Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 10:25 PM JST

PDB ID	:	6JXK
Title	:	Rb+-bound E2-MgF state of the gastric proton pump (Wild-type)
Authors	:	Abe, K.; Irie, K.; Yamamoto, K.
Deposited on	:	2019-04-23
Resolution	:	4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

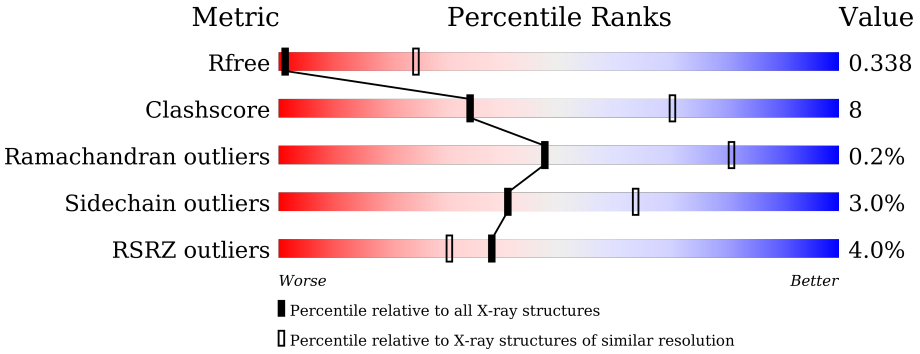
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	987	3% 75% 24% •
1	E	987	4% 80% 20% •
2	B	289	10% 67% 25% • 6%
2	F	289	78% 14% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MF4	A	1101	-	-	X	-
3	MF4	E	1101	-	-	X	-
5	CLR	A	1103	-	-	-	X
5	CLR	F	307	-	-	-	X
6	K	A	1104	-	-	-	X
6	K	E	1103	-	-	-	X
7	NAG	B	301	-	-	-	X
7	NAG	B	302	-	-	-	X
7	NAG	F	306	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19807 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 Potassium-transporting ATPase alpha chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	987	7659	4890	1292	1423	54	0	0	0
1	E	987	7659	4890	1292	1423	54	0	0	0

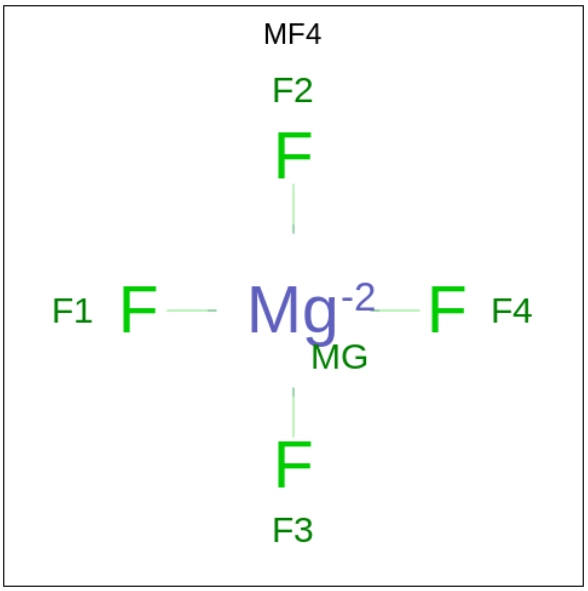
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP P19156
A	220	CYS	ARG	engineered mutation	UNP P19156
A	593	CYS	SER	engineered mutation	UNP P19156
A	1005	SER	GLY	engineered mutation	UNP P19156
E	47	GLY	-	expression tag	UNP P19156
E	220	CYS	ARG	engineered mutation	UNP P19156
E	593	CYS	SER	engineered mutation	UNP P19156
E	1005	SER	GLY	engineered mutation	UNP P19156

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	271	2175	1411	360	391	13	0	0	0
2	F	266	2128	1379	353	384	12	0	0	0

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).

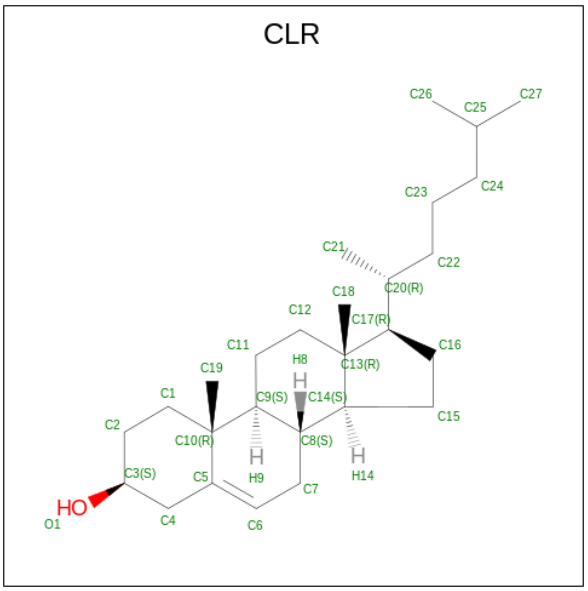


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total F Mg 5 4 1	0	0
3	E	1	Total F Mg 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).

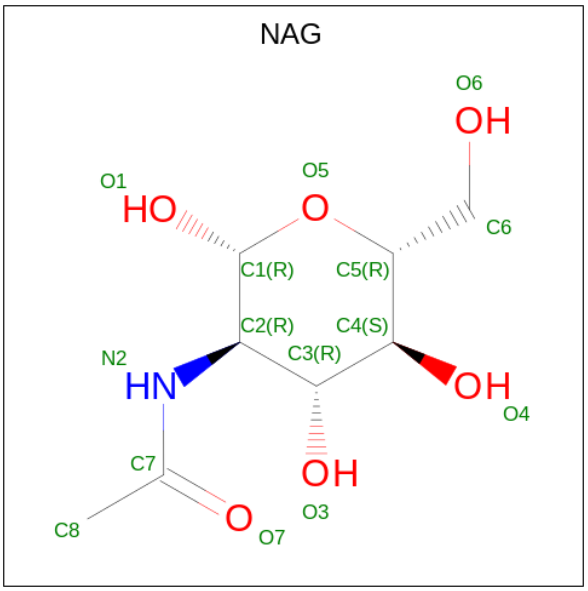


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 28 27 1	0	0
5	F	1	Total C O 28 27 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total K 3 3	0	0
6	E	3	Total K 3 3	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



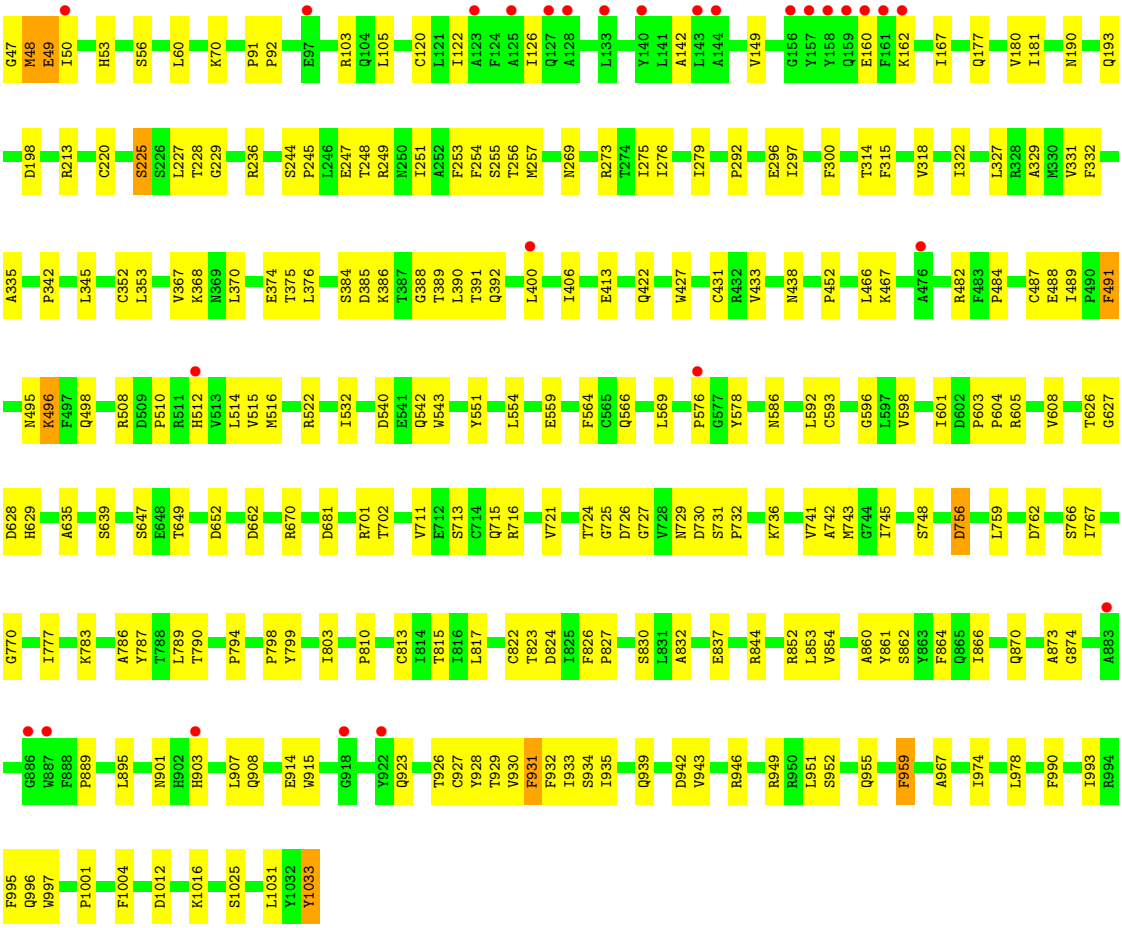
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	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.

