHE:HB3	1:A:505:LEU:HD21	1.92	0.52
1:A:337:SER:O	1:A:339:SER:N	2.43	0.52
7:F:30:THR:HA	7:F:53:PRO:HB2	1.92	0.52
3:H:109:ASP:OD1	3:H:110:SER:N	2.42	0.51
7:F:12:VAL:HG11	7:F:18:VAL:HB	1.93	0.51
2:L:16:GLY:H	2:L:78:LEU:HB3	1.75	0.50
1:A:138:ILE:HD12	1:A:164:LEU:HD22	1.92	0.50
3:H:40:MET:HG2	3:H:92:ALA:HB2	1.93	0.50
6:E:90:HIS:CD2	6:E:97:THR:H	2.29	0.49
5:D:162:SER:HB2	5:D:206:ASN:HB2	1.93	0.49
4:C:119:PHE:HB3	5:D:133:LEU:HD22	1.95	0.49
1:A:189:GLU:HA	1:A:192:ASP:OD2	2.12	0.49
1:A:34:VAL:HG13	1:A:55:VAL:HB	1.94	0.49
1:A:169:GLN:HG2	1:A:170:LEU:HG	1.93	0.49
5:D:11:LEU:HD13	5:D:156:PRO:HG3	1.95	0.49
1:A:107:GLN:O	1:A:109:ASN:ND2	2.46	0.49
2:L:11:LEU:HD11	2:L:104:VAL:HG22	1.96	0.48
6:E:33:LEU:HD13	6:E:34:ALA:H	1.77	0.48
5:D:106:PHE:O	5:D:108:SER:N	2.44	0.48
7:F:33:TRP:HA	7:F:53:PRO:HD3	1.95	0.48
4:C:30:TYR:O	4:C:65:ASN:ND2	2.47	0.48
1:A:468:TYR:HB3	3:H:33:TRP:HZ2	1.78	0.48
5:D:10:GLY:HA3	5:D:211:PRO:HG3	1.96	0.47
5:D:18:LEU:HB3	5:D:86:LEU:HB3	1.95	0.47
1:A:513:LEU:HB2	1:A:537:LEU:HD23	1.96	0.47
1:A:592:ASP:HA	1:A:616:ASN:HB2	1.96	0.47
2:L:7:SER:OG	2:L:22:THR:OG1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:114:SER:HB2	2:L:137:ASN:HB3	1.96	0.47
1:A:362:MET:O	1:A:365:ASN:ND2	2.47	0.47
1:A:460:GLU:HB3	1:A:484:ARG:HB2	1.96	0.47
1:A:493:LYS:HE2	3:H:57:TYR:CD1	2.50	0.46
5:D:23:ALA:HA	5:D:81:GLN:HG2	1.97	0.46
1:A:155:SER:O	1:A:157:ASN:ND2	2.48	0.46
5:D:206:ASN:ND2	5:D:217:ASP:OD2	2.49	0.46
5:D:14:PRO:HD2	5:D:122:SER:HB3	1.97	0.46
6:E:143:ARG:CZ	6:E:164:VAL:HG11	2.46	0.45
1:A:179:SER:O	1:A:181:ASN:ND2	2.49	0.45
3:H:97:ALA:HB1	3:H:108:PHE:HB3	1.99	0.45
5:D:38:TRP:CE2	5:D:84:LEU:HB2	2.51	0.45
2:L:214:CYS:OXT	3:H:221:HIS:NE2	2.44	0.45
1:A:278:MET:HG3	8:A:806:NAG:H61	1.98	0.45
5:D:38:TRP:O	5:D:50:LEU:HB2	2.17	0.45
3:H:208:HIS:CD2	3:H:210:PRO:HD2	2.52	0.45
1:A:192:ASP:HB2	5:D:57:SER:HB3	1.98	0.45
1:A:49:LEU:HB2	1:A:74:TYR:HE1	1.82	0.45
1:A:55:VAL:HG22	1:A:79:SER:HB3	1.99	0.44
1:A:37:CYS:HB2	1:A:58:LEU:HD23	2.00	0.44
1:A:460:GLU:CB	1:A:484:ARG:HB2	2.48	0.44
2:L:148:TRP:CE2	2:L:179:LEU:HB2	2.52	0.44
3:H:199:THR:HG22	3:H:200:LYS:HG3	1.99	0.44
1:A:468:TYR:HB3	3:H:33:TRP:CZ2	2.52	0.44
4:C:135:CYS:HB3	4:C:177:SER:HB3	2.00	0.44
1:A:281:LEU:HB2	1:A:305:LEU:HD23	1.99	0.44
6:E:193:TYR:HE2	6:E:212:ARG:HB2	1.83	0.44
5:D:168:LEU:HD21	5:D:191:VAL:HG21	2.00	0.44
5:D:6:GLN:HE21	5:D:116:THR:HG22	1.83	0.44
4:C:37:GLN:OE1	5:D:41:GLN:NE2	2.51	0.44
7:F:58:ILE:HG23	7:F:70:LEU:HD12	2.00	0.44
4:C:16:GLN:HG2	4:C:17:THR:H	1.83	0.44
1:A:117:LYS:HE2	4:C:31:TYR:CD2	2.53	0.43
