



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:30 PM UTC

PDB ID : 6JXK / pdb_00006jxk
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 ⓘ 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

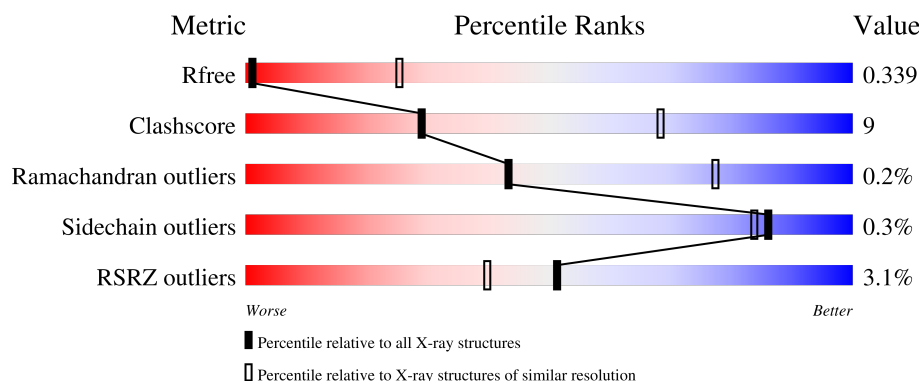
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	987	0% 77% 23%
1	E	987	3% 80% 20%
2	B	289	7% 70% 23% 6%
2	F	289	4% 79% 13% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MF4	A	1101	-	-	X	-
3	MF4	E	1101	-	-	X	-

2 Entry composition

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
1	A	987	Total	C	N	O	S	0	0	0
			7659	4890	1292	1423	54			
1	E	987	Total	C	N	O	S	0	0	0
			7659	4890	1292	1423	54			

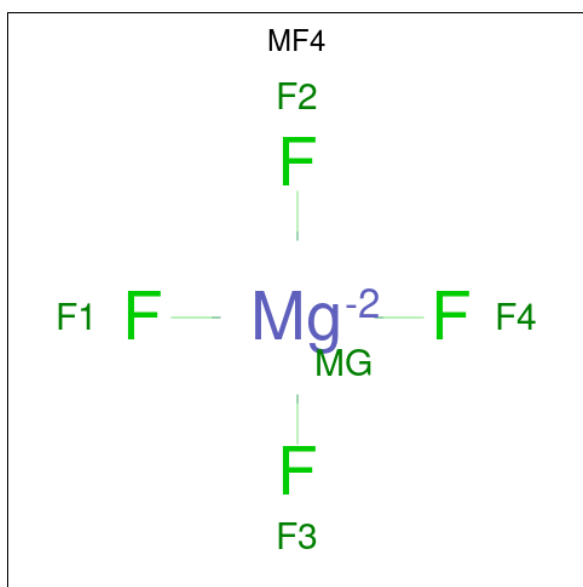
There are 8 discrepancies between the modelled and reference sequences:

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
2	B	271	Total	C	N	O	S	0	0	0
			2175	1411	360	391	13			
2	F	266	Total	C	N	O	S	0	0	0
			2128	1379	353	384	12			

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (CCD ID: MF4) (formula: F₄Mg).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