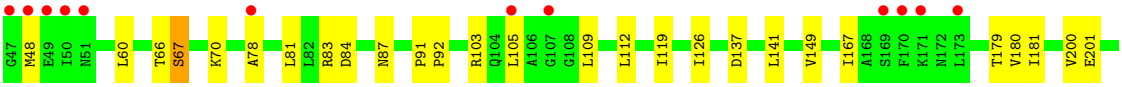
• Molecule 1: Potassium-transporting ATPase alpha chain 1

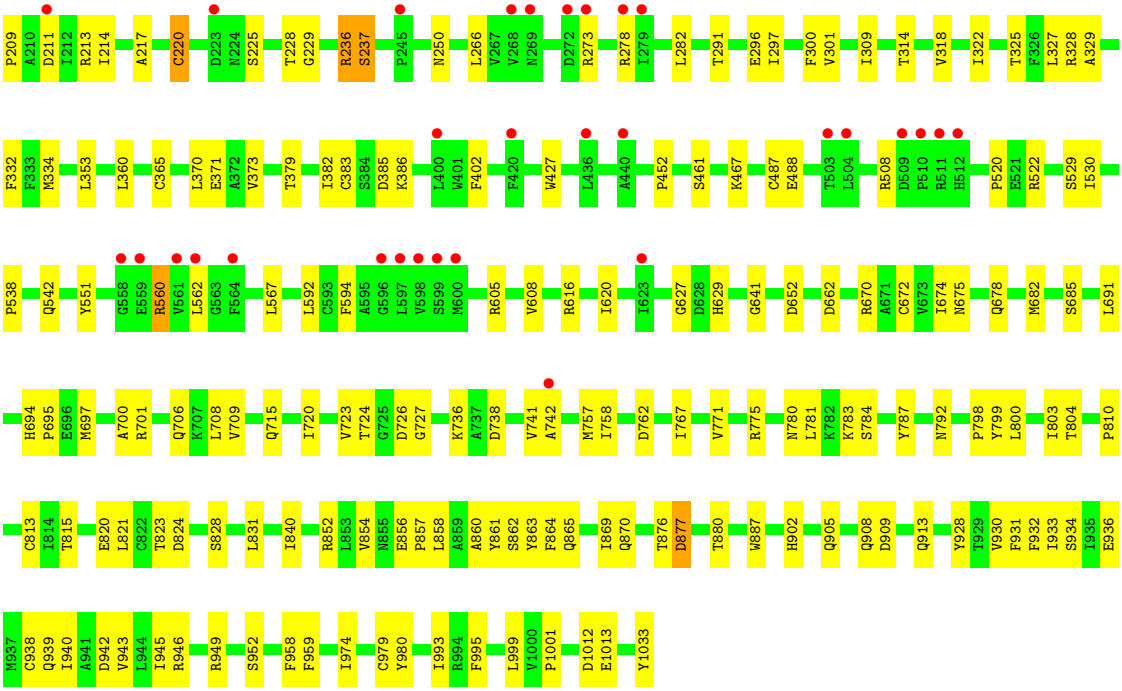
Chain A: 3% 75% 24%



• Molecule 1: Potassium-transporting ATPase alpha chain 1

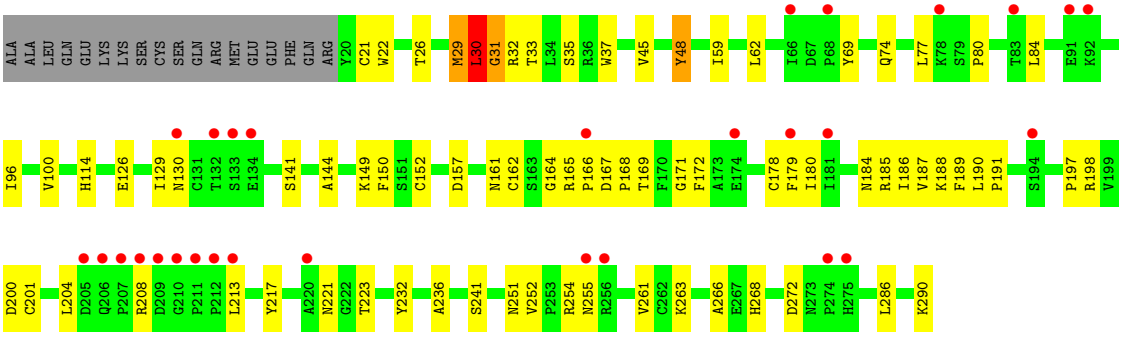
Chain E: 4% 80% 20%





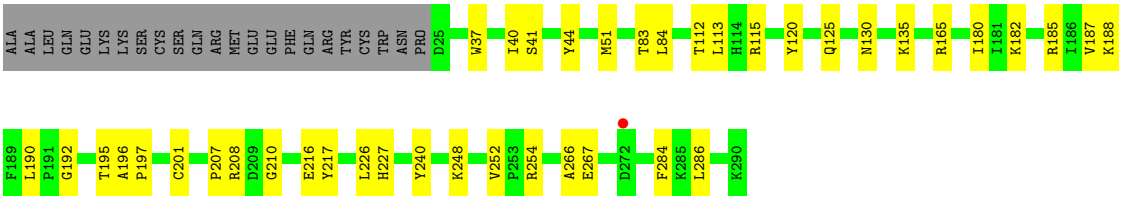
- Molecule 2: Potassium-transporting ATPase subunit beta

Chain B:



- Molecule 2: Potassium-transporting ATPase subunit beta

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	191.51Å 106.43Å 250.96Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	47.79 – 4.30 47.79 – 4.05	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.79-4.30) 82.1 (47.79-4.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.263 , 0.338 0.263 , 0.338	Depositor DCC
R_{free} test set	1546 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	160.3	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 154.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	19807	wwPDB-VP
Average B, all atoms (Å^2)	244.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MF4, NAG, CLR, MG, K

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	0.28	0/7817	0.51	0/10618
1	E	0.27	0/7817	0.50	0/10618
2	B	0.34	0/2246	0.57	0/3057
2	F	0.28	0/2195	0.52	0/2985
All	All	0.28	0/20075	0.51	0/27278

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	7659	0	7686	147	0
1	E	7659	0	7685	111	0
2	B	2175	0	2105	56	0
2	F	2128	0	2065	23	0
3	A	5	0	0	4	0
3	E	5	0	0	4	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
5	A	28	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	28	0	46	3	0
6	A	3	0	0	0	0
6	E	3	0	0	0	0
7	B	28	0	26	0	0
7	F	84	0	78	0	0
All	All	19807	0	19737	333	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 8.