1:A:60:HIS:H	1:A:84:PHE:HB2	1.84	0.43
5:D:8:GLY:HA3	5:D:20:LEU:HD23	1.99	0.43
4:C:112:ALA:HB3	4:C:140:PHE:HA	1.99	0.43
1:A:194:PHE:HB3	1:A:197:SER:HB2	1.99	0.43
7:F:152:PHE:HA	7:F:153:PRO:HA	1.74	0.43
1:A:590:ILE:HG23	1:A:614:SER:HB2	2.01	0.43
3:H:13:LYS:HD2	3:H:121:SER:HA	1.99	0.43
5:D:27:ASP:OD1	5:D:28:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:126:GLY:HA2	3:H:127:PRO:HD3	1.84	0.43
4:C:109:GLN:HG2	4:C:110:PRO:HD2	2.00	0.43
4:C:119:PHE:HA	4:C:120:PRO:HD3	1.87	0.43
3:H:98:ARG:NH2	3:H:109:ASP:OD2	2.48	0.43
5:D:16:GLN:HG2	5:D:17:THR:H	1.84	0.43
6:E:15:VAL:HB	6:E:108:ARG:HD3	2.00	0.43
7:F:201:THR:HA	7:F:216:ARG:HA	2.00	0.42
1:A:483:GLN:HA	1:A:508:LEU:HA	2.00	0.42
1:A:514:SER:O	1:A:516:ASN:ND2	2.53	0.42
5:D:195:SER:HA	5:D:198:LEU:HG	2.01	0.42
1:A:351:PHE:HB3	1:A:378:LEU:HD21	2.01	0.42
4:C:125:GLU:HG2	4:C:130:LYS:O	2.19	0.42
5:D:52:ILE:HG22	5:D:102:TYR:CZ	2.54	0.42
1:A:648:ASP:HA	1:A:679:THR:HG23	2.02	0.42
6:E:167:GLN:HE21	6:E:172:SER:HB3	1.85	0.42
7:F:130:LEU:HD11	7:F:147:LEU:HB2	2.02	0.42
1:A:47:ASP:OD1	1:A:47:ASP:N	2.53	0.42
2:L:36:TYR:CZ	2:L:46:LEU:HD13	2.55	0.42
5:D:49:TRP:HZ2	5:D:52:ILE:HG23	1.84	0.42
5:D:6:GLN:NE2	5:D:116:THR:HG22	2.34	0.42
7:F:131:ALA:HA	7:F:132:PRO:HD3	1.94	0.42
7:F:129:PRO:HD3	7:F:215:LYS:HE2	2.01	0.42
7:F:48:ILE:HG23	7:F:64:PHE:HD2	1.85	0.42
1:A:654:ILE:HG12	1:A:658:VAL:HG23	2.03	0.41
1:A:449:GLY:HA2	1:A:475:SER:O	2.20	0.41
5:D:155:PHE:HA	5:D:156:PRO:HA	1.83	0.41
1:A:482:LEU:HD21	1:A:485:LEU:HD13	2.01	0.41
2:L:198:HIS:CD2	2:L:199:GLN:H	2.38	0.41
3:H:60:TYR:HE2	3:H:70:ILE:HG13	1.85	0.41
2:L:120:PRO:HD3	2:L:132:VAL:HG22	2.02	0.41
5:D:133:LEU:HD11	5:D:150:LEU:HB2	2.02	0.41
1:A:49:LEU:HB2	1:A:74:TYR:CE1	2.56	0.41
6:E:14:SER:HB3	6:E:108:ARG:HG2	2.02	0.41
4:C:160:VAL:HG22	4:C:179:LEU:HD13	2.03	0.41
7:F:12:VAL:HG21	7:F:86:LEU:HD13	2.01	0.41
1:A:73:ARG:HD3	1:A:74:TYR:CZ	2.55	0.41
5:D:148:GLY:HA3	5:D:190:VAL:HG12	2.02	0.41
1:A:686:PHE:HA	1:A:687:PRO:HD3	1.92	0.41
3:H:168:THR:OG1	3:H:169:SER:N	2.54	0.41
5:D:49:TRP:CZ2	5:D:52:ILE:HG23	2.56	0.41
1:A:569:LEU:HB3	1:A:574:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HA	1:A:224:PHE:HB2	2.03	0.41
2:L:93:THR:HG22	2:L:95:SER:H	1.86	0.41
2:L:49:TYR:HB2	3:H:107:THR:HG21	2.03	0.41
7:F:51:ILE:HD12	7:F:70:LEU:HB3	2.02	0.40
5:D:153:ASP:HB3	5:D:184:LEU:HD13	2.03	0.40
1:A:569:LEU:HB2	1:A:593:LEU:HD23	2.03	0.40
1:A:510:ILE:HG13	1:A:534:ILE:HB	2.03	0.40
1:A:603:ALA:HA	1:A:629:VAL:HG22	2.02	0.40
1:A:32:HIS:C	1:A:34:VAL:H	2.24	0.40
5:D:138:ARG:HD2	5:D:140:THR:HG22	2.04	0.40