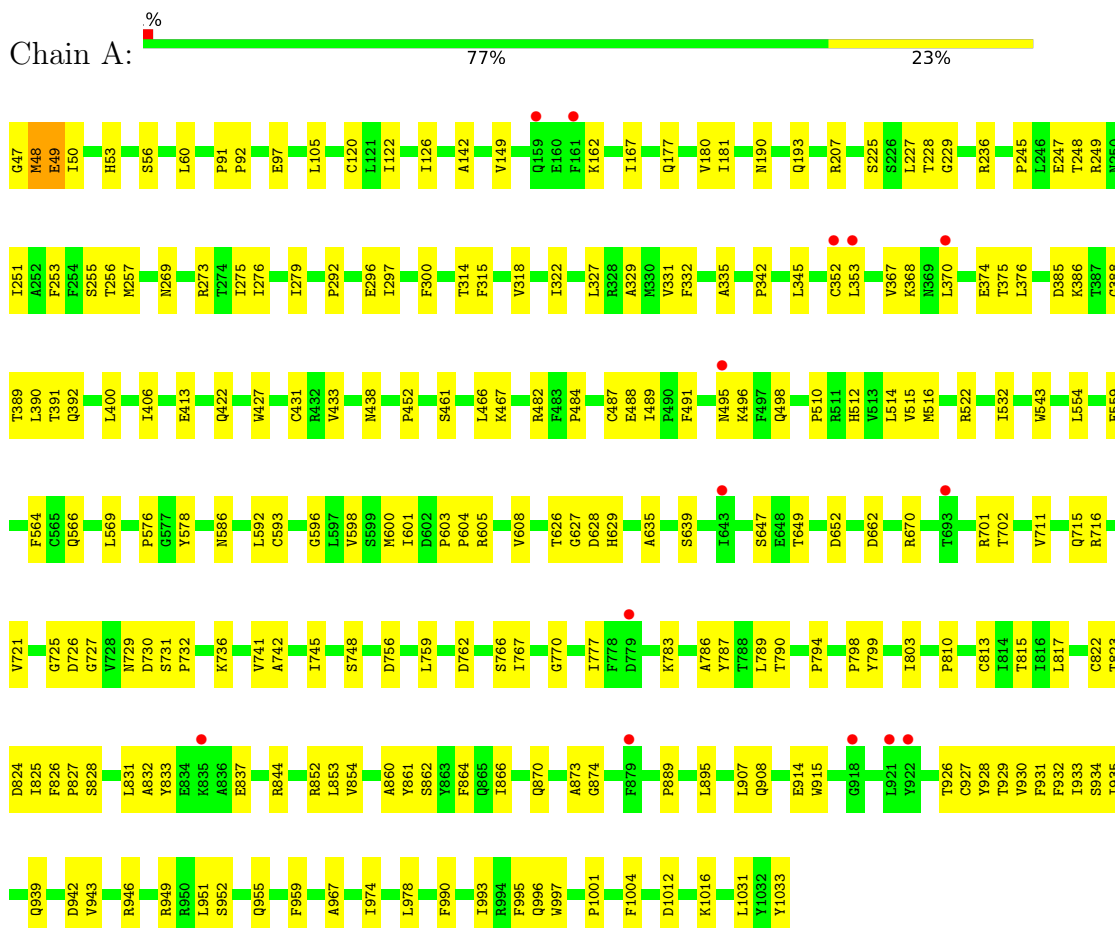


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

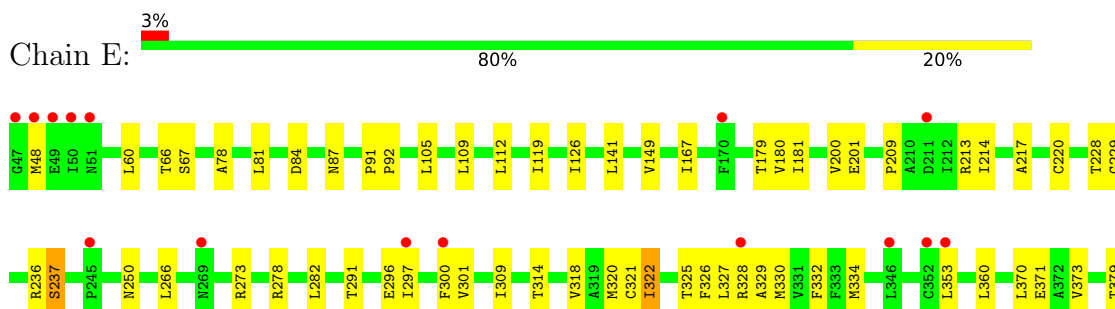
3 Residue-property plots

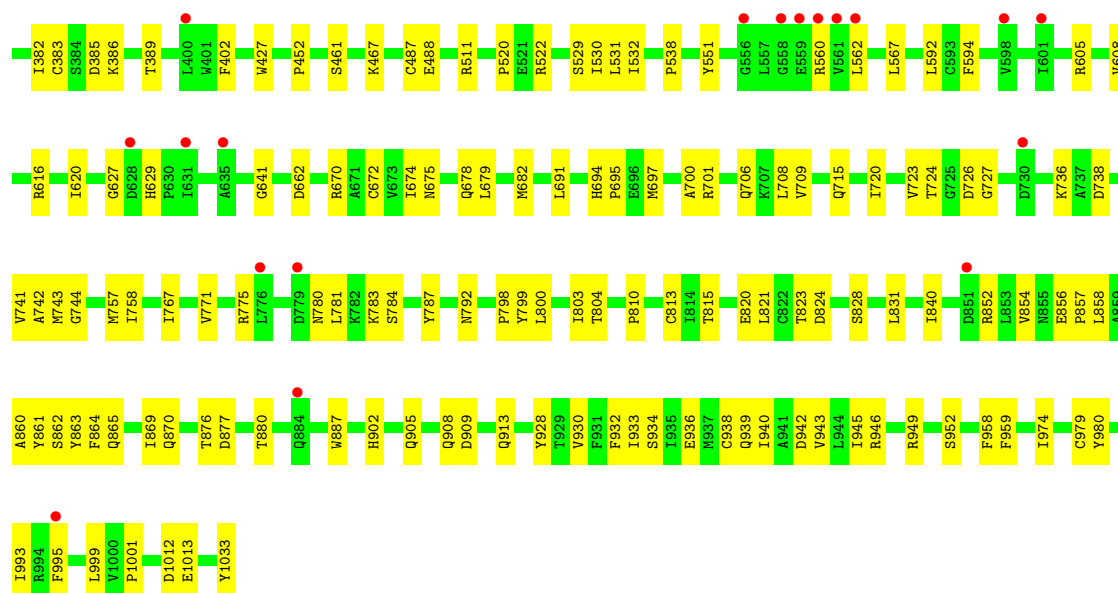
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

