



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:10 AM UTC

PDB ID : 7W7B / pdb_00007w7b
Title : Heme exporter HrtBA in complex with protoporphyrin IX containing manganese(III), high resolution data
Authors : Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shirouzu, M.; Shiro, Y.
Deposited on : 2021-12-04
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

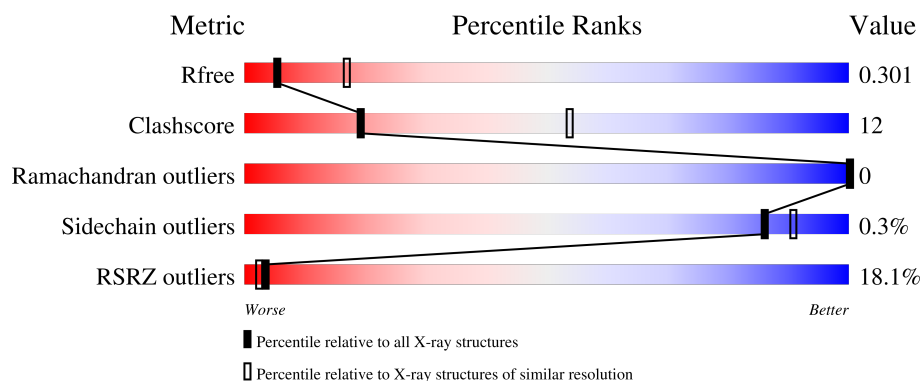
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	231	14% 71% 23% 6%
1	C	231	12% 63% 31% 6%
1	E	231	14% 71% 23% 6%
1	G	231	8% 67% 31% .
1	I	231	7% 72% 23% .

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Mol	Chain	Length	Quality of chain
1	K	231	6% 74% 21% 5%
2	B	344	21% 71% 28%
2	D	344	18% 75% 25%
2	F	344	17% 77% 22%
2	H	344	30% 74% 26%
2	J	344	28% 73% 26%
2	L	344	22% 80% 19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25131 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 Putative ABC transport system, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1618	1010	293	312	3			
1	C	218	Total	C	N	O	S	0	0	0
			1634	1019	296	316	3			
1	E	217	Total	C	N	O	S	0	0	0
			1629	1016	295	315	3			
1	G	225	Total	C	N	O	S	0	0	0
			1693	1059	307	324	3			
1	I	221	Total	C	N	O	S	0	0	0
			1652	1031	299	319	3			
1	K	219	Total	C	N	O	S	0	0	0
			1639	1022	297	317	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LYS	-	expression tag	UNP Q6NEF2
A	223	LEU	-	expression tag	UNP Q6NEF2
A	224	TRP	-	expression tag	UNP Q6NEF2
A	225	SER	-	expression tag	UNP Q6NEF2
A	226	HIS	-	expression tag	UNP Q6NEF2
A	227	PRO	-	expression tag	UNP Q6NEF2
A	228	GLN	-	expression tag	UNP Q6NEF2
A	229	PHE	-	expression tag	UNP Q6NEF2
A	230	GLU	-	expression tag	UNP Q6NEF2
A	231	LYS	-	expression tag	UNP Q6NEF2
C	222	LYS	-	expression tag	UNP Q6NEF2
C	223	LEU	-	expression tag	UNP Q6NEF2
C	224	TRP	-	expression tag	UNP Q6NEF2
C	225	SER	-	expression tag	UNP Q6NEF2
C	226	HIS	-	expression tag	UNP Q6NEF2
C	227	PRO	-	expression tag	UNP Q6NEF2
C	228	GLN	-	expression tag	UNP Q6NEF2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	229	PHE	-	expression tag	UNP Q6NEF2
C	230	GLU	-	expression tag	UNP Q6NEF2
C	231	LYS	-	expression tag	UNP Q6NEF2
E	222	LYS	-	expression tag	UNP Q6NEF2
E	223	LEU	-	expression tag	UNP Q6NEF2
E	224	TRP	-	expression tag	UNP Q6NEF2
E	225	SER	-	expression tag	UNP Q6NEF2
E	226	HIS	-	expression tag	UNP Q6NEF2
E	227	PRO	-	expression tag	UNP Q6NEF2
E	228	GLN	-	expression tag	UNP Q6NEF2
E	229	PHE	-	expression tag	UNP Q6NEF2
E	230	GLU	-	expression tag	UNP Q6NEF2
E	231	LYS	-	expression tag	UNP Q6NEF2
G	222	LYS	-	expression tag	UNP Q6NEF2
G	223	LEU	-	expression tag	UNP Q6NEF2
G	224	TRP	-	expression tag	UNP Q6NEF2
G	225	SER	-	expression tag	UNP Q6NEF2
G	226	HIS	-	expression tag	UNP Q6NEF2
G	227	PRO	-	expression tag	UNP Q6NEF2
G	228	GLN	-	expression tag	UNP Q6NEF2
G	229	PHE	-	expression tag	UNP Q6NEF2
G	230	GLU	-	expression tag	UNP Q6NEF2
G	231	LYS	-	expression tag	UNP Q6NEF2
I	222	LYS	-	expression tag	UNP Q6NEF2
I	223	LEU	-	expression tag	UNP Q6NEF2
I	224	TRP	-	expression tag	UNP Q6NEF2
I	225	SER	-	expression tag	UNP Q6NEF2
I	226	HIS	-	expression tag	UNP Q6NEF2
I	227	PRO	-	expression tag	UNP Q6NEF2
I	228	GLN	-	expression tag	UNP Q6NEF2
I	229	PHE	-	expression tag	UNP Q6NEF2
I	230	GLU	-	expression tag	UNP Q6NEF2
I	231	LYS	-	expression tag	UNP Q6NEF2
K	222	LYS	-	expression tag	UNP Q6NEF2
K	223	LEU	-	expression tag	UNP Q6NEF2
K	224	TRP	-	expression tag	UNP Q6NEF2
K	225	SER	-	expression tag	UNP Q6NEF2
K	226	HIS	-	expression tag	UNP Q6NEF2
K	227	PRO	-	expression tag	UNP Q6NEF2
K	228	GLN	-	expression tag	UNP Q6NEF2
K	229	PHE	-	expression tag	UNP Q6NEF2
K	230	GLU	-	expression tag	UNP Q6NEF2

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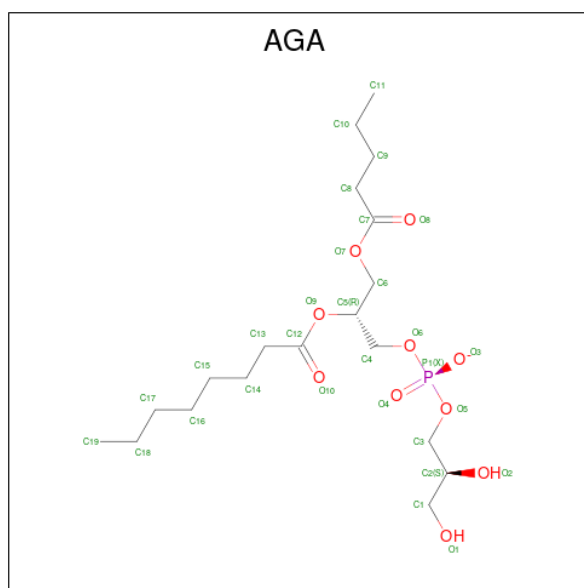
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Chain	Residue	Modelled	Actual	Comment	Reference
K	231	LYS	-	expression tag	UNP Q6NEF2

- Molecule 2 is a protein called Putative ABC transport system integral membrane protein.