All (333) 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)
2:B:30:LEU:O	2:B:32:ARG:N	1.90	1.04
2:B:29:MET:O	2:B:31:GLY:N	2.03	0.91
1:E:370:LEU:O	1:E:373:VAL:HG12	1.73	0.89
1:E:297:ILE:O	1:E:301:VAL:HG23	1.76	0.86
2:B:30:LEU:O	2:B:32:ARG:O	1.94	0.86
2:B:26:THR:OG1	2:B:29:MET:SD	2.38	0.81
2:B:187:VAL:HG12	2:B:188:LYS:HG2	1.64	0.78
1:A:48:MET:HA	1:A:48:MET:CE	2.13	0.77
2:B:21:CYS:SG	2:B:22:TRP:N	2.57	0.77
1:A:487:CYS:SG	1:A:488:GLU:N	2.58	0.76
1:A:126:ILE:HG21	1:A:327:LEU:HD11	1.68	0.75
1:E:567:LEU:HB2	1:E:592:LEU:HD23	1.69	0.73
2:B:252:VAL:O	2:B:254:ARG:NH1	2.22	0.72
2:B:191:PRO:HA	2:B:268:HIS:HB2	1.72	0.71
2:B:198:ARG:HG2	2:B:223:THR:HG22	1.72	0.71
2:B:26:THR:OG1	2:B:29:MET:HB2	1.91	0.70
1:E:383:CYS:HB2	1:E:723:VAL:HG22	1.72	0.70
2:B:29:MET:C	2:B:31:GLY:H	1.93	0.70
1:A:438:ASN:HD21	1:A:466:LEU:HB2	1.57	0.69
2:F:120:TYR:HA	2:F:125:GLN:HE21	1.57	0.69
1:A:91:PRO:HA	1:A:167:ILE:HD13	1.74	0.69
1:A:228:THR:O	3:A:1101:MF4:F1	2.00	0.69
2:F:252:VAL:O	2:F:254:ARG:NH1	2.26	0.69
1:A:628:ASP:OD1	1:A:629:HIS:N	2.25	0.69
1:A:47:GLY:O	1:A:48:MET:HB2	1.92	0.69
2:F:192:GLY:HA3	2:F:267:GLU:HB3	1.75	0.68
1:E:84:ASP:HB3	1:E:273:ARG:HH12	1.57	0.68
1:A:385:ASP:OD1	1:A:386:LYS:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HG	1:A:598:VAL:HG13	1.76	0.68
1:A:783:LYS:HE2	1:A:949:ARG:HG3	1.77	0.67
1:E:856:GLU:HB2	1:E:857:PRO:HD3	1.77	0.67
1:A:578:TYR:OH	1:A:586:ASN:ND2	2.28	0.67
1:E:60:LEU:HD21	1:E:213:ARG:HG2	1.77	0.66
2:B:26:THR:O	2:B:29:MET:HB2	1.95	0.66
1:A:374:GLU:HG2	1:A:374:GLU:O	1.96	0.66
1:A:391:THR:HA	1:A:604:PRO:HA	1.78	0.66
1:E:854:VAL:HG13	1:E:858:LEU:HD22	1.77	0.65
1:E:228:THR:O	3:E:1101:MF4:F1	2.05	0.64
2:F:197:PRO:HB3	2:F:266:ALA:HB2	1.77	0.64
1:E:126:ILE:HG21	1:E:327:LEU:HD11	1.80	0.64
2:B:190:LEU:O	2:B:268:HIS:ND1	2.32	0.64
1:E:724:THR:HG22	1:E:741:VAL:HB	1.79	0.64
1:A:385:ASP:OD1	3:A:1101:MF4:F3	2.06	0.63
1:A:452:PRO:O	1:A:467:LYS:NZ	2.31	0.63
1:E:329:ALA:HA	1:E:332:PHE:HD2	1.63	0.63
2:F:37:TRP:HZ3	5:F:307:CLR:H193	1.63	0.63
1:A:860:ALA:HB1	5:A:1103:CLR:H6	1.81	0.63
1:E:385:ASP:OD1	1:E:386:LYS:N	2.31	0.63
2:F:187:VAL:HG12	2:F:188:LYS:HG2	1.80	0.63
1:A:952:SER:HB3	1:A:955:GLN:HG3	1.82	0.62
1:E:385:ASP:OD1	3:E:1101:MF4:F3	2.07	0.62
1:A:711:VAL:HG13	1:A:721:VAL:HG11	1.82	0.62
1:E:799:TYR:O	1:E:803:ILE:HG13	2.00	0.62
1:A:949:ARG:NH1	1:A:1033:TYR:OXT	2.32	0.61
1:A:225:SER:O	1:A:229:GLY:N	2.29	0.61
1:A:120:CYS:HB3	1:A:142:ALA:HB2	1.83	0.61
1:E:627:GLY:N	3:E:1101:MF4:F4	2.21	0.60
5:A:1103:CLR:H193	2:B:37:TRP:CZ3	2.37	0.60
1:A:276:ILE:HA	1:A:279:ILE:HD12	1.84	0.60
1:E:332:PHE:CD1	1:E:803:ILE:HG12	2.36	0.60
2:F:112:THR:HG22	2:F:115:ARG:NH1	2.17	0.59
1:A:406:ILE:HG21	1:A:554:LEU:HD21	1.83	0.59
2:B:29:MET:C	2:B:31:GLY:N	2.52	0.59
2:B:221:ASN:HB3	2:B:223:THR:HG23	1.85	0.59
1:E:949:ARG:NH1	1:E:1033:TYR:OXT	2.36	0.58
1:E:529:SER:HA	1:E:538:PRO:HA	1.86	0.58
1:A:914:GLU:OE1	2:B:184:ASN:HA	2.02	0.58
2:F:201:CYS:N	2:F:217:TYR:OH	2.36	0.58
1:A:512:HIS:O	1:A:569:LEU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ALA:HA	1:A:332:PHE:CD2	2.38	0.58
1:E:674:ILE:HG23	1:E:678:GLN:HB3	1.86	0.57
1:E:815:THR:HG21	1:E:928:TYR:HB3	1.87	0.57
1:A:837:GLU:HB3	1:A:951:LEU:HG	1.87	0.57
1:E:952:SER:OG	1:E:1013:GLU:OE1	2.21	0.57
2:B:198:ARG:HA	2:B:223:THR:HA	1.85	0.56
1:A:559:GLU:HG2	1:A:601:ILE:HD12	1.85	0.56
1:A:942:ASP:O	1:A:946:ARG:HG2	2.05	0.56
2:B:188:LYS:HE2	2:B:232:TYR:HD1	1.70	0.56
1:A:332:PHE:CD1	1:A:803:ILE:HG12	2.40	0.55
1:A:296:GLU:OE1	1:A:852:ARG:NE	2.32	0.55
2:F:207:PRO:HG2	2:F:210:GLY:HA3	1.89	0.55
1:A:759:LEU:HD13	1:A:766:SER:HB2	1.88	0.55
1:A:815:THR:HG21	1:A:928:TYR:HB3	1.88	0.55
1:A:227:LEU:HD21	1:A:275:ILE:HG21	1.89	0.54
1:A:49:GLU:OE2	1:A:49:GLU:HA	2.07	0.54
1:A:908:GLN:HG2	1:A:914:GLU:HG2	1.90	0.54
1:E:932:PHE:O	1:E:936:GLU:HG2	2.07	0.54
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.90	0.54
2:F:83:THR:OG1	2:F:182:LYS:HE3	2.09	0.53
1:E:112:LEU:HD21	1:E:309:ILE:HD11	1.91	0.53
2:F:195:THR:OG1	2:F:196:ALA:N	2.40	0.53
2:F:112:THR:HG22	2:F:115:ARG:HH11	1.73	0.53
1:E:214:ILE:HG21	1:E:217:ALA:HB2	1.91	0.53
1:A:927:CYS:HA	1:A:930:VAL:HG12	1.91	0.53
1:A:959:PHE:HZ	1:E:999:LEU:HD12	1.73	0.53
1:E:783:LYS:HE2	1:E:949:ARG:HG3	1.89	0.53
1:A:177:GLN:NE2	1:A:190:ASN:OD1	2.42	0.53
2:B:59:ILE:HA	2:B:62:LEU:HB3	1.91	0.53
1:A:48:MET:HA	1:A:48:MET:HE2	1.88	0.52
1:E:672:CYS:HB2	1:E:694:HIS:CG	2.44	0.52
1:A:92:PRO:HD2	1:A:167:ILE:HG21	1.92	0.52
1:E:876:THR:O	1:E:880:THR:OG1	2.25	0.52
2:B:144:ALA:HA	2:B:150:PHE:CE1	2.45	0.52
1:A:715:GLN:OE1	1:A:736:LYS:NZ	2.43	0.51
2:B:45:VAL:HA	2:B:48:TYR:HB2	1.91	0.51
1:A:253:PHE:O	1:A:256:THR:OG1	2.19	0.51
1:A:532:ILE:HG12	1:A:543:TRP:CH2	2.46	0.51
1:A:566:GLN:O	1:A:593:CYS:N	2.42	0.51
1:E:66:THR:OG1	1:E:67:SER:N	2.41	0.51
1:E:715:GLN:OE1	1:E:736:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:OE1	1:A:413:GLU:HB3	2.10	0.51
1:E:862:SER:OG	1:E:946:ARG:NH2	2.43	0.51
1:E:325:THR:HG23	1:E:328:ARG:H	1.75	0.51
1:A:48:MET:CE	1:A:48:MET:CA	2.87	0.50
1:A:932:PHE:CD2	1:A:933:ILE:HG13	2.46	0.50
1:E:60:LEU:HD23	1:E:266:LEU:HD12	1.92	0.50
1:E:402:PHE:CZ	1:E:427:TRP:HB2	2.46	0.50
1:E:522:ARG:NH1	1:E:522:ARG:HB3	2.25	0.50
1:A:247:GLU:OE2	1:A:701:ARG:NE	2.42	0.50
1:A:390:LEU:HB3	1:A:608:VAL:HG11	1.93	0.50
1:E:452:PRO:O	1:E:467:LYS:NZ	2.45	0.50
1:A:53:HIS:HB3	1:A:251:ILE:HD11	1.92	0.50
1:A:874:GLY:HA3	1:A:931:PHE:CE1	2.47	0.50
1:E:824:ASP:OD2	1:E:939:GLN:NE2	2.42	0.50
1:A:292:PRO:HG2	1:A:375:THR:HG23	1.93	0.50
1:E:87:ASN:ND2	1:E:209:PRO:O	2.42	0.50
1:A:993:ILE:HB	1:A:997:TRP:HE3	1.77	0.50
1:E:798:PRO:HB3	1:E:810:PRO:HB2	1.94	0.50
1:A:318:VAL:O	1:A:322:ILE:HG13	2.12	0.50
1:E:706:GLN:HA	1:E:709:VAL:HB	1.93	0.50
1:A:300:PHE:HB3	1:A:854:VAL:HB	1.94	0.49
1:A:510:PRO:HB2	1:A:576:PRO:HG3	1.92	0.49
1:A:635:ALA:O	1:A:639:SER:OG	2.29	0.49
1:E:522:ARG:HB3	1:E:522:ARG:HH11	1.77	0.49
1:E:91:PRO:HA	1:E:167:ILE:HD13	1.95	0.49
1:A:787:TYR:CE1	1:A:943:VAL:HB	2.47	0.49
1:A:726:ASP:O	1:A:748:SER:N	2.35	0.49
1:A:427:TRP:CH2	1:A:431:CYS:HB2	2.47	0.49
1:A:491:PHE:HB2	1:A:498:GLN:HE21	1.77	0.49
1:A:933:ILE:HD12	1:A:993:ILE:HD11	1.94	0.49
2:B:26:THR:O	2:B:29:MET:CB	2.60	0.49
2:B:69:TYR:CD1	2:B:236:ALA:HB2	2.48	0.49
2:F:40:ILE:HD12	2:F:41:SER:N	2.28	0.49
2:B:188:LYS:HE2	2:B:232:TYR:CD1	2.48	0.49
1:E:863:TYR:HB3	1:E:864:PHE:CD1	2.48	0.49
1:E:870:GLN:HG2	1:E:938:CYS:HB3	1.94	0.49
1:E:670:ARG:HG2	1:E:695:PRO:HG2	1.94	0.49
1:E:940:ILE:O	1:E:943:VAL:HG12	2.13	0.49
1:A:56:SER:O	1:A:60:LEU:HD13	2.13	0.48
1:A:162:LYS:HB2	1:A:368:LYS:HE3	1.95	0.48
1:E:520:PRO:HG2	1:E:551:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:678:GLN:O	1:E:682:MET:HG3	2.13	0.48
1:E:979:CYS:HB2	1:E:980:TYR:CD1	2.49	0.48
1:E:229:GLY:HA3	3:E:1101:MF4:F2	2.02	0.48
1:E:297:ILE:O	1:E:301:VAL:CG2	2.56	0.48
1:A:269:ASN:ND2	1:A:273:ARG:O	2.46	0.48
1:E:530:ILE:HB	1:E:594:PHE:HB3	1.94	0.48
1:E:282:LEU:HD22	1:E:708:LEU:HD13	1.96	0.48
1:E:78:ALA:HA	1:E:81:LEU:HB3	1.96	0.48
1:E:823:THR:HG22	1:E:974:ILE:HG23	1.95	0.48
1:A:489:ILE:HG21	1:A:495:ASN:ND2	2.29	0.48
1:A:741:VAL:HG11	1:A:767:ILE:HD11	1.95	0.48
2:B:149:LYS:N	2:B:236:ALA:O	2.44	0.48
1:A:1012:ASP:O	1:A:1016:LYS:HG3	2.14	0.47
1:E:109:LEU:HD13	1:E:301:VAL:HG13	1.95	0.47
2:B:179:PHE:HZ	2:B:286:LEU:HD13	1.79	0.47
2:B:254:ARG:O	2:B:255:ASN:HB2	2.13	0.47
1:E:616:ARG:NH1	1:E:641:GLY:O	2.47	0.47
1:E:958:PHE:HB2	1:E:959:PHE:CD1	2.49	0.47
2:B:96:ILE:O	2:B:286:LEU:HD12	2.14	0.47
1:A:564:PHE:HB2	1:A:596:GLY:O	2.15	0.47
1:A:662:ASP:OD1	1:A:662:ASP:N	2.48	0.47
2:F:185:ARG:HD2	2:F:240:TYR:CE1	2.49	0.47
5:F:307:CLR:H6	1:E:860:ALA:HB1	1.97	0.47