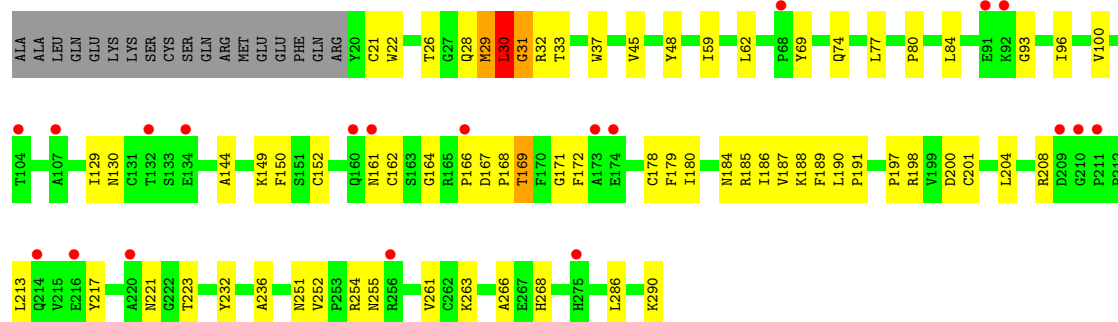


• Molecule 1: Potassium-transporting ATPase alpha chain 1

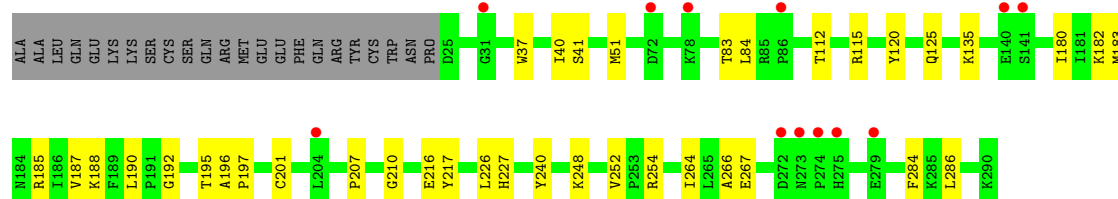
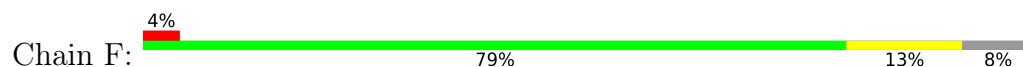




• Molecule 2: Potassium-transporting ATPase subunit beta



• Molecule 2: Potassium-transporting ATPase subunit beta



4 Data and refinement statistics

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 – 4.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.79-4.30) 95.0 (47.79-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.263 , 0.338 0.266 , 0.339	Depositor DCC
R_{free} test set	1546 reflections (3.90%)	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)	0.25 , 200.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	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.*

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: NAG, CLR, MF4, K, MG

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	0.20	0/7817	0.50	0/10618
1	E	0.17	0/7817	0.48	3/10618 (0.0%)
2	B	0.27	0/2246	0.60	3/3057 (0.1%)
2	F	0.19	0/2195	0.49	0/2985
All	All	0.20	0/20075	0.50	6/27278 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	511	ARG	N-CA-C	6.76	120.49	110.48
1	E	321	CYS	N-CA-C	6.04	117.87	111.28
1	E	744	GLY	N-CA-C	5.93	122.02	114.66
2	B	93	GLY	N-CA-C	5.68	118.17	111.63
2	B	28	GLN	N-CA-C	-5.61	107.02	112.97
2	B	169	THR	CB-CA-C	-5.27	101.59	110.44

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	7659	0	7686	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	7659	0	7685	118	0
2	B	2175	0	2105	56	0
2	F	2128	0	2065	24	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
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	344	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 9.