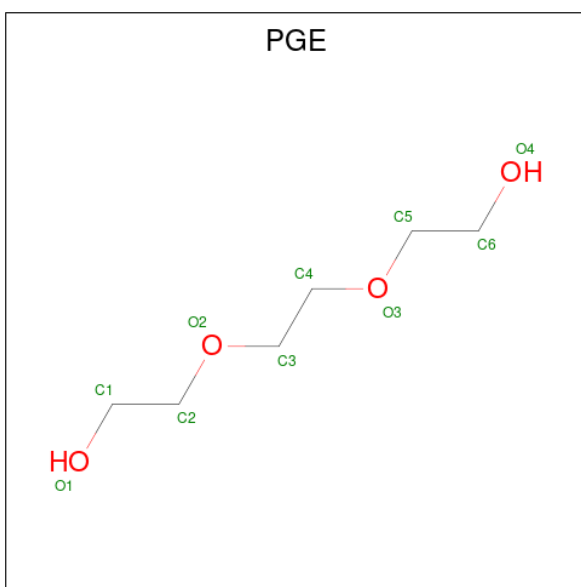
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	341	Total	C	N	O	S	0	1	0
			2518	1617	425	471	5			
2	D	343	Total	C	N	O	S	0	1	0
			2530	1624	427	474	5			
2	F	342	Total	C	N	O	S	0	1	0
			2523	1620	426	472	5			
2	H	341	Total	C	N	O	S	0	0	0
			2510	1612	422	471	5			
2	J	343	Total	C	N	O	S	0	1	0
			2530	1624	427	474	5			
2	L	343	Total	C	N	O	S	0	0	0
			2522	1619	424	474	5			

- Molecule 3 is (1S)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (CCD ID: AGA) (formula: C₁₉H₃₆O₁₀P).



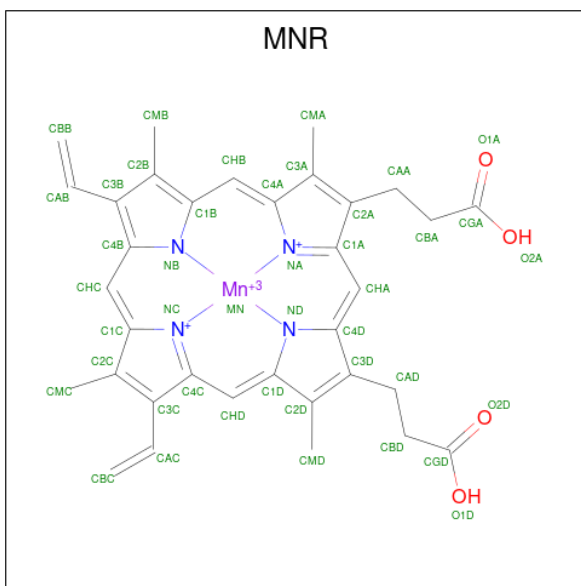
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			23	14	8	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



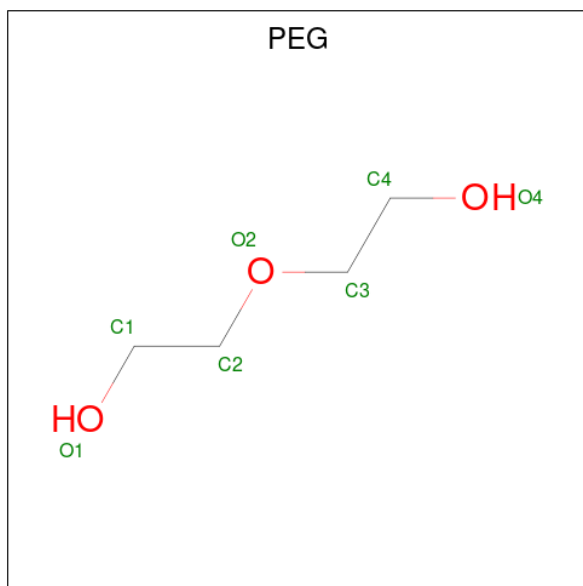
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O		0	0
			10	6	4			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING MN (CCD ID: MNR) (formula: $C_{34}H_{32}MnN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Mn	N	O	0
			43	34	1	4	4	
5	H	1	Total	C	Mn	N	O	0
			43	34	1	4	4	

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

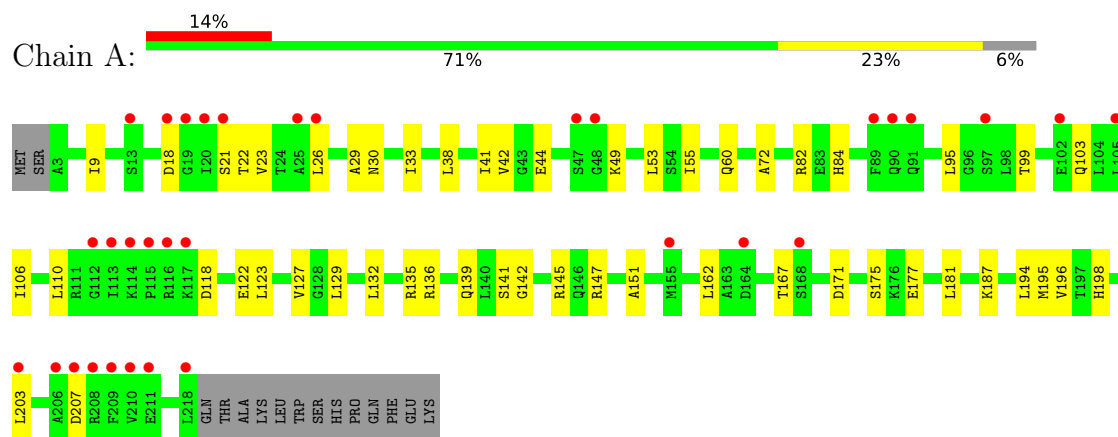


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			7	4	3		
6	H	1	Total	C	O	0	0
			7	4	3		

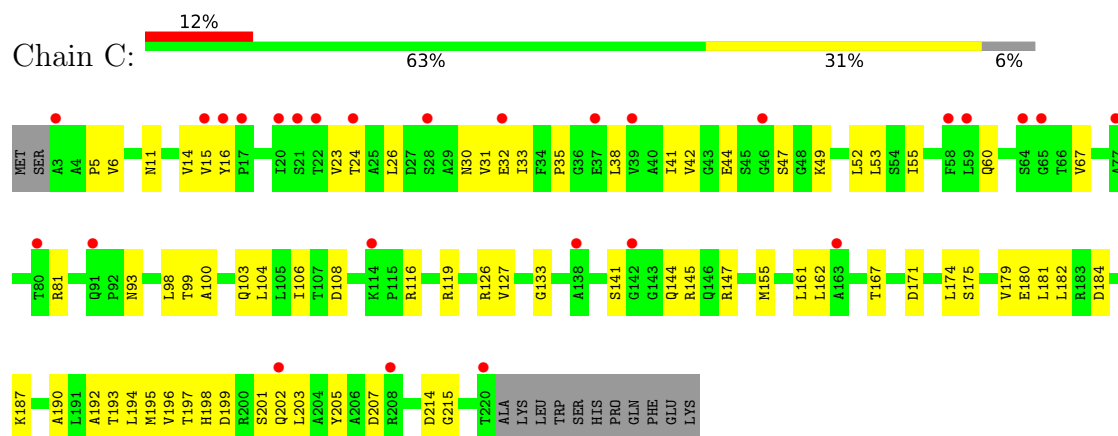
3 Residue-property plots [i](#)

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.