1:A:853:LEU:HA	1:A:853:LEU:HD23	1.74	0.47
2:B:261:VAL:HG12	2:B:263:LYS:HG3	1.96	0.47
1:E:382:ILE:HG13	1:E:620:ILE:HG21	1.97	0.47
1:A:315:PHE:HA	1:A:318:VAL:HB	1.97	0.47
1:E:820:GLU:O	1:E:821:LEU:HD23	2.15	0.47
1:A:498:GLN:O	1:A:516:MET:HG3	2.16	0.46
1:A:756:ASP:OD1	1:A:756:ASP:N	2.47	0.46
1:A:823:THR:HG22	1:A:974:ILE:HG23	1.97	0.46
1:E:360:LEU:HD12	1:E:373:VAL:HG23	1.96	0.46
1:A:190:ASN:HB2	1:A:193:GLN:HG2	1.96	0.46
1:A:929:THR:HG23	1:A:990:PHE:HD1	1.80	0.46
1:A:236:ARG:HA	1:A:249:ARG:HB3	1.98	0.46
1:A:649:THR:OG1	1:A:652:ASP:N	2.49	0.46
1:A:122:ILE:HG22	1:A:122:ILE:O	2.16	0.46
2:B:164:GLY:HA2	2:B:168:PRO:HA	1.98	0.46
1:E:141:LEU:HD11	1:E:813:CYS:HB3	1.97	0.46
1:A:245:PRO:HA	1:A:248:THR:HG22	1.97	0.46
1:A:813:CYS:O	1:A:817:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLN:NE2	1:A:939:GLN:OE1	2.41	0.46
5:A:1103:CLR:H193	2:B:37:TRP:HZ3	1.81	0.46
2:B:167:ASP:OD2	2:B:171:GLY:N	2.49	0.46
1:A:385:ASP:HB3	1:A:389:THR:OG1	2.16	0.45
1:A:729:ASN:ND2	3:A:1101:MF4:F4	2.39	0.45
2:B:186:ILE:HB	2:B:189:PHE:HB2	1.97	0.45
1:E:605:ARG:HB2	1:E:608:VAL:HG23	1.99	0.45
1:A:384:SER:HG	1:A:724:THR:HG1	1.58	0.45
1:A:934:SER:HA	1:A:1001:PRO:HG3	1.98	0.45
2:B:30:LEU:HD13	2:B:30:LEU:HA	1.75	0.45
1:A:727:GLY:N	1:A:730:ASP:OD2	2.37	0.45
1:A:895:LEU:HD11	1:A:907:LEU:HD21	1.97	0.45
1:A:908:GLN:OE1	2:B:185:ARG:NH1	2.50	0.45
2:B:169:THR:O	2:B:172:PHE:HB2	2.17	0.45
1:A:297:ILE:HA	1:A:300:PHE:CE2	2.52	0.45
1:E:179:THR:OG1	1:E:201:GLU:O	2.35	0.45
1:E:220:CYS:HB3	1:E:236:ARG:HB2	1.98	0.45
1:A:743:MET:HE3	1:A:762:ASP:HB3	1.98	0.44
2:B:201:CYS:HA	2:B:261:VAL:O	2.17	0.44
1:A:331:VAL:HG12	1:A:331:VAL:O	2.17	0.44
1:E:105:LEU:HD22	1:E:149:VAL:HG12	1.98	0.44
1:E:675:ASN:HB2	1:E:701:ARG:HB3	1.99	0.44
1:E:908:GLN:HA	1:E:913:GLN:O	2.17	0.44
1:A:790:THR:HB	1:A:862:SER:HB3	1.99	0.44
1:E:314:THR:O	1:E:318:VAL:HG23	2.17	0.44
1:E:995:PHE:O	1:E:999:LEU:HG	2.17	0.44
1:A:601:ILE:O	1:A:603:PRO:HD3	2.18	0.44
1:A:314:THR:O	1:A:318:VAL:HG23	2.17	0.44
1:A:388:GLY:N	1:A:391:THR:OG1	2.51	0.44
1:A:794:PRO:HB2	1:A:935:ILE:HD11	2.00	0.44
2:B:204:LEU:HD13	2:B:261:VAL:HG21	1.99	0.44
1:E:379:THR:HA	1:E:720:ILE:HB	1.99	0.44
1:E:942:ASP:O	1:E:946:ARG:HG2	2.18	0.44
1:E:691:LEU:HD23	1:E:697:MET:HG2	2.00	0.44
1:E:877:ASP:CG	1:E:930:VAL:HG22	2.38	0.44
2:B:30:LEU:C	2:B:32:ARG:N	2.66	0.44
2:B:162:CYS:HB3	2:B:178:CYS:HB3	1.86	0.44
1:E:353:LEU:HD21	1:E:781:LEU:HD11	2.00	0.44
1:A:826:PHE:CD2	1:A:967:ALA:HA	2.52	0.43
1:A:798:PRO:HB3	1:A:810:PRO:HD2	1.98	0.43
1:A:873:ALA:HB2	1:A:1004:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:ALA:HB3	1:E:237:SER:HA	2.00	0.43
1:E:742:ALA:HB3	1:E:758:ILE:HD13	1.99	0.43
1:A:745:ILE:HB	1:A:762:ASP:OD2	2.18	0.43
1:A:799:TYR:O	1:A:803:ILE:HG13	2.18	0.43
2:B:33:THR:O	2:B:37:TRP:HD1	2.01	0.43
1:A:374:GLU:O	1:A:374:GLU:CG	2.59	0.43
1:A:627:GLY:HA2	1:A:702:THR:H	1.82	0.43
1:A:647:SER:HB3	1:A:670:ARG:HB3	2.01	0.43
2:B:197:PRO:HB3	2:B:266:ALA:HB2	1.99	0.43
1:E:720:ILE:HA	1:E:738:ASP:OD2	2.18	0.43
2:B:200:ASP:HA	2:B:217:TYR:OH	2.18	0.43
1:E:933:ILE:HD12	1:E:993:ILE:HD11	2.00	0.43
1:A:353:LEU:HB2	1:A:370:LEU:HD13	2.00	0.43
1:A:496:LYS:HB2	1:A:522:ARG:NH1	2.34	0.43
2:B:32:ARG:HG3	2:B:37:TRP:NE1	2.33	0.43
1:E:780:ASN:ND2	1:E:831:LEU:O	2.52	0.43
1:A:824:ASP:HA	1:A:827:PRO:HD2	2.00	0.43
1:A:335:ALA:HB1	1:A:799:TYR:CE1	2.54	0.43
1:A:794:PRO:HG3	1:A:870:GLN:HB3	2.01	0.43
1:E:92:PRO:HD2	1:E:167:ILE:HG21	2.01	0.43
1:A:433:VAL:HG13	1:A:515:VAL:HB	2.01	0.42
1:E:767:ILE:O	1:E:771:VAL:HG23	2.19	0.42
1:E:787:TYR:CE1	1:E:943:VAL:HB	2.55	0.42
1:A:352:CYS:SG	1:A:832:ALA:HB2	2.58	0.42
1:A:995:PHE:CD1	1:A:996:GLN:HG3	2.53	0.42
2:B:213:LEU:HD12	2:B:251:ASN:HB3	2.01	0.42
2:F:185:ARG:HD2	2:F:240:TYR:HE1	1.84	0.42
1:A:514:LEU:HD22	1:A:592:LEU:HD22	2.01	0.42
2:F:196:ALA:HA	2:F:226:LEU:HD21	2.02	0.42
1:E:784:SER:HB2	1:E:828:SER:O	2.19	0.42
1:A:342:PRO:HG3	1:A:789:LEU:CD2	2.50	0.42
1:A:736:LYS:HG3	1:A:736:LYS:O	2.18	0.42
1:A:926:THR:HG22	1:A:926:THR:O	2.19	0.42
2:B:129:ILE:O	2:B:152:CYS:HA	2.20	0.42
2:B:161:ASN:HA	2:B:166:PRO:HD2	2.01	0.42
2:F:190:LEU:HD23	2:F:190:LEU:HA	1.91	0.42
1:A:725:GLY:O	1:A:742:ALA:HA	2.20	0.42
1:E:675:ASN:HA	1:E:700:ALA:O	2.19	0.42
1:E:945:ILE:HB	1:E:1012:ASP:OD2	2.19	0.42
1:E:887:TRP:CE2	1:E:909:ASP:HB3	2.54	0.42
1:A:731:SER:OG	1:A:732:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:LEU:HD21	2:F:284:PHE:CD1	2.55	0.42
1:E:180:VAL:HG22	1:E:181:ILE:H	1.83	0.42
1:E:861:TYR:O	1:E:865:GLN:HB2	2.19	0.42
1:A:257:MET:HB2	1:A:257:MET:HE2	1.95	0.42
1:E:291:THR:HG21	1:E:371:GLU:HB3	2.01	0.42
1:E:792:ASN:ND2	1:E:820:GLU:OE1	2.53	0.42
1:A:915:TRP:NE1	2:B:77:LEU:HD11	2.35	0.42
2:B:129:ILE:HG22	2:B:130:ASN:N	2.35	0.42
1:E:318:VAL:O	1:E:322:ILE:HG13	2.19	0.42
1:A:105:LEU:HD22	1:A:149:VAL:HG12	2.01	0.41
2:F:84:LEU:HA	2:F:180:ILE:O	2.19	0.41
2:F:216:GLU:HB3	2:F:248:LYS:HB3	2.02	0.41
1:E:461:SER:OG	1:E:560:ARG:NH2	2.53	0.41
1:E:757:MET:HG2	1:E:758:ILE:N	2.36	0.41
1:A:861:TYR:CE2	1:A:866:ILE:HD11	2.55	0.41
5:F:307:CLR:H8	5:F:307:CLR:H182	1.79	0.41
2:B:84:LEU:HA	2:B:180:ILE:O	2.21	0.41
1:A:53:HIS:CD2	1:A:248:THR:HG21	2.56	0.41
2:B:80:PRO:HD3	2:B:189:PHE:CZ	2.55	0.41
1:E:180:VAL:HA	1:E:200:VAL:HA	2.02	0.41
1:A:376:LEU:HD12	1:A:770:GLY:HA3	2.03	0.41
1:A:860:ALA:HA	1:A:864:PHE:HD1	1.85	0.41
1:E:296:GLU:OE2	1:E:852:ARG:HB3	2.20	0.41
1:A:1031:LEU:HD23	1:A:1031:LEU:HA	1.86	0.41
2:B:100:VAL:HG21	2:B:290:LYS:HE3	2.03	0.41
1:A:422:GLN:HA	1:A:427:TRP:CD1	2.55	0.41
1:A:701:ARG:HD2	1:A:701:ARG:HA	1.98	0.41
1:A:716:ARG:O	1:A:716:ARG:HG3	2.21	0.41
1:A:729:ASN:N	1:A:729:ASN:OD1	2.52	0.41
1:A:844:ARG:HA	1:A:844:ARG:HD3	1.91	0.41
1:A:974:ILE:O	1:A:978:LEU:HG	2.21	0.41
1:E:629:HIS:HA	1:E:701:ARG:HD3	2.03	0.41
1:A:180:VAL:HG22	1:A:181:ILE:H	1.86	0.41
1:A:626:THR:O	1:A:702:THR:OG1	2.28	0.41
1:E:560:ARG:HH22	1:E:562:LEU:HD11	1.86	0.41
1:E:800:LEU:O	1:E:804:THR:HG23	2.21	0.41
1:A:786:ALA:HB1	1:A:946:ARG:CZ	2.51	0.40
2:B:186:ILE:HB	2:B:189:PHE:CB	2.51	0.40
1:E:48:MET:O	1:E:278:ARG:NH1	2.54	0.40
1:E:487:CYS:SG	1:E:488:GLU:N	2.94	0.40
1:E:934:SER:HA	1:E:1001:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:662:ASP:N	1:E:662:ASP:OD1	2.49	0.40
1:E:726:ASP:OD1	1:E:727:GLY:N	2.55	0.40
1:E:775:ARG:HB3	1:E:840:ILE:HD11	2.03	0.40
1:A:385:ASP:OD2	3:A:1101:MF4:F2	2.29	0.40
1:A:482:ARG:O	1:A:484:PRO:HD3	2.22	0.40
2:F:51:MET:SD	1:E:869:ILE:HG12	2.62	0.40
1:E:119:ILE:HG21	1:E:334:MET:HB2	2.04	0.40
1:E:250:ASN:OD1	1:E:250:ASN:N	2.53	0.40
1:E:902:HIS:O	1:E:905:GLN:NE2	2.55	0.40
1:A:329:ALA:HA	1:A:332:PHE:CE2	2.56	0.40
1:A:342:PRO:HB2	1:A:345:LEU:HB2	2.03	0.40
1:A:367:VAL:HG12	1:A:368:LYS:H	1.86	0.40
1:A:822:CYS:SG	1:A:974:ILE:HG12	2.61	0.40
2:F:135:LYS:O	2:F:227:HIS:HA	2.21	0.40
2:F:286:LEU:HD12	2:F:286:LEU:HA	1.93	0.40
1:A:777:ILE:HD12	1:A:777:ILE:HA	1.87	0.40
2:B:74:GLN:HB3	2:B:77:LEU:HB2	2.02	0.40
2:B:208:ARG:HD3	2:B:208: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	985/987 (100%)	895 (91%)	88 (9%)	2 (0%)	47 81
1	E	985/987 (100%)	900 (91%)	84 (8%)	1 (0%)	51 85
2	B	269/289 (93%)	237 (88%)	30 (11%)	2 (1%)	22 62
2	F	264/289 (91%)	246 (93%)	18 (7%)	0	100 100
All	All	2503/2552 (98%)	2278 (91%)	220 (9%)	5 (0%)	47 81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	LEU
2	B	31	GLY
1	A	50	ILE
1	A	889	PRO
1	E	237	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/834 (100%)	805 (96%)	29 (4%)	36	60
1	E	834/834 (100%)	815 (98%)	19 (2%)	50	70
2	B	237/253 (94%)	226 (95%)	11 (5%)	27	53
2	F	232/253 (92%)	227 (98%)	5 (2%)	52	71
All	All	2137/2174 (98%)	2073 (97%)	64 (3%)	41	64