All (344) 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
1:A:48:MET:HE2	1:A:48:MET:HA	1.49	0.94
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
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
2:B:29:MET:C	2:B:31:GLY:H	1.93	0.76
1:A:48:MET:HE2	1:A:48:MET:CA	2.17	0.75
1:A:126:ILE:HG21	1:A:327:LEU:HD11	1.68	0.75
1:A:48:MET:HA	1:A:48:MET:CE	2.13	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:452:PRO:O	1:A:467:LYS:NZ	2.31	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
2:B:29:MET:C	2:B:31:GLY:N	2.52	0.63
1:A:385:ASP:OD1	3:A:1101:MF4:F3	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:679:LEU:HA	1:E:682:MET:HE2	1.84	0.58
1:A:461:SER:HA	1:A:600:MET:HE1	1.85	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:207:ARG:HG2	1:A:257:MET:HE2	1.85	0.58
1:A:512:HIS:O	1:A:569:LEU:N	2.36	0.58
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
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:908:GLN:HG2	1:A:914:GLU:HG2	1.90	0.54
1:E:119:ILE:HG23	1:E:330:MET:HE3	1.88	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
1:A:253:PHE:O	1:A:256:THR:OG1	2.19	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ILE:HA	2:B:62:LEU:HB3	1.91	0.53
1:A:715:GLN:OE1	1:A:736:LYS:NZ	2.43	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
2:B:45:VAL:HA	2:B:48:TYR:HB2	1.91	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:715:GLN:OE1	1:E:736:LYS:NZ	2.44	0.51
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: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:A:49:GLU:OE2	1:A:49:GLU:HA	2.07	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:320:MET:HE1	1:E:326:PHE:HB2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:952:SER:OG	1:E:1013:GLU:OE1	2.21	0.48
1:A:162:LYS:HB2	1:A:368:LYS:HE3	1.95	0.48
2:B:30:LEU:C	2:B:32:ARG:N	2.66	0.48
1:E:520:PRO:HG2	1:E:551:TYR:CE1	2.48	0.48
1:E:389:THR:HA	1:E:743:MET:HE2	1.95	0.48
1:E:678:GLN:O	1:E:682:MET:HG3	2.13	0.48
1:E:877:ASP:CG	1:E:930:VAL:HG22	2.38	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:48:MET:HE2	1:E:48:MET:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:THR:OG1	1:E:67:SER:N	2.41	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
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: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:48:MET:HE2	1:A:48:MET:N	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:995:PHE:O	1:E:999:LEU:HG	2.17	0.44
1:A:255:SER:O	1:A:255:SER:OG	2.36	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:185:ARG:HD2	2:F:240:TYR:HE1	1.84	0.42
1:E:300:PHE:CD1	1:E:300:PHE:C	2.97	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: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:A:736:LYS:O	1:A:736:LYS:HG3	2.18	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
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: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
1:A:825:ILE:O	1:A:828:SER:OG	2.38	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:531:LEU:C	1:E:532:ILE:HD12	2.45	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
2:F:183:MET:HE2	2:F:264:ILE:HD12	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LEU:C	1:A:833:TYR:H	2.28	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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	985/987 (100%)	895 (91%)	88 (9%)	2 (0%)	43	77
1	E	985/987 (100%)	900 (91%)	84 (8%)	1 (0%)	48	83
2	B	269/289 (93%)	237 (88%)	30 (11%)	2 (1%)	18	55
2	F	264/289 (91%)	246 (93%)	18 (7%)	0	100	100
All	All	2503/2552 (98%)	2278 (91%)	220 (9%)	5 (0%)	43	77