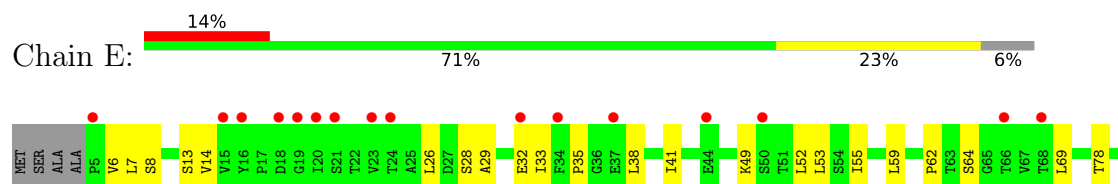
- Molecule 1: Putative ABC transport system, ATP-binding protein

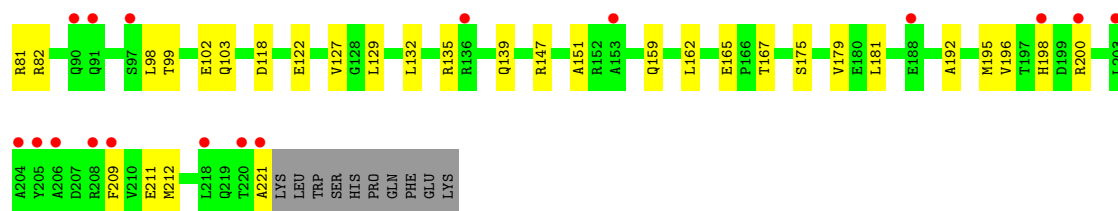


- Molecule 1: Putative ABC transport system, ATP-binding protein

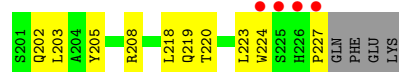
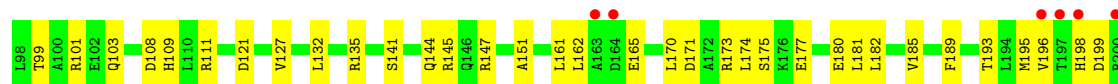


- Molecule 1: Putative ABC transport system, ATP-binding protein

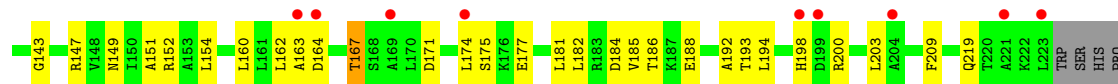




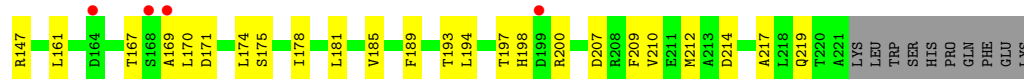
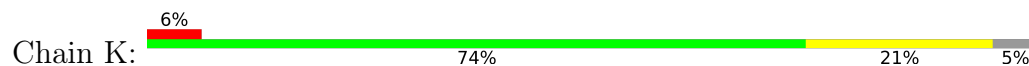
- Molecule 1: Putative ABC transport system, ATP-binding protein



- Molecule 1: Putative ABC transport system, ATP-binding protein

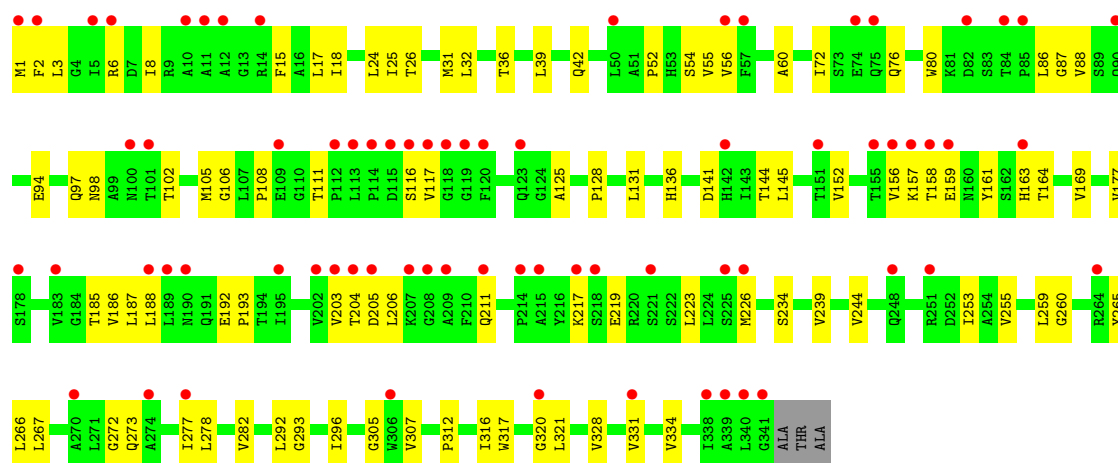


- Molecule 1: Putative ABC transport system, ATP-binding protein

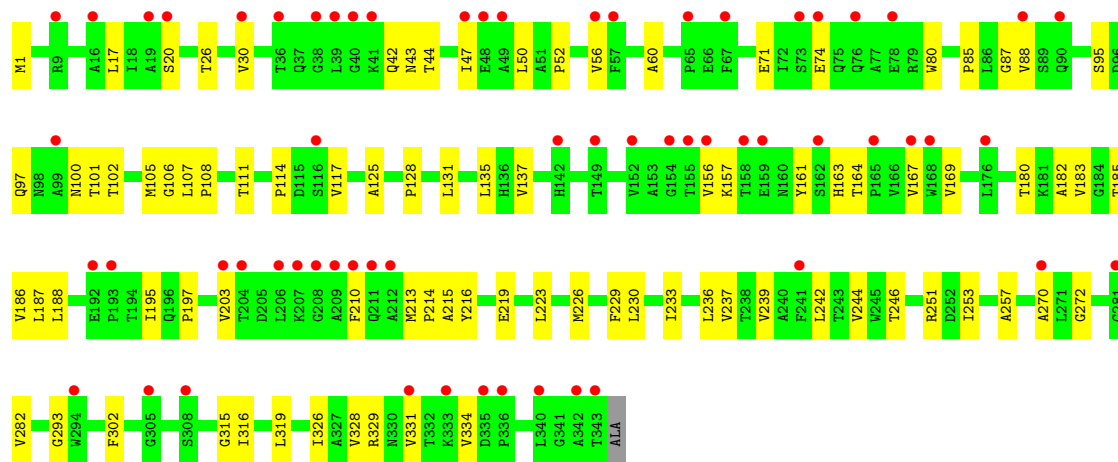
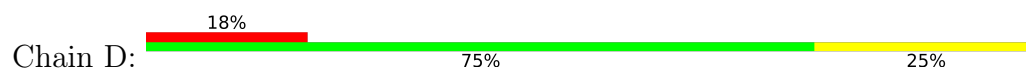


- Molecule 2: Putative ABC transport system integral membrane protein

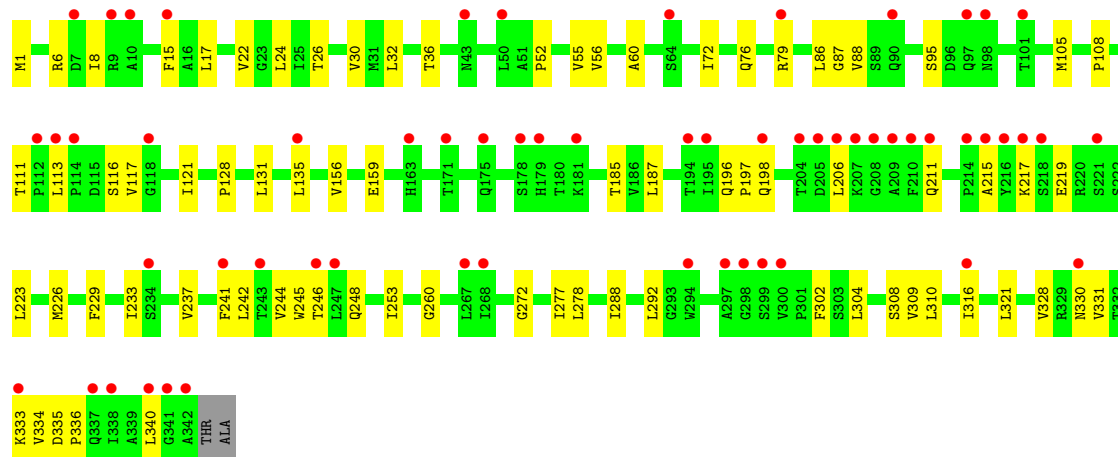
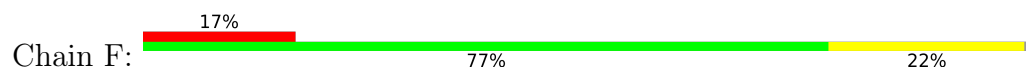