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET
1	A	49	GLU
1	A	70	LYS
1	A	103	ARG
1	A	160	GLU
1	A	198	ASP
1	A	213	ARG
1	A	220	CYS
1	A	225	SER
1	A	244	SER
1	A	254	PHE
1	A	255	SER
1	A	491	PHE
1	A	496	LYS
1	A	508	ARG
1	A	540	ASP
1	A	542	GLN

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Mol	Chain	Res	Type
1	A	551	TYR
1	A	681	ASP
1	A	713	SER
1	A	756	ASP
1	A	830	SER
1	A	901	ASN
1	A	903	HIS
1	A	923	GLN
1	A	931	PHE
1	A	959	PHE
1	A	1025	SER
1	A	1033	TYR
2	B	29	MET
2	B	30	LEU
2	B	35	SER
2	B	48	TYR
2	B	114	HIS
2	B	126	GLU
2	B	141	SER
2	B	157	ASP
2	B	165	ARG
2	B	241	SER
2	B	272	ASP
2	F	44	TYR
2	F	113	LEU
2	F	130	ASN
2	F	165	ARG
2	F	208	ARG
1	E	67	SER
1	E	70	LYS
1	E	83	ARG
1	E	103	ARG
1	E	137	ASP
1	E	211	ASP
1	E	220	CYS
1	E	225	SER
1	E	236	ARG
1	E	300	PHE
1	E	365	CYS
1	E	508	ARG
1	E	542	GLN
1	E	560	ARG