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

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%)	831 (100%)	3 (0%)	84	82
1	E	834/834 (100%)	833 (100%)	1 (0%)	88	88
2	B	237/253 (94%)	235 (99%)	2 (1%)	73	77
2	F	232/253 (92%)	232 (100%)	0	100	100
All	All	2137/2174 (98%)	2131 (100%)	6 (0%)	86	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET
1	A	49	GLU
1	A	97	GLU
2	B	29	MET
2	B	30	LEU
1	E	322	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	193	GLN
1	A	224	ASN
1	A	288	ASN
1	A	438	ASN
1	A	498	GLN
1	A	586	ASN
1	A	870	GLN
1	A	939	GLN
2	B	160	GLN
2	F	125	GLN
2	F	237	GLN
2	F	289	GLN
1	E	415	GLN
1	E	780	ASN
1	E	902	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.68	0	48,48,48	1.26	3 (6%)
3	MF4	E	1101	1	0,4,4	-	-	-		
7	NAG	F	302	2	14,14,15	1.91	2 (14%)	17,19,21	1.27	2 (11%)
7	NAG	F	303	2	14,14,15	0.21	0	17,19,21	0.60	0
7	NAG	F	305	2	14,14,15	0.67	1 (7%)	17,19,21	0.61	0
7	NAG	F	301	2	14,14,15	0.57	1 (7%)	17,19,21	0.62	0
7	NAG	F	304	2	14,14,15	0.55	0	17,19,21	0.50	0
7	NAG	B	301	2	14,14,15	0.82	1 (7%)	17,19,21	0.91	1 (5%)
3	MF4	A	1101	1	0,4,4	-	-	-		
7	NAG	B	302	2	14,14,15	1.15	1 (7%)	17,19,21	0.80	1 (5%)
7	NAG	F	306	2	14,14,15	0.56	0	17,19,21	0.36	0
5	CLR	F	307	-	31,31,31	0.71	0	48,48,48	1.30	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	F	301	2	-	2/6/23/26	0/1/1/1
7	NAG	F	304	2	-	0/6/23/26	0/1/1/1
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1
7	NAG	B	302	2	-	3/6/23/26	0/1/1/1
7	NAG	F	306	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	F	307	-	-	5/10/68/68	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	302	NAG	C1-C2	5.47	1.59	1.52
7	B	302	NAG	C1-C2	4.17	1.58	1.52
7	F	302	NAG	O5-C1	-3.85	1.37	1.43
7	B	301	NAG	C1-C2	2.73	1.56	1.52
7	F	305	NAG	C1-C2	2.38	1.55	1.52
7	F	301	NAG	C1-C2	2.02	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	CLR	C19-C10-C5	-5.10	100.59	108.38
5	F	307	CLR	C8-C7-C6	-4.89	105.98	112.76
7	F	302	NAG	C4-C3-C2	3.47	116.11	111.02
5	F	307	CLR	C13-C14-C8	-3.30	109.73	114.41
7	B	301	NAG	C1-O5-C5	3.23	116.52	112.19
5	A	1103	CLR	C9-C10-C5	3.22	114.36	109.65
7	B	302	NAG	C1-O5-C5	2.88	116.04	112.19
7	F	302	NAG	O5-C5-C4	-2.84	103.91	110.83
5	A	1103	CLR	C19-C10-C1	2.54	113.29	109.43
5	F	307	CLR	C9-C10-C5	2.52	113.34	109.65
5	F	307	CLR	C19-C10-C5	-2.21	105.00	108.38
5	F	307	CLR	C17-C13-C14	2.05	102.45	100.10

There are no chirality outliers.

All (25) 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	F	306	NAG	O5-C5-C6-O6
7	B	301	NAG	C4-C5-C6-O6
7	B	302	NAG	O5-C5-C6-O6
5	A	1103	CLR	C17-C20-C22-C23
7	F	302	NAG	C4-C5-C6-O6