1:A:138:ILE:HD13	1:A:143:PHE:CE2	2.56	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	657/694 (95%)	603 (92%)	50 (8%)	4 (1%)	30	74
2	L	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	34	77
3	H	223/225 (99%)	209 (94%)	12 (5%)	2 (1%)	21	67
4	C	208/213 (98%)	192 (92%)	12 (6%)	4 (2%)	10	51
5	D	222/226 (98%)	207 (93%)	14 (6%)	1 (0%)	34	77
6	E	213/215 (99%)	198 (93%)	10 (5%)	5 (2%)	8	47
7	F	213/223 (96%)	197 (92%)	15 (7%)	1 (0%)	34	77
All	All	1948/2010 (97%)	1811 (93%)	119 (6%)	18 (1%)	21	67

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
3	H	193	PRO
4	C	50	ASP
6	E	108	ARG
6	E	111	VAL
5	D	107	TYR
1	A	643	ARG
3	H	197	LEU
6	E	110	THR
7	F	121	SER
1	A	467	LYS
1	A	491	ALA
6	E	205	PRO
2	L	138	ASN
4	C	93	PRO
4	C	108	GLY
4	C	152	ASP
6	E	139	ASN

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	613/644 (95%)	609 (99%)	4 (1%)	88	96
2	L	186/186 (100%)	182 (98%)	4 (2%)	60	86
3	H	194/194 (100%)	189 (97%)	5 (3%)	54	83
4	C	178/181 (98%)	175 (98%)	3 (2%)	68	89
5	D	197/199 (99%)	192 (98%)	5 (2%)	55	84
6	E	188/188 (100%)	184 (98%)	4 (2%)	61	86
7	F	189/195 (97%)	183 (97%)	6 (3%)	46	80
All	All	1745/1787 (98%)	1714 (98%)	31 (2%)	66	88

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	303	PHE
1	A	498	SER
1	A	607	ASN
2	L	11	LEU
2	L	33	LEU
2	L	55	GLN
2	L	100	GLN
3	H	76	ILE
3	H	118	THR
3	H	158	VAL
3	H	178	LEU
3	H	222	HIS
4	C	95	PHE
4	C	164	THR
4	C	210	THR
5	D	17	THR
5	D	32	ASN
5	D	47	LEU
5	D	67	VAL
5	D	217	ASP
6	E	33	LEU
6	E	81	GLU
6	E	90	HIS
6	E	108	ARG
7	F	57	ARG
7	F	72	VAL
7	F	104	THR
7	F	165	LEU
7	F	217	VAL
7	F	219	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	65	ASN
6	E	167	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 ⓘ

15 carbohydrates 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	$\# Z > 2$
10	NAG	A	803	1,10	14,14,15	0.58	0	15,19,21	0.77	0
10	NAG	A	804	10	14,14,15	0.46	0	15,19,21	0.83	1 (6%)
10	NAG	A	807	1,10	14,14,15	0.55	0	15,19,21	0.89	1 (6%)
10	NAG	A	808	10	14,14,15	0.47	0	15,19,21	0.65	0
10	NAG	A	810	1,10	14,14,15	0.55	0	15,19,21	0.72	0
10	NAG	A	811	10	14,14,15	0.52	0	15,19,21	0.62	0
10	NAG	A	812	1,10	14,14,15	0.51	0	15,19,21	0.72	0
10	NAG	A	813	10	14,14,15	0.51	0	15,19,21	0.58	0
11	NAG	A	814	1,11	14,14,15	0.49	0	15,19,21	0.74	0
11	NAG	A	815	11	14,14,15	0.53	0	15,19,21	0.82	0
11	BMA	A	816	11	11,11,12	0.62	0	14,15,17	0.75	0
11	MAN	A	817	11	11,11,12	0.60	0	14,15,17	0.92	0
12	NAG	A	818	1,12	14,14,15	0.51	0	15,19,21	0.69	0
12	NAG	A	819	12	14,14,15	0.47	0	15,19,21	0.76	0