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Mol	Chain	Res	Type
1	E	652	ASP
1	E	685	SER
1	E	762	ASP
1	E	877	ASP
1	E	931	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	586	ASN
1	A	923	GLN
2	F	125	GLN
2	F	289	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are 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	CLR	A	1103	-	31,31,31	0.66	0	48,48,48	1.20	3 (6%)
3	MF4	A	1101	1	0,4,4	-	-	-		
7	NAG	F	302	2	14,14,15	1.84	2 (14%)	17,19,21	1.26	2 (11%)
7	NAG	F	303	2	14,14,15	0.21	0	17,19,21	0.58	0
7	NAG	F	305	2	14,14,15	0.62	1 (7%)	17,19,21	0.59	0
7	NAG	B	302	2	14,14,15	1.05	1 (7%)	17,19,21	0.79	1 (5%)
7	NAG	F	306	2	14,14,15	0.54	0	17,19,21	0.34	0
7	NAG	B	301	2	14,14,15	0.77	1 (7%)	17,19,21	0.90	1 (5%)
7	NAG	F	301	2	14,14,15	0.52	0	17,19,21	0.60	0
7	NAG	F	304	2	14,14,15	0.57	0	17,19,21	0.48	0
3	MF4	E	1101	1	0,4,4	-	-	-		
5	CLR	F	307	-	31,31,31	0.69	0	48,48,48	1.25	5 (10%)

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
5	CLR	A	1103	-	-	4/10/68/68	0/4/4/4
7	NAG	F	302	2	-	4/6/23/26	0/1/1/1
7	NAG	F	303	2	-	0/6/23/26	0/1/1/1
7	NAG	F	305	2	-	2/6/23/26	0/1/1/1
7	NAG	B	302	2	-	2/6/23/26	0/1/1/1
7	NAG	F	306	2	-	2/6/23/26	0/1/1/1
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1
7	NAG	F	301	2	-	2/6/23/26	0/1/1/1
7	NAG	F	304	2	-	0/6/23/26	0/1/1/1
5	CLR	F	307	-	-	5/10/68/68	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	302	NAG	C1-C2	4.99	1.59	1.52
7	F	302	NAG	O5-C1	-4.06	1.37	1.43
7	B	302	NAG	C1-C2	3.81	1.58	1.52
7	B	301	NAG	C1-C2	2.49	1.56	1.52
7	F	305	NAG	C1-C2	2.17	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1103	CLR	C19-C10-C5	-4.79	100.59	108.34
5	F	307	CLR	C8-C7-C6	-4.70	105.98	112.73
7	F	302	NAG	C4-C3-C2	3.47	116.11	111.02
7	B	301	NAG	C1-O5-C5	3.19	116.52	112.19
5	F	307	CLR	C13-C14-C8	-3.14	109.73	114.38
5	A	1103	CLR	C9-C10-C5	3.01	114.36	109.65
7	F	302	NAG	O5-C5-C4	-2.84	103.91	110.83
7	B	302	NAG	C1-O5-C5	2.84	116.04	112.19
5	A	1103	CLR	C19-C10-C1	2.45	113.29	109.43
5	F	307	CLR	C9-C10-C5	2.35	113.34	109.65
5	F	307	CLR	C19-C10-C5	-2.06	105.00	108.34
5	F	307	CLR	C17-C13-C14	2.01	102.45	100.07

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	301	NAG	O5-C5-C6-O6
7	F	305	NAG	O5-C5-C6-O6
7	F	301	NAG	C4-C5-C6-O6
7	B	301	NAG	O5-C5-C6-O6
7	B	302	NAG	O5-C5-C6-O6
7	F	306	NAG	O5-C5-C6-O6
7	F	302	NAG	O5-C5-C6-O6
7	B	301	NAG	C4-C5-C6-O6
7	F	302	NAG	C4-C5-C6-O6
7	F	305	NAG	C4-C5-C6-O6
5	A	1103	CLR	C17-C20-C22-C23
5	F	307	CLR	C17-C20-C22-C23
7	B	302	NAG	C4-C5-C6-O6
7	F	302	NAG	C8-C7-N2-C2
7	F	302	NAG	O7-C7-N2-C2
5	A	1103	CLR	C21-C20-C22-C23
5	F	307	CLR	C21-C20-C22-C23
7	F	306	NAG	C4-C5-C6-O6
5	A	1103	CLR	C23-C24-C25-C27
5	A	1103	CLR	C23-C24-C25-C26
5	F	307	CLR	C23-C24-C25-C27
5	F	307	CLR	C23-C24-C25-C26
5	F	307	CLR	C20-C22-C23-C24