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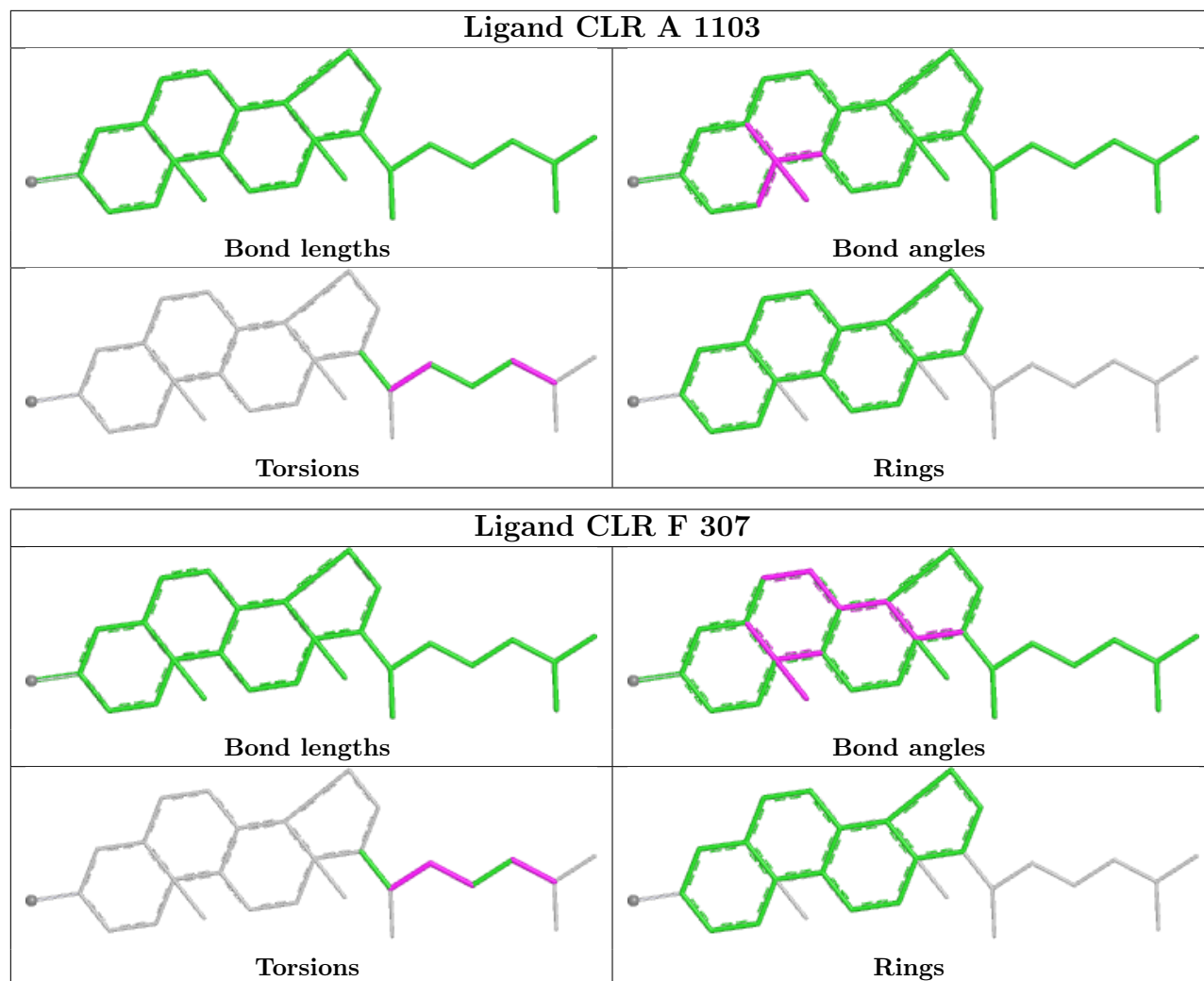
Mol	Chain	Res	Type	Atoms
7	F	305	NAG	C4-C5-C6-O6
7	F	302	NAG	O5-C5-C6-O6
5	F	307	CLR	C17-C20-C22-C23
7	B	302	NAG	C4-C5-C6-O6
5	A	1103	CLR	C21-C20-C22-C23
7	F	302	NAG	C8-C7-N2-C2
7	F	302	NAG	O7-C7-N2-C2
5	F	307	CLR	C21-C20-C22-C23
7	F	306	NAG	C4-C5-C6-O6
5	A	1103	CLR	C23-C24-C25-C27
5	A	1103	CLR	C23-C24-C25-C26
5	F	307	CLR	C23-C24-C25-C27
5	F	307	CLR	C23-C24-C25-C26
5	F	307	CLR	C20-C22-C23-C24
7	B	302	NAG	C1-C2-N2-C7
7	F	306	NAG	C1-C2-N2-C7