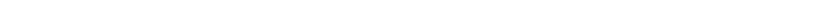


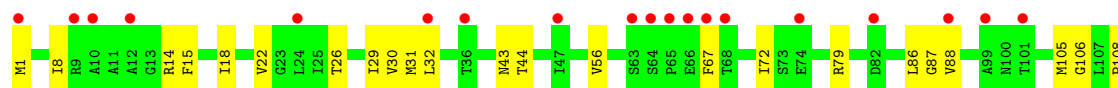
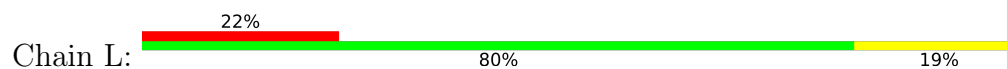
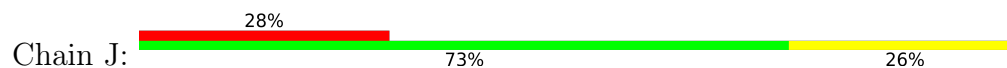
• Molecule 2: Putative ABC transport system integral membrane protein

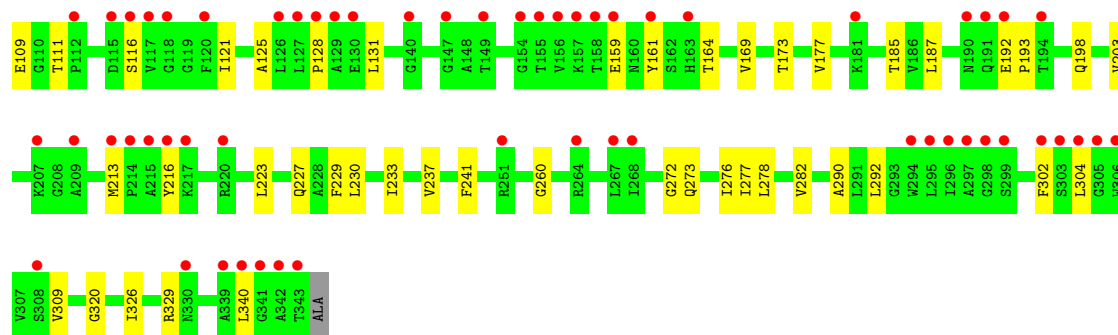


• Molecule 2: Putative ABC transport system integral membrane protein



- Chain H:  30% 74% 26%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.00Å 133.49Å 159.34Å 111.65° 99.69° 94.64°	Depositor
Resolution (Å)	49.39 – 3.00 49.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.39-3.00) 80.4 (49.39-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.266 , 0.299 0.267 , 0.301	Depositor DCC
R_{free} test set	3813 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	25131	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGA, PGE, MNR, PEG

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	0/1637	0.52	0/2216
1	C	0.19	0/1653	0.50	0/2238
1	E	0.16	0/1648	0.45	0/2230
1	G	0.19	0/1716	0.45	0/2325
1	I	0.19	0/1671	0.48	0/2263
1	K	0.20	0/1658	0.52	0/2245
2	B	0.16	0/2567	0.47	0/3509
2	D	0.21	0/2579	0.49	0/3526
2	F	0.15	0/2572	0.45	0/3516
2	H	0.16	0/2556	0.48	0/3495
2	J	0.16	0/2579	0.45	0/3526
2	L	0.16	0/2568	0.45	0/3512
All	All	0.18	0/25404	0.47	0/34601

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	1618	0	1664	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1634	0	1679	54	0
1	E	1629	0	1675	39	0
1	G	1693	0	1737	47	0
1	I	1652	0	1697	45	0
1	K	1639	0	1684	36	0
2	B	2518	0	2601	78	0
2	D	2530	0	2613	63	0
2	F	2523	0	2606	59	0
2	H	2510	0	2588	66	0
2	J	2530	0	2613	62	0
2	L	2522	0	2600	44	0
3	B	23	0	19	2	0
4	B	10	0	14	1	0
5	D	43	0	30	6	0
5	H	43	0	30	6	0
6	D	7	0	10	0	0
6	H	7	0	10	0	0
All	All	25131	0	25870	595	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 12.