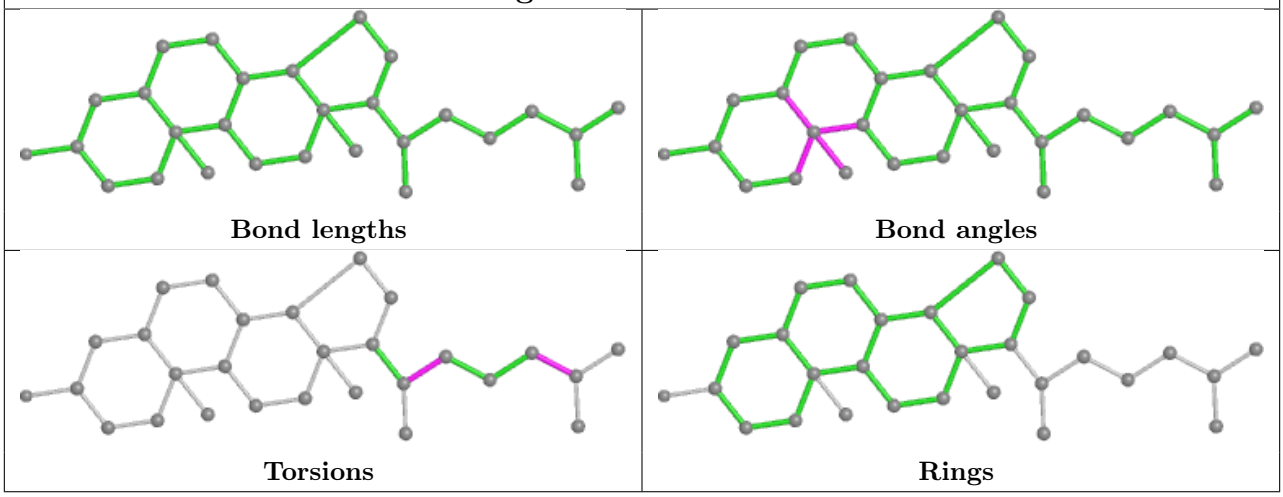
There are no ring outliers.

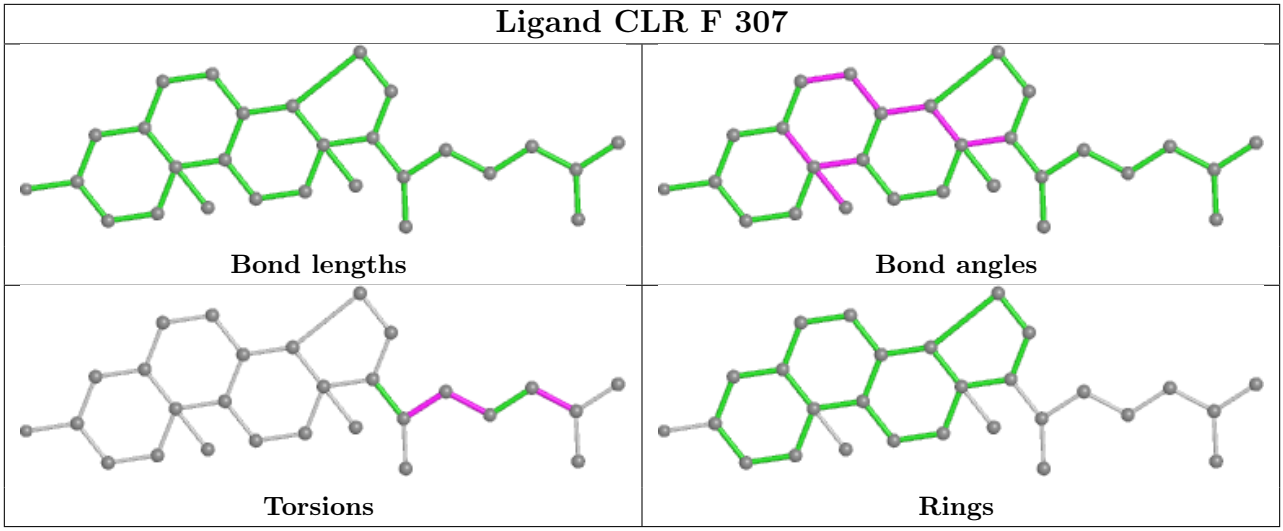
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1103	CLR	3	0
3	A	1101	MF4	4	0
3	E	1101	MF4	4	0
5	F	307	CLR	3	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 then 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.

Ligand CLR A 1103





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	987/987 (100%)	-0.35	27 (2%)	54	44	56, 182, 332, 418	0
1	E	987/987 (100%)	-0.06	43 (4%)	34	28	91, 278, 430, 517	0
2	B	271/289 (93%)	0.33	29 (10%)	6	6	220, 340, 459, 529	0
2	F	266/289 (92%)	-0.59	1 (0%)	92	87	97, 204, 318, 415	0
All	All	2511/2552 (98%)	-0.19	100 (3%)	38	30	56, 233, 409, 529	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	210	GLY	11.6
2	B	208	ARG	10.9
2	B	207	PRO	8.5
2	B	92	LYS	8.1
2	B	91	GLU	8.0
1	E	50	ILE	7.5
2	B	255	ASN	7.3
1	E	561	VAL	7.3
1	E	269	ASN	7.2
1	E	51	ASN	6.7
1	E	599	SER	6.1
1	E	170	PHE	5.9
1	E	49	GLU	5.9
1	E	48	MET	5.7
2	B	209	ASP	5.7
1	E	562	LEU	5.5
1	E	211	ASP	5.5
2	B	213	LEU	5.3
1	E	558	GLY	5.2
1	E	559	GLU	5.2
1	A	158	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	211	PRO	5.2
2	B	134	GLU	5.2
2	B	132	THR	5.0
2	B	256	ARG	4.9
2	B	130	ASN	4.9
1	A	159	GLN	4.7
1	A	143	LEU	4.5
1	E	597	LEU	4.5
1	E	598	VAL	4.4
1	A	903	HIS	4.4
1	E	171	LYS	4.3
1	E	742	ALA	4.2
1	E	596	GLY	4.0
2	F	272	ASP	4.0
1	E	400	LEU	4.0
1	A	162	LYS	3.9
1	A	157	TYR	3.8
2	B	66	ILE	3.7
2	B	275	HIS	3.7
1	A	161	PHE	3.6
2	B	274	PRO	3.6
1	A	140	TYR	3.5
2	B	179	PHE	3.5
1	E	510	PRO	3.4
1	E	273	ARG	3.3
1	A	133	LEU	3.3
1	A	97	GLU	3.3
1	E	268	VAL	3.2
1	E	223	ASP	3.2
1	A	156	GLY	3.1
1	A	125	ALA	3.1
2	B	166	PRO	3.1
1	A	918	GLY	3.1
1	E	420	PHE	3.0
1	A	160	GLU	2.9
2	B	174	GLU	2.9
2	B	68	PRO	2.9
1	E	278	ARG	2.8
1	E	78	ALA	2.8
2	B	133	SER	2.8
1	E	105	LEU	2.8
1	E	436	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	600	MET	2.7
1	E	272	ASP	2.6
1	E	503	THR	2.6
2	B	194	SER	2.6
1	E	511	ARG	2.6
1	E	47	GLY	2.6
1	E	512	HIS	2.6
1	E	504	LEU	2.5
1	A	127	GLN	2.5
1	E	440	ALA	2.5
1	A	883	ALA	2.5
2	B	83	THR	2.4
1	E	509	ASP	2.4
1	E	279	ILE	2.3
1	A	512	HIS	2.3
1	E	169	SER	2.3
1	A	50	ILE	2.3
2	B	220	ALA	2.3
2	B	212	PRO	2.3
2	B	181	ILE	2.3
1	E	173	LEU	2.2
1	E	564	PHE	2.2
2	B	206	GLN	2.2
1	A	887	TRP	2.2
1	A	144	ALA	2.2
1	E	107	GLY	2.2
1	A	400	LEU	2.2
1	A	576	PRO	2.2
1	A	476	ALA	2.1
1	A	123	ALA	2.1
1	A	922	TYR	2.1
2	B	205	ASP	2.1
1	E	245	PRO	2.1
1	A	128	ALA	2.0
1	A	886	GLY	2.0
1	E	623	ILE	2.0
2	B	78	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