12	BMA	A	820	12	11,11,12	0.62	0	14,15,17	0.66	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
10	NAG	A	803	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	804	10	-	0/6/23/26	0/1/1/1
10	NAG	A	807	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	808	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	810	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	811	10	-	0/6/23/26	0/1/1/1
10	NAG	A	812	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	813	10	-	0/6/23/26	0/1/1/1
11	NAG	A	814	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	815	11	-	0/6/23/26	0/1/1/1
11	BMA	A	816	11	-	0/2/19/22	0/1/1/1
11	MAN	A	817	11	-	0/2/19/22	0/1/1/1
12	NAG	A	818	1,12	-	0/6/23/26	0/1/1/1
12	NAG	A	819	12	-	0/6/23/26	0/1/1/1
12	BMA	A	820	12	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	804	NAG	C1-O5-C5	2.05	114.85	112.25
10	A	807	NAG	C4-C3-C2	2.08	114.46	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
8	NAG	A	801	1	14,14,15	0.56	0	15,19,21	0.83	1 (6%)
8	NAG	A	802	1	14,14,15	0.52	0	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	805	1	14,14,15	0.47	0	15,19,21	0.81	0
8	NAG	A	806	1	14,14,15	0.50	0	15,19,21	0.60	0
8	NAG	A	809	1	14,14,15	0.45	0	15,19,21	0.86	0
9	SO4	A	821	-	4,4,4	0.22	0	6,6,6	0.16	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
8	NAG	A	801	1	-	0/6/23/26	0/1/1/1
8	NAG	A	802	1	-	0/6/23/26	0/1/1/1
8	NAG	A	805	1	-	0/6/23/26	0/1/1/1
8	NAG	A	806	1	-	0/6/23/26	0/1/1/1
8	NAG	A	809	1	-	0/6/23/26	0/1/1/1
9	SO4	A	821	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801	NAG	C1-O5-C5	2.33	115.21	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	806	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	659/694 (94%)	-0.07	8 (1%) 81 73	51, 94, 175, 221	0
2	L	214/214 (100%)	0.23	14 (6%) 22 17	62, 117, 183, 210	0
3	H	225/225 (100%)	0.70	26 (11%) 6 6	69, 122, 222, 272	0
4	C	210/213 (98%)	0.13	5 (2%) 62 52	80, 124, 172, 212	0
5	D	224/226 (99%)	0.30	11 (4%) 33 25	68, 117, 214, 242	0
6	E	215/215 (100%)	0.28	16 (7%) 17 14	59, 112, 185, 208	0
7	F	217/223 (97%)	0.26	11 (5%) 32 24	66, 121, 198, 223	0
All	All	1964/2010 (97%)	0.19	91 (4%) 36 28	51, 111, 191, 272	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	146	LEU	10.6
3	H	147	GLY	7.8
3	H	145	ALA	5.8
2	L	132	VAL	5.2
7	F	131	ALA	4.9
7	F	144	LEU	4.7
3	H	132	LEU	4.6
3	H	138	SER	4.6
3	H	139	THR	4.5
3	H	129	VAL	4.5
2	L	131	SER	4.4
2	L	193	ALA	4.4
3	H	190	VAL	4.3
5	D	139	SER	4.1
5	D	138	ARG	4.1
3	H	137	ARG	4.1
2	L	133	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