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	E	1101	MF4	4	0
3	A	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 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	987/987 (100%)	-0.16	14 (1%) 73 58	56, 182, 332, 418	0
1	E	987/987 (100%)	-0.05	33 (3%) 49 39	91, 278, 430, 517	0
2	B	271/289 (93%)	0.54	20 (7%) 20 23	220, 340, 459, 529	0
2	F	266/289 (92%)	-0.03	12 (4%) 38 33	97, 204, 318, 415	0
All	All	2511/2552 (98%)	-0.03	79 (3%) 51 40	56, 233, 409, 529	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	THR	10.0
2	B	166	PRO	9.6
1	E	598	VAL	7.9
2	F	78	LYS	7.6
2	B	134	GLU	6.3
2	B	220	ALA	5.7
1	E	50	ILE	5.5
2	F	272	ASP	4.6
2	B	174	GLU	4.5
1	A	918	GLY	4.5
1	E	561	VAL	4.3
2	B	161	ASN	4.1
1	E	400	LEU	3.9
1	E	558	GLY	3.7
1	E	51	ASN	3.7
2	B	107	ALA	3.5
1	E	47	GLY	3.4
2	F	273	ASN	3.4
1	E	562	LEU	3.4
2	B	92	LYS	3.3
1	A	353	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	173	ALA	3.1
1	E	300	PHE	3.1
1	E	779	ASP	3.1
1	E	730	ASP	3.0
1	E	49	GLU	3.0
1	A	159	GLN	3.0
2	F	274	PRO	3.0
2	B	210	GLY	3.0
2	B	275	HIS	3.0
1	E	48	MET	2.9
1	E	884	GLN	2.9
1	A	922	TYR	2.8
1	E	269	ASN	2.8
2	B	211	PRO	2.7
1	E	560	ARG	2.7
2	B	160	GLN	2.7
1	E	601	ILE	2.7
1	E	211	ASP	2.6
2	B	209	ASP	2.6
1	E	346	LEU	2.6
1	E	776	LEU	2.6
1	E	995	PHE	2.6
1	E	631	ILE	2.6
2	F	279	GLU	2.6
2	B	104	THR	2.6
2	F	72	ASP	2.5
1	E	556	GLY	2.5
1	A	643	ILE	2.5
2	B	91	GLU	2.4
2	B	214	GLN	2.4
1	A	161	PHE	2.4
1	A	495	ASN	2.4
1	A	370	LEU	2.4
2	F	204	LEU	2.4
1	A	352	CYS	2.3
1	E	245	PRO	2.3
2	F	275	HIS	2.3
2	B	68	PRO	2.3
1	E	635	ALA	2.3
1	E	297	ILE	2.2
1	A	779	ASP	2.2
1	E	628	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	851	ASP	2.2
2	B	256	ARG	2.2
2	F	86	PRO	2.2
1	A	693	THR	2.2
1	E	352	CYS	2.2
1	A	835	LYS	2.1
1	A	921	LEU	2.1
1	E	328	ARG	2.1
2	F	140	GLU	2.1
1	E	170	PHE	2.1
1	E	353	LEU	2.0
1	A	879	PHE	2.0
2	F	141	SER	2.0
2	F	31	GLY	2.0
1	E	559	GLU	2.0
2	B	216	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