All (595) 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:F:79:ARG:HH12	2:F:198:GLN:HB2	1.31	0.93
1:I:198:HIS:HB3	1:K:198:HIS:CE1	2.07	0.90
1:A:53:LEU:HD11	1:A:162:LEU:HB3	1.56	0.87
1:E:59:LEU:HD13	2:F:340:LEU:HD11	1.55	0.86
1:E:127:VAL:HG13	1:E:181:LEU:HD21	1.58	0.86
1:E:53:LEU:HD11	1:E:162:LEU:HB3	1.60	0.83
2:F:304:LEU:HD21	2:F:309:VAL:HG23	1.59	0.82
2:D:253:ILE:HD13	2:D:331:VAL:HG23	1.63	0.81
2:H:180:THR:HG22	2:H:182:ALA:H	1.46	0.80
2:H:86:LEU:HD21	2:H:105:MET:HE2	1.64	0.80
1:I:132:LEU:HB3	1:I:135:ARG:HD3	1.62	0.79
2:B:253:ILE:HD13	2:B:331:VAL:HG23	1.64	0.79
1:K:55:ILE:HG23	1:K:67:VAL:HG21	1.64	0.79
1:G:127:VAL:HG13	1:G:181:LEU:HD21	1.64	0.78
1:I:127:VAL:HG13	1:I:181:LEU:HD21	1.66	0.77
1:A:127:VAL:HG13	1:A:181:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:PRO:HG3	2:H:203:VAL:HG11	1.68	0.76
2:L:79:ARG:HH12	2:L:198:GLN:HB2	1.50	0.75
1:I:95:LEU:O	1:I:103:GLN:NE2	2.20	0.74
2:B:72:ILE:HG12	2:B:187:LEU:HG	1.70	0.74
1:C:104:LEU:HB3	1:C:155:MET:HG3	1.69	0.73
1:G:53:LEU:HD11	1:G:162:LEU:HB3	1.70	0.73
1:K:41:ILE:HD11	1:K:194:LEU:HD22	1.71	0.72
1:E:49:LYS:HD2	1:E:196:VAL:HG13	1.72	0.72
2:H:56:VAL:HG22	2:H:203:VAL:HG22	1.72	0.71
2:D:185:THR:HG23	2:D:186:VAL:HG23	1.72	0.71
2:D:180:THR:HG22	2:D:182:ALA:H	1.56	0.71
1:G:55:ILE:HG22	1:G:67:VAL:HG21	1.73	0.71
1:C:53:LEU:HD11	1:C:162:LEU:HB3	1.73	0.70
2:H:88:VAL:HG22	2:H:105:MET:HG2	1.73	0.70
2:F:253:ILE:HD13	2:F:331:VAL:HG23	1.74	0.70
1:E:14:VAL:HG23	1:E:55:ILE:HD11	1.73	0.69
2:J:253:ILE:HD13	2:J:331:VAL:HG13	1.73	0.69
1:G:7:LEU:HB3	1:G:33:ILE:HG22	1.73	0.69
2:B:305:GLY:HA2	4:B:502:PGE:H2	1.74	0.69
1:K:132:LEU:HD22	1:K:135:ARG:HE	1.57	0.69
2:H:42:GLN:HG3	2:H:163:HIS:HA	1.72	0.69
1:E:7:LEU:HD23	1:E:33:ILE:HD13	1.75	0.68
2:D:108:PRO:HG2	2:D:111:THR:HG21	1.74	0.68
2:B:42:GLN:HG3	2:B:163:HIS:HA	1.74	0.68
2:B:26:THR:HG21	2:B:282:VAL:HG22	1.74	0.68
2:D:56:VAL:HG22	2:D:203:VAL:HG22	1.75	0.67
1:C:127:VAL:HG13	1:C:181:LEU:HD21	1.76	0.67
1:C:14:VAL:HG23	1:C:55:ILE:HD11	1.75	0.67
1:G:51:THR:O	1:G:55:ILE:HG12	1.96	0.66
2:F:1:MET:HE2	2:F:272:GLY:HA3	1.76	0.66
2:L:326:ILE:O	2:L:329:ARG:NH1	2.26	0.66
1:K:42:VAL:HG11	1:K:200:ARG:HE	1.60	0.66
2:B:31:MET:HE1	2:B:292:LEU:HB2	1.78	0.66
1:A:33:ILE:HD11	1:A:194:LEU:HG	1.76	0.66
1:C:55:ILE:HG23	1:C:67:VAL:HG21	1.76	0.65
1:A:171:ASP:HB2	1:C:214:ASP:OD1	1.97	0.65
1:C:47:SER:O	1:C:215:GLY:N	2.24	0.65
2:H:41:LYS:NZ	2:H:48:GLU:OE1	2.30	0.65
2:F:304:LEU:CD2	2:F:309:VAL:HG23	2.26	0.65
2:B:223:LEU:HD21	5:D:401:MNR:HMB3	1.78	0.64
1:G:108:ASP:OD1	1:G:111:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:LEU:HD12	2:H:227:GLN:HG2	1.79	0.64
2:H:108:PRO:HD2	2:H:111:THR:HG21	1.80	0.64
1:I:182:LEU:O	1:I:186:THR:HG23	1.98	0.64
2:L:44:THR:HA	2:L:213:MET:HE1	1.80	0.64
1:K:82:ARG:HB2	2:L:260:GLY:HA3	1.80	0.63
2:D:326:ILE:O	2:D:329:ARG:NH1	2.29	0.63
1:G:73:GLU:HG2	1:K:84:HIS:HE1	1.62	0.63
2:D:102:THR:HG21	2:D:131:LEU:HD22	1.81	0.63
1:A:167:THR:HB	1:A:175:SER:HB3	1.81	0.63
2:B:1:MET:HE1	2:B:272:GLY:HA3	1.81	0.62
2:D:156:VAL:HG12	2:D:157:LYS:H	1.64	0.62
2:H:125:ALA:HA	2:H:169:VAL:HG12	1.81	0.62
2:H:253:ILE:HG22	2:H:334:VAL:HG11	1.82	0.62
2:F:32:LEU:O	2:F:36:THR:HG23	1.99	0.62
2:L:72:ILE:HG12	2:L:187:LEU:HG	1.81	0.62
2:B:226:MET:HE1	2:D:226:MET:HE1	1.80	0.61
2:F:226:MET:HE1	2:H:226:MET:SD	2.40	0.61
2:B:128:PRO:HB3	2:B:158:THR:HG22	1.81	0.61
2:L:8:ILE:HD11	2:L:273:GLN:HG3	1.82	0.61
1:K:127:VAL:HG13	1:K:181:LEU:HD21	1.80	0.61
2:B:219:GLU:HB2	5:D:401:MNR:C2C	2.30	0.61
1:A:187:LYS:NZ	1:A:207:ASP:OD2	2.29	0.60
2:D:42:GLN:HG3	2:D:163:HIS:HA	1.83	0.60
2:F:196:GLN:HG3	2:F:197:PRO:HD2	1.82	0.60
2:D:74:GLU:HG3	2:D:183:VAL:HG21	1.83	0.60
2:D:26:THR:HG21	2:D:282:VAL:HG22	1.82	0.60
2:F:246:THR:HG21	2:F:328:VAL:HG22	1.84	0.60
2:J:72:ILE:HG12	2:J:187:LEU:HG	1.83	0.60
1:I:7:LEU:HB3	1:I:33:ILE:HG22	1.84	0.60
2:B:239:VAL:HG12	2:D:17:LEU:HD21	1.83	0.60
2:H:117:VAL:HG13	2:H:156:VAL:HB	1.84	0.60
1:K:55:ILE:CG2	1:K:67:VAL:HG21	2.32	0.59
2:B:97:GLN:HG3	2:B:136:HIS:HB2	1.84	0.59
1:C:81:ARG:NH1	2:D:257:ALA:O	2.29	0.59
2:H:26:THR:HG21	2:H:282:VAL:HG22	1.83	0.59
2:J:32:LEU:O	2:J:36:THR:HG23	2.02	0.59
2:F:86:LEU:HD21	2:F:105:MET:HE2	1.85	0.59
2:B:253:ILE:HG22	2:B:334:VAL:HG11	1.84	0.59
2:F:223:LEU:HD21	5:H:401:MNR:HMB2	1.85	0.59