6	E	132	SER	3.7
3	H	224	HIS	3.7
3	H	128	SER	3.5
3	H	223	HIS	3.5
6	E	121	PRO	3.4
3	H	133	ALA	3.3
7	F	143	ALA	3.3
3	H	219	VAL	3.3
7	F	128	PHE	3.2
6	E	147	VAL	3.1
3	H	131	PRO	3.1
6	E	118	ILE	3.1
7	F	145	GLY	3.1
3	H	149	LEU	3.0
3	H	97	ALA	3.0
2	L	147	GLN	2.9
2	L	116	PHE	2.9
5	D	145	ALA	2.9
3	H	130	PHE	2.9
3	H	191	THR	2.9
5	D	221	HIS	2.8
3	H	134	PRO	2.8
4	C	119	PHE	2.8
7	F	132	PRO	2.8
4	C	210	THR	2.8
7	F	129	PRO	2.8
2	L	114	SER	2.7
5	D	197	SER	2.7
1	A	647	PHE	2.7
1	A	648	ASP	2.6
1	A	683	TYR	2.6
6	E	145	ALA	2.6
3	H	203	THR	2.6
4	C	208	ALA	2.6
3	H	150	VAL	2.6
2	L	135	LEU	2.6
5	D	203	TYR	2.6
6	E	108	ARG	2.5
2	L	134	CYS	2.5
7	F	208	PRO	2.5
6	E	122	SER	2.5
5	D	222	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
6	E	179	THR	2.4
5	D	224	HIS	2.4
6	E	181	THR	2.4
7	F	197	THR	2.4
2	L	118	PHE	2.4
1	A	657	PHE	2.4
6	E	150	LYS	2.3
7	F	157	THR	2.3
6	E	136	LEU	2.2
6	E	178	SER	2.2
3	H	215	VAL	2.2
2	L	178	THR	2.2
6	E	193	TYR	2.2
4	C	207	VAL	2.2
1	A	659	ASN	2.2
5	D	146	ALA	2.2
6	E	149	TRP	2.2
2	L	177	SER	2.2
1	A	651	CYS	2.2
2	L	117	ILE	2.1
1	A	35	ALA	2.1
3	H	201	THR	2.1
7	F	130	LEU	2.1
6	E	131	ALA	2.1
5	D	196	SER	2.1
5	D	198	LEU	2.0
1	A	630	PHE	2.0
6	E	133	VAL	2.0
4	C	2	SER	2.0
2	L	115	VAL	2.0
3	H	127	PRO	2.0
3	H	189	VAL	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](#)

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
11	NAG	A	814	14/15	0.92	0.27	0.81	74,100,115,130	0
12	NAG	A	819	14/15	0.81	0.23	-	130,166,194,196	0
12	NAG	A	818	14/15	0.91	0.18	-	90,126,147,159	0
10	NAG	A	804	14/15	0.80	0.30	-	178,197,217,223	0
12	BMA	A	820	11/12	0.69	0.20	-	186,201,220,226	0
10	NAG	A	812	14/15	0.94	0.15	-	104,123,140,140	0
10	NAG	A	810	14/15	0.82	0.20	-	103,117,145,157	0
11	MAN	A	817	11/12	0.80	0.20	-	163,189,200,201	0
10	NAG	A	807	14/15	0.84	0.22	-	98,146,164,166	0
10	NAG	A	813	14/15	0.76	0.26	-	104,162,173,176	0
10	NAG	A	803	14/15	0.89	0.17	-	91,162,179,181	0
11	BMA	A	816	11/12	0.78	0.23	-	135,161,183,183	0
10	NAG	A	811	14/15	0.71	0.41	-	112,156,175,185	0
10	NAG	A	808	14/15	0.78	0.29	-	133,159,168,173	0
11	NAG	A	815	14/15	0.88	0.23	-	104,138,153,163	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	SO4	A	821	5/5	0.88	0.32	2.21	111,114,140,154	0
8	NAG	A	802	14/15	0.73	0.25	-0.33	132,155,165,171	0
8	NAG	A	805	14/15	0.89	0.19	-0.69	81,103,127,135	0
8	NAG	A	809	14/15	0.79	0.22	-	94,141,163,173	0
8	NAG	A	801	14/15	0.72	0.20	-	159,187,198,200	0
8	NAG	A	806	14/15	0.83	0.22	-	110,138,153,155	0

6.5 Other polymers ⓘ

There are no such residues in this entry.