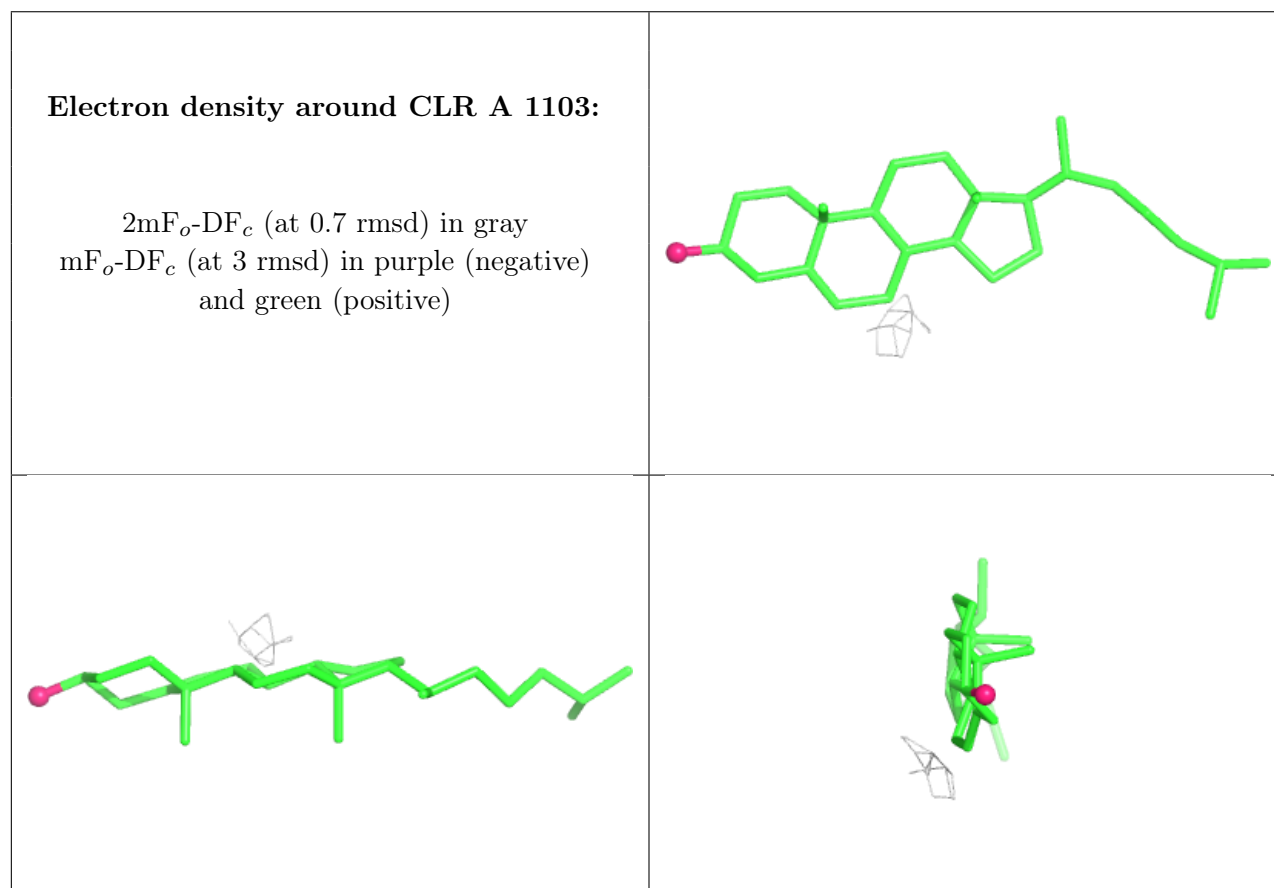
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	E	1103	1/1	-0.11	0.16	381,381,381,381	0
7	NAG	F	306	14/15	0.37	0.09	298,313,325,328	0
7	NAG	F	302	14/15	0.38	0.13	273,280,298,302	0
7	NAG	F	305	14/15	0.42	0.13	235,273,278,281	0
7	NAG	B	301	14/15	0.50	0.16	330,341,347,351	0
7	NAG	F	301	14/15	0.56	0.11	255,276,289,289	0
7	NAG	B	302	14/15	0.59	0.11	361,376,384,387	0

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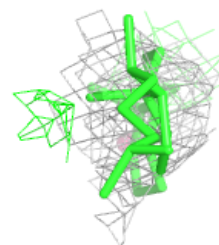
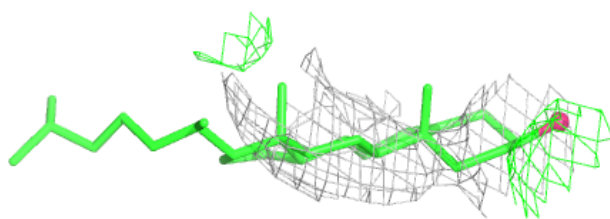
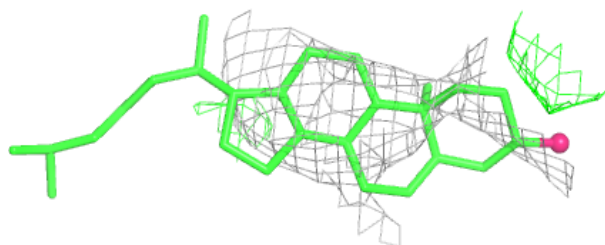
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	F	304	14/15	0.63	0.08	302,318,325,326	0
5	CLR	A	1103	28/28	0.76	0.18	311,365,379,385	0
5	CLR	F	307	28/28	0.76	0.25	297,312,318,323	0
6	K	E	1104	1/1	0.77	0.11	333,333,333,333	0
7	NAG	F	303	14/15	0.81	0.15	276,290,303,310	0
6	K	A	1104	1/1	0.85	0.29	245,245,245,245	0
6	K	A	1105	1/1	0.87	0.09	171,171,171,171	0
3	MF4	E	1101	5/5	0.90	0.07	337,343,348,349	0
4	MG	E	1102	1/1	0.94	0.09	320,320,320,320	0
6	K	A	1106	1/1	0.95	0.05	179,179,179,179	0
3	MF4	A	1101	5/5	0.96	0.06	93,110,113,128	0
6	K	E	1105	1/1	0.99	0.03	170,170,170,170	0
4	MG	A	1102	1/1	1.00	0.06	80,80,80,80	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 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.