1:A:44:GLU:OE1	1:A:198:HIS:NE2	2.35	0.59
2:J:80:TRP:HA	2:J:195:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:SER:OG	2:H:76:GLN:HB2	2.03	0.58
2:D:125:ALA:HA	2:D:169:VAL:HG12	1.85	0.58
2:B:156:VAL:HG12	2:B:157:LYS:N	2.18	0.58
2:J:92:ARG:NH1	2:J:94:GLU:OE1	2.36	0.58
2:L:116:SER:OG	2:L:159:GLU:OE2	2.22	0.58
1:G:10:THR:HG21	1:K:73:GLU:HG2	1.86	0.58
2:B:17:LEU:HD21	2:D:239:VAL:HG12	1.86	0.58
2:B:219:GLU:HB2	5:D:401:MNR:C1C	2.34	0.57
1:I:33:ILE:HG12	1:I:192:ALA:HB1	1.86	0.57
1:A:127:VAL:O	1:A:147:ARG:HD3	2.05	0.57
1:C:141:SER:OG	1:C:144:GLN:HG3	2.05	0.57
1:E:26:LEU:HD11	1:E:29:ALA:HB2	1.87	0.57
1:C:190:ALA:HB1	1:K:66:THR:HG23	1.85	0.57
1:G:141:SER:O	1:G:145:ARG:HG3	2.04	0.57
2:H:32:LEU:O	2:H:36:THR:HG23	2.05	0.57
1:I:126:ARG:NH2	1:I:188:GLU:OE1	2.36	0.57
2:B:94:GLU:HB3	2:B:144:THR:HB	1.86	0.57
2:F:26:THR:HG22	2:F:316:ILE:HG21	1.87	0.57
1:I:55:ILE:HG22	1:I:67:VAL:HG21	1.87	0.56
2:J:205:ASP:OD1	2:J:206:LEU:N	2.34	0.56
2:J:326:ILE:O	2:J:329:ARG:NH1	2.37	0.56
2:H:137:VAL:HG13	2:H:141:ASP:HB2	1.87	0.56
2:B:36:THR:HG22	2:B:223:LEU:HB3	1.87	0.56
1:K:212:MET:HG2	1:K:217:ALA:HA	1.87	0.56
2:J:245:TRP:NE1	2:J:273:GLN:OE1	2.38	0.56
2:B:116:SER:OG	2:B:159:GLU:OE2	2.24	0.56
1:C:141:SER:O	1:C:145:ARG:HG3	2.06	0.56
2:B:145:LEU:HG	2:B:177:VAL:HG11	1.88	0.56
2:D:80:TRP:HA	2:D:195:ILE:HD13	1.88	0.55
1:C:33:ILE:HG22	1:C:192:ALA:HB1	1.88	0.55
1:K:141:SER:OG	1:K:144:GLN:HG3	2.07	0.55
2:F:302:PHE:CE2	2:F:304:LEU:HD12	2.41	0.55
2:F:108:PRO:HG2	2:F:111:THR:HG21	1.89	0.55
2:H:94:GLU:HG3	2:H:99:ALA:HB2	1.89	0.55
2:H:335:ASP:OD1	2:H:336:PRO:HD2	2.07	0.55
1:I:127:VAL:HG12	1:I:147:ARG:HB3	1.88	0.55
2:B:86:LEU:HD22	2:B:188:LEU:HD11	1.89	0.55
2:F:244:VAL:HG12	2:H:244:VAL:HG12	1.88	0.55
2:L:125:ALA:HA	2:L:169:VAL:HG12	1.88	0.54
1:K:127:VAL:HG12	1:K:147:ARG:HB3	1.89	0.54
2:L:87:GLY:O	2:L:105:MET:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:PRO:HD2	2:L:111:THR:HG21	1.89	0.54
1:A:123:LEU:O	1:A:127:VAL:HG23	2.06	0.54
1:A:198:HIS:O	1:A:198:HIS:ND1	2.40	0.54
1:C:41:ILE:HD13	1:C:52:LEU:HD23	1.89	0.54
1:C:44:GLU:OE2	1:C:198:HIS:NE2	2.40	0.54
2:J:59:THR:N	2:J:200:ASN:O	2.36	0.54
1:K:40:ALA:HB3	1:K:209:PHE:HB3	1.89	0.54
1:C:41:ILE:CD1	1:C:194:LEU:HD11	2.37	0.54
1:E:49:LYS:NZ	1:E:165:GLU:OE2	2.39	0.54
2:L:302:PHE:CE1	2:L:304:LEU:HD13	2.42	0.54
1:E:13:SER:OG	1:E:28:SER:N	2.26	0.54
2:J:116:SER:OG	2:J:159:GLU:OE2	2.24	0.54
2:D:26:THR:HG22	2:D:316:ILE:HD13	1.89	0.54
1:I:107:THR:O	1:I:111:ARG:HG3	2.08	0.54
2:J:186:VAL:HG12	2:J:187:LEU:N	2.23	0.54
2:B:55:VAL:O	2:B:204:THR:HG22	2.08	0.54
1:C:15:VAL:HG22	1:C:24:THR:HA	1.89	0.54
2:D:100:ASN:OD1	2:D:101:THR:N	2.40	0.54
2:D:186:VAL:HG12	2:D:187:LEU:N	2.23	0.54
1:A:147:ARG:NH2	1:A:177:GLU:OE1	2.40	0.53
2:H:197:PRO:HB2	2:H:201:GLU:HB2	1.89	0.53
1:K:14:VAL:CG2	1:K:55:ILE:HD11	2.38	0.53
1:C:127:VAL:HG11	1:C:147:ARG:O	2.09	0.53
2:J:95:SER:HB3	2:J:135:LEU:HD13	1.89	0.53
2:L:290:ALA:HB2	2:L:309:VAL:HG21	1.89	0.53
2:F:72:ILE:HG23	2:F:76:GLN:HB3	1.91	0.53
1:I:11:ASN:O	1:I:65:GLY:HA3	2.08	0.53
1:I:203:LEU:HB3	1:I:209:PHE:CE1	2.43	0.53
2:J:15:PHE:CD1	2:J:277:ILE:HG13	2.43	0.53
2:J:26:THR:HG22	2:J:316:ILE:HD13	1.89	0.53
1:E:6:VAL:O	1:E:69:LEU:HD12	2.08	0.53
1:E:14:VAL:CG2	1:E:55:ILE:HD11	2.38	0.53
1:A:42:VAL:HG21	1:A:203:LEU:HD11	1.91	0.53
2:F:24:LEU:HD12	2:H:236:LEU:HD12	1.89	0.53
1:I:51:THR:O	1:I:55:ILE:HG12	2.09	0.53
1:A:127:VAL:HG21	1:A:151:ALA:HB2	1.91	0.53
1:C:108:ASP:OD2	1:C:116:ARG:HG2	2.08	0.53
1:E:129:LEU:HD22	1:E:132:LEU:HD12	1.91	0.53
1:I:200:ARG:HA	1:I:203:LEU:HG	1.91	0.53
1:C:93:ASN:OD1	2:D:251:ARG:NH2	2.35	0.53
1:C:42:VAL:CG2	1:C:203:LEU:HD21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1:MET:HE1	2:J:276:ILE:HD11	1.91	0.52
2:F:72:ILE:HG12	2:F:187:LEU:HG	1.90	0.52
2:H:128:PRO:HG2	2:H:131:LEU:HB3	1.91	0.52
2:B:36:THR:HG22	2:B:223:LEU:HD13	1.91	0.52
2:B:52:PRO:HD2	2:B:206:LEU:HD13	1.90	0.52
2:B:117:VAL:HG13	2:B:156:VAL:HG11	1.92	0.52
2:D:186:VAL:HG12	2:D:187:LEU:H	1.75	0.52
1:A:9:ILE:O	1:A:30:ASN:HA	2.08	0.52
2:D:161:TYR:O	2:D:164:THR:OG1	2.26	0.52
1:K:127:VAL:HG11	1:K:147:ARG:O	2.09	0.52
2:J:26:THR:HG21	2:J:282:VAL:HG22	1.91	0.52
2:F:52:PRO:HD2	2:F:206:LEU:HD13	1.92	0.52
2:H:36:THR:HG22	2:H:223:LEU:HD13	1.92	0.52
2:J:278:LEU:HD13	2:J:320:GLY:HA3	1.92	0.52