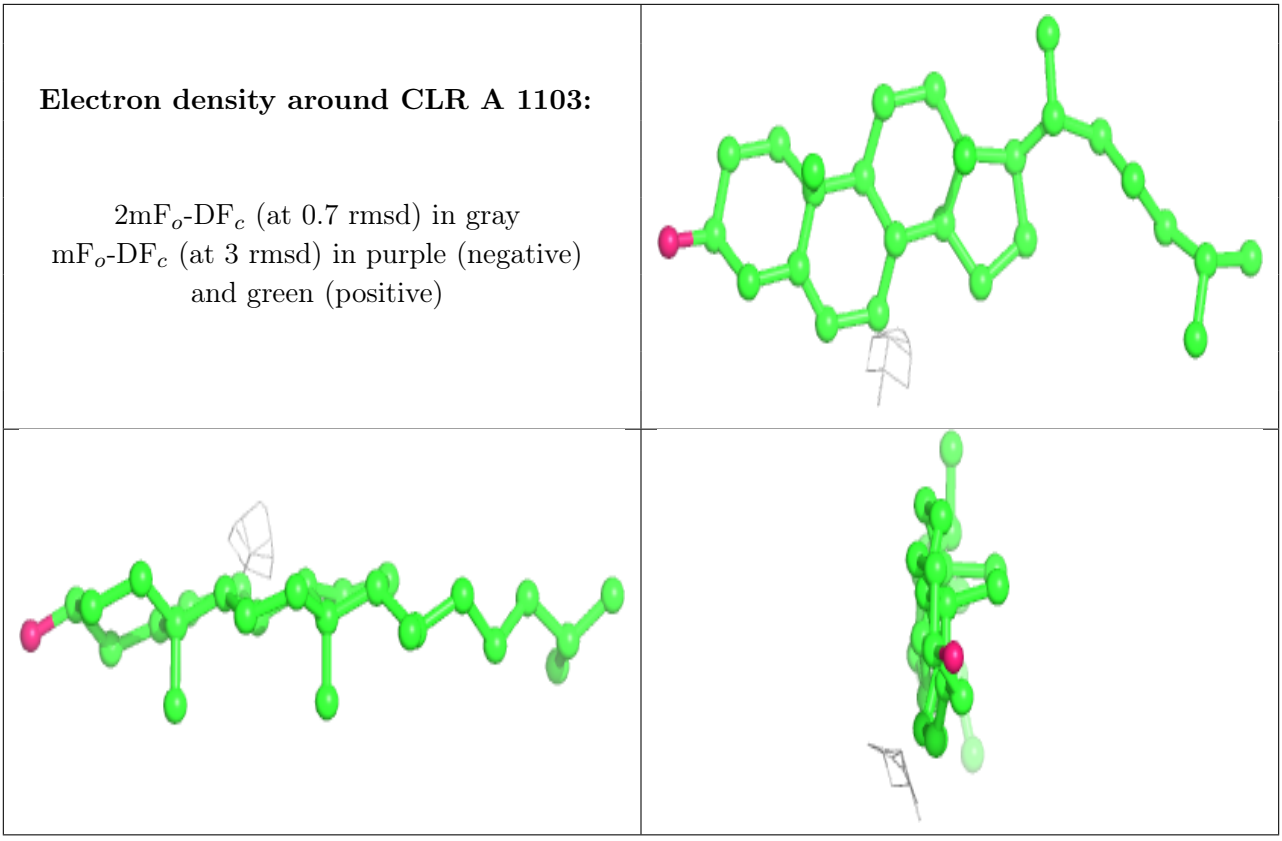
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	K	A	1104	1/1	0.55	0.47	245,245,245,245	0
6	K	E	1103	1/1	0.57	1.15	381,381,381,381	0
7	NAG	F	306	14/15	0.57	0.74	298,313,325,328	0
5	CLR	A	1103	28/28	0.61	1.13	311,365,379,385	0
7	NAG	F	305	14/15	0.62	0.27	235,273,278,281	0
5	CLR	F	307	28/28	0.64	0.52	297,312,318,323	0
7	NAG	B	301	14/15	0.65	0.47	330,341,347,351	0
7	NAG	F	301	14/15	0.72	0.28	255,276,289,289	0
7	NAG	B	302	14/15	0.79	0.43	361,376,384,387	0
7	NAG	F	303	14/15	0.80	0.41	276,290,303,310	0
6	K	A	1106	1/1	0.85	0.23	179,179,179,179	0
7	NAG	F	304	14/15	0.86	0.23	302,318,325,326	0
3	MF4	E	1101	5/5	0.88	0.16	337,343,348,349	0
7	NAG	F	302	14/15	0.91	0.37	273,280,298,302	0
6	K	E	1104	1/1	0.93	0.24	333,333,333,333	0
6	K	A	1105	1/1	0.95	0.23	171,171,171,171	0
3	MF4	A	1101	5/5	0.95	0.15	93,110,113,128	0
6	K	E	1105	1/1	0.96	0.20	170,170,170,170	0
4	MG	A	1102	1/1	0.98	0.21	80,80,80,80	0
4	MG	E	1102	1/1	0.98	0.17	320,320,320,320	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.

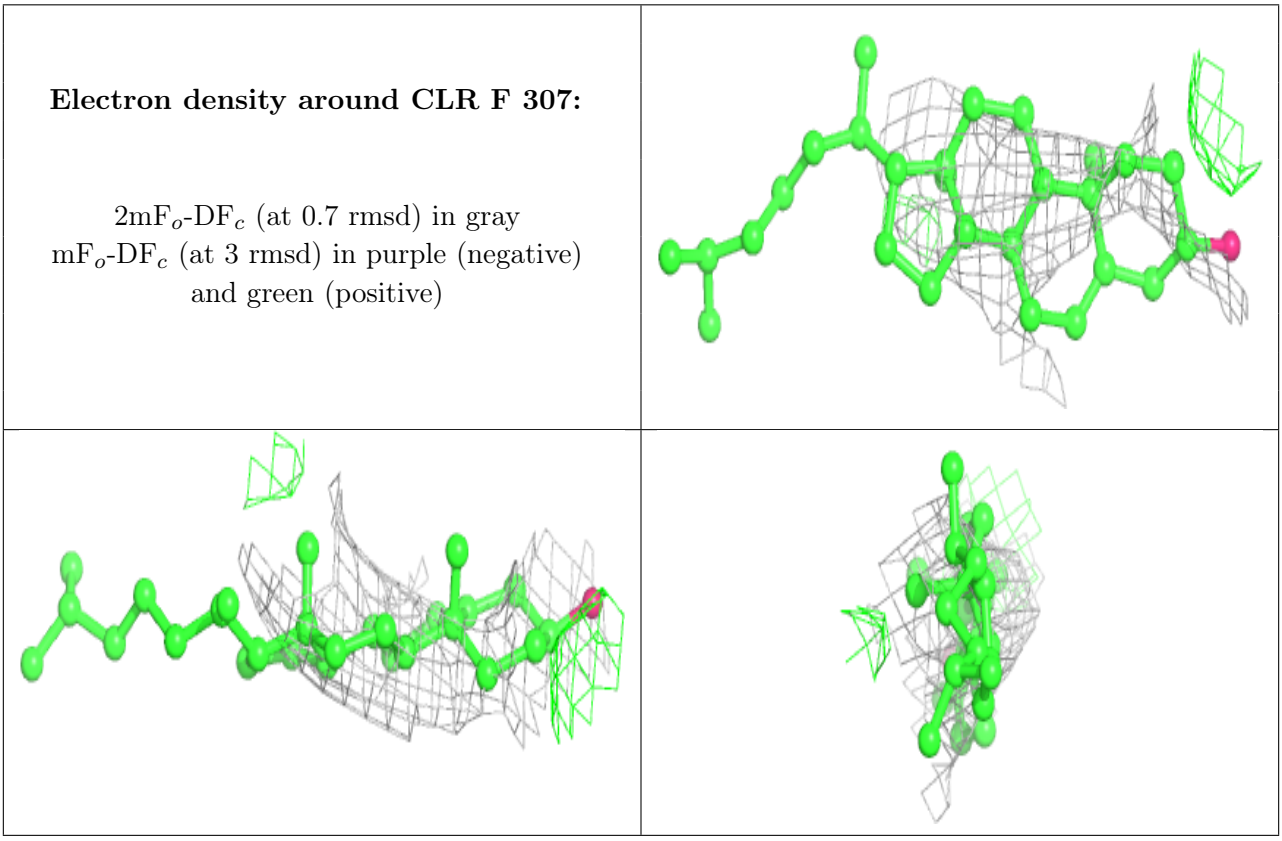
Electron density around CLR A 1103:

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



Electron density around CLR F 307:

$2mF_o$-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.