2:B:24:LEU:HD12	2:D:236:LEU:HD12	1.91	0.52
1:G:171:ASP:OD1	1:G:174:LEU:HB2	2.10	0.52
2:F:241:PHE:HD2	2:F:242:LEU:HD22	1.74	0.51
2:J:113:LEU:HD21	2:J:121:ILE:HD11	1.92	0.51
2:L:26:THR:HG21	2:L:282:VAL:HG22	1.90	0.51
1:A:41:ILE:HD11	1:A:194:LEU:HD22	1.92	0.51
2:F:17:LEU:HD21	2:H:239:VAL:HG12	1.91	0.51
1:G:199:ASP:OD2	1:G:202:GLN:HG3	2.11	0.51
2:L:15:PHE:CD1	2:L:277:ILE:HG13	2.46	0.51
2:F:302:PHE:CZ	2:F:304:LEU:HD12	2.45	0.51
2:H:104:VAL:HG22	2:H:167:VAL:HB	1.92	0.51
2:J:25:ILE:HG21	2:J:234:SER:HB3	1.90	0.51
2:J:117:VAL:HG13	2:J:156:VAL:HB	1.91	0.51
1:A:95:LEU:O	1:A:103:GLN:NE2	2.43	0.51
2:B:32:LEU:O	2:B:36:THR:HG23	2.10	0.51
1:I:55:ILE:CG2	1:I:67:VAL:HG21	2.41	0.51
1:K:21:SER:OG	1:K:22:THR:N	2.43	0.51
1:K:95:LEU:O	1:K:103:GLN:NE2	2.44	0.51
2:H:145:LEU:HG	2:H:177:VAL:HG11	1.93	0.51
1:I:132:LEU:HD22	1:I:135:ARG:HH11	1.76	0.51
2:J:161:TYR:O	2:J:164:THR:OG1	2.29	0.51
2:H:161:TYR:O	2:H:164:THR:OG1	2.27	0.51
1:A:129:LEU:HD22	1:A:132:LEU:HD12	1.91	0.50
1:A:135:ARG:HD2	1:A:139:GLN:HB3	1.93	0.50
2:H:86:LEU:O	2:H:185:THR:HG22	2.11	0.50
2:B:205:ASP:OD1	2:B:206:LEU:N	2.43	0.50
1:C:119:ARG:NH1	1:C:155:MET:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:GLU:H	1:I:73:GLU:CD	2.16	0.50
1:E:82:ARG:NH1	2:F:260:GLY:O	2.44	0.50
1:E:127:VAL:HG21	1:E:151:ALA:HB2	1.93	0.50
2:L:106:GLY:HA2	2:L:169:VAL:O	2.12	0.50
1:A:21:SER:OG	1:A:22:THR:N	2.44	0.50
2:L:14:ARG:O	2:L:18:ILE:HG13	2.12	0.50
1:C:42:VAL:HG21	1:C:203:LEU:HD21	1.94	0.50
1:E:41:ILE:HD13	1:E:52:LEU:HD23	1.93	0.50
1:I:171:ASP:HB2	1:K:214:ASP:OD1	2.11	0.50
2:D:17:LEU:O	2:D:20:SER:OG	2.24	0.50
2:F:304:LEU:HD23	2:F:308:SER:HB3	1.93	0.50
2:B:211:GLN:HG2	2:B:217:LYS:HD2	1.93	0.50
1:C:126:ARG:HH22	1:C:184:ASP:HB3	1.77	0.50
1:C:167:THR:HB	1:C:175:SER:HB3	1.94	0.50
1:C:198:HIS:O	1:C:198:HIS:ND1	2.35	0.50
1:E:6:VAL:HG11	1:E:159:GLN:O	2.12	0.50
1:E:33:ILE:HG22	1:E:192:ALA:HB1	1.94	0.50
1:E:135:ARG:NH2	1:E:139:GLN:O	2.43	0.50
2:H:86:LEU:HD11	2:H:105:MET:HB3	1.94	0.50
2:L:31:MET:HE1	2:L:292:LEU:HD23	1.94	0.50
1:E:175:SER:O	1:E:179:VAL:HG23	2.12	0.50
2:L:56:VAL:HG22	2:L:203:VAL:HG22	1.93	0.50
2:B:328:VAL:O	2:B:331:VAL:HG12	2.12	0.50
1:G:41:ILE:HB	1:G:196:VAL:HG22	1.92	0.50
2:H:197:PRO:HG3	2:H:203:VAL:HG23	1.94	0.50
2:D:328:VAL:HG12	2:D:328:VAL:O	2.12	0.49
1:G:101:ARG:HD3	1:G:121:ASP:OD1	2.12	0.49
1:I:203:LEU:HB3	1:I:209:PHE:HE1	1.77	0.49
2:H:26:THR:HG22	2:H:316:ILE:HD13	1.93	0.49
2:B:108:PRO:HD2	2:B:111:THR:HG21	1.92	0.49
2:B:128:PRO:HD2	2:B:131:LEU:HD23	1.95	0.49
2:B:317:TRP:CH2	2:B:321:LEU:HD11	2.47	0.49
1:E:14:VAL:HG22	1:E:62:PRO:HA	1.94	0.49
2:F:211:GLN:HG3	2:F:217:LYS:HD2	1.94	0.49
1:I:41:ILE:HD11	1:I:194:LEU:HD22	1.95	0.49
1:E:99:THR:O	1:E:103:GLN:HG2	2.11	0.49
2:D:108:PRO:HG2	2:D:111:THR:CG2	2.41	0.49
2:L:1:MET:SD	2:L:272:GLY:HA3	2.52	0.49
1:C:49:LYS:HB3	1:C:196:VAL:HG13	1.95	0.49
2:D:71:GLU:OE2	2:D:180:THR:HG21	2.13	0.49
2:F:335:ASP:OD1	2:F:336:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ILE:CG2	1:G:67:VAL:HG21	2.40	0.49
1:I:149:ASN:ND2	1:I:152:ARG:HH21	2.11	0.49
2:B:72:ILE:HG23	2:B:76:GLN:HB3	1.94	0.49
2:J:14:ARG:O	2:J:18:ILE:HG13	2.12	0.49
1:A:141:SER:O	1:A:145:ARG:HG3	2.12	0.48
2:B:267:LEU:HD12	2:B:328:VAL:HG12	1.94	0.48
1:I:7:LEU:HD22	1:I:160:LEU:HD21	1.94	0.48
2:J:135:LEU:HB2	2:J:137:VAL:HG22	1.95	0.48
1:C:31:VAL:HG21	1:C:52:LEU:HD21	1.94	0.48
2:D:87:GLY:O	2:D:105:MET:HA	2.12	0.48
2:F:26:THR:HG22	2:F:316:ILE:HD13	1.95	0.48
2:F:116:SER:OG	2:F:159:GLU:OE2	2.31	0.48
2:J:76:GLN:HE21	2:J:201:GLU:HG2	1.78	0.48
2:B:88:VAL:HG22	2:B:105:MET:HG2	1.94	0.48
2:L:86:LEU:HD21	2:L:105:MET:HE2	1.96	0.48
1:I:143:GLY:O	1:I:147:ARG:HG3	2.13	0.48
2:B:312:PRO:HD3	3:B:501:AGA:H131	1.95	0.48
1:I:200:ARG:HG2	1:I:203:LEU:HD11	1.96	0.48
2:B:307:VAL:HG12	3:B:501:AGA:H41	1.95	0.48
1:E:102:GLU:OE2	2:F:6:ARG:NH1	2.47	0.48
2:H:93:ILE:HA	2:H:144:THR:O	2.14	0.48
2:J:55:VAL:O	2:J:204:THR:HG22	2.13	0.48
1:A:72:ALA:HB2	1:A:84:HIS:CD2	2.49	0.48
2:B:87:GLY:HA2	2:B:185:THR:H	1.79	0.48
1:I:81:ARG:HG2	1:I:87:PHE:HZ	1.79	0.48
1:A:49:LYS:HB3	1:A:196:VAL:HG13	1.96	0.47
1:A:99:THR:HG22	1:A:136:ARG:HG2	1.94	0.47
1:G:109:HIS:HD1	2:H:265:TYR:HE1	1.60	0.47
1:C:26:LEU:HD23	1:C:55:ILE:HD12	1.96	0.47
1:G:165:GLU:OE2	1:G:198:HIS:NE2	2.46	0.47
1:A:18:ASP:CG	1:C:141:SER:HB2	2.38	0.47
2:B:185:THR:HG23	2:B:186:VAL:HG22	1.97	0.47
2:H:47:ILE:HD12	2:H:213:MET:HE3	1.96	0.47
2:F:229:PHE:O	2:F:233:ILE:HG13	2.15	0.47
1:I:53:LEU:HD21	1:I:164:ASP:HB2	1.95	0.47
2:L:161:TYR:O	2:L:164:THR:OG1	2.28	0.47
2:B:25:ILE:HG21	2:B:234:SER:HB3	1.95	0.47
1:A:55:ILE:HD13	1:A:60:GLN:O	2.15	0.47
1:C:187:LYS:NZ	1:C:207:ASP:OD2	2.42	0.47
2:J:231:TYR:O	2:J:234:SER:OG	2.27	0.47
2:J:245:TRP:O	2:J:249:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:TYR:HE1	1:C:60:GLN:HE22	1.63	0.47
1:E:38:LEU:HD21	1:E:195:MET:HE3	1.97	0.47
2:F:229:PHE:HE1	2:H:27:LEU:HD23	1.80	0.47
2:H:112:PRO:HA	2:H:120:PHE:CD1	2.49	0.47
2:H:223:LEU:HD21	5:H:401:MNR:HMB1	1.97	0.47
1:I:127:VAL:CG1	1:I:147:ARG:HB3	2.44	0.47
1:C:104:LEU:HB3	1:C:155:MET:CG	2.42	0.47
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.65	0.47
1:G:15:VAL:H	1:G:63:THR:HG21	1.80	0.47
1:G:127:VAL:HG21	1:G:151:ALA:HB2	1.97	0.47
1:G:18:ASP:HB2	1:G:23:VAL:CG1	2.45	0.47
1:K:95:LEU:N	1:K:103:GLN:HE22	2.13	0.47
2:B:117:VAL:HG13	2:B:156:VAL:CG1	2.45	0.46
2:B:87:GLY:O	2:B:105:MET:HA	2.15	0.46
2:D:88:VAL:HG22	2:D:105:MET:HG2	1.97	0.46
2:H:137:VAL:HG11	2:H:152:VAL:HG21	1.98	0.46
1:I:167:THR:HB	1:I:175:SER:HB3	1.97	0.46
1:E:127:VAL:HG12	1:E:147:ARG:HB3	1.96	0.46
2:F:223:LEU:HD21	5:H:401:MNR:CMB	2.45	0.46
2:H:53:HIS:HD2	2:H:192:GLU:HA	1.80	0.46
2:J:128:PRO:HG3	2:J:165:PRO:HB2	1.97	0.46
2:J:189:LEU:HD13	2:J:193:PRO:HB3	1.97	0.46
1:A:26:LEU:HD11	1:A:29:ALA:HB2	1.98	0.46
2:D:128:PRO:HD2	2:D:167:VAL:HG22	1.96	0.46
2:H:53:HIS:N	2:H:189:LEU:O	2.42	0.46
2:L:56:VAL:HB	2:L:187:LEU:HB2	1.98	0.46
1:E:118:ASP:O	1:E:122:GLU:HG3	2.14	0.46
1:I:88:VAL:HB	1:I:163:ALA:HA	1.98	0.46
2:J:29:ILE:CG1	2:J:230:LEU:HB3	2.46	0.46
2:J:74:GLU:HG2	2:J:183:VAL:HG13	1.98	0.46
2:L:29:ILE:HD11	2:L:230:LEU:HB2	1.98	0.46
2:B:161:TYR:O	2:B:164:THR:OG1	2.33	0.46
1:C:180:GLU:HG2	1:C:205:TYR:CE1	2.50	0.46
1:G:208:ARG:NH2	1:G:219:GLN:OE1	2.49	0.46
1:C:98:LEU:HD11	1:C:106:ILE:HD12	1.98	0.46
1:G:38:LEU:HD11	1:G:195:MET:HE2	1.96	0.46
1:I:126:ARG:HH22	1:I:184:ASP:CG	2.23	0.46
2:J:18:ILE:HG12	2:J:241:PHE:CD1	2.51	0.46
2:J:29:ILE:HG12	2:J:230:LEU:HB3	1.97	0.46
1:K:41:ILE:HG22	1:K:49:LYS:HG2	1.97	0.46
1:A:18:ASP:HB2	1:A:23:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:SER:OG	1:G:144:GLN:HG3	2.15	0.46
1:G:218:LEU:HG	1:G:220:THR:HG23	1.97	0.46
1:I:154:LEU:HD11	1:I:185:VAL:HG11	1.98	0.46
2:B:56:VAL:HB	2:B:187:LEU:HB2	1.98	0.46
1:C:11:ASN:N	1:C:30:ASN:OD1	2.48	0.46
2:D:223:LEU:HD23	2:D:226:MET:HE2	1.97	0.46
2:F:309:VAL:HG12	2:F:310:LEU:HD23	1.97	0.46
1:G:59:LEU:HD12	2:H:340:LEU:HD11	1.98	0.46
2:D:43:ASN:HD22	2:D:216:TYR:HA	1.80	0.45
2:D:253:ILE:HG22	2:D:334:VAL:HG11	1.97	0.45
2:F:241:PHE:CE1	2:H:244:VAL:HG21	2.51	0.45
1:G:72:ALA:HB2	1:G:84:HIS:CD2	2.51	0.45
2:L:223:LEU:O	2:L:227:GLN:HG3	2.16	0.45
2:F:8:ILE:HA	2:F:15:PHE:CD2	2.51	0.45
1:G:127:VAL:HG11	1:G:147:ARG:O	2.16	0.45
2:J:87:GLY:O	2:J:105:MET:HA	2.16	0.45
1:C:99:THR:O	1:C:103:GLN:HG2	2.17	0.45
1:C:179:VAL:HG21	1:C:202:GLN:CD	2.41	0.45
2:D:80:TRP:CZ2	2:D:197:PRO:HB3	2.51	0.45
1:G:185:VAL:HG13	1:G:189:PHE:CD2	2.51	0.45
1:K:129:LEU:HD11	1:K:147:ARG:HB2	1.98	0.45
2:L:26:THR:HG21	2:L:282:VAL:HA	1.98	0.45
2:B:39:LEU:HD12	2:B:223:LEU:HD11	1.98	0.45
1:E:127:VAL:O	1:E:147:ARG:HD3	2.16	0.45
2:F:245:TRP:O	2:F:248:GLN:HB3	2.16	0.45
1:A:38:LEU:HD11	1:A:195:MET:HE2	1.99	0.45
1:E:49:LYS:HD2	1:E:196:VAL:CG1	2.42	0.45
2:H:112:PRO:HA	2:H:120:PHE:HD1	1.81	0.45
2:J:15:PHE:HD1	2:J:277:ILE:HG13	1.81	0.45
2:B:125:ALA:HA	2:B:169:VAL:HG12	1.98	0.45
2:F:88:VAL:HG22	2:F:105:MET:HG2	1.99	0.45
1:G:180:GLU:HG2	1:G:205:TYR:CE1	2.51	0.45
2:J:293:GLY:O	2:J:297:ALA:N	2.50	0.45
2:B:36:THR:CG2	2:B:223:LEU:HB3	2.47	0.45
2:D:114:PRO:O	2:D:117:VAL:N	2.45	0.45
2:D:229:PHE:O	2:D:233:ILE:HG13	2.17	0.45
1:E:127:VAL:HG11	1:E:147:ARG:O	2.17	0.45
2:F:108:PRO:HG2	2:F:111:THR:CG2	2.47	0.45
2:L:18:ILE:HG12	2:L:241:PHE:CD1	2.52	0.45
1:G:99:THR:O	1:G:103:GLN:HG2	2.17	0.45
2:H:26:THR:O	2:H:30:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:192:GLU:HG3	2:L:193:PRO:HD2	1.99	0.45
1:A:42:VAL:CG2	1:A:203:LEU:HD21	2.47	0.45
2:B:102:THR:HG21	2:B:131:LEU:CD2	2.46	0.45
1:C:116:ARG:HG2	1:C:116:ARG:H	1.59	0.45
2:F:253:ILE:HG22	2:F:334:VAL:HG11	1.99	0.45
2:H:145:LEU:HD23	2:H:177:VAL:HG21	1.99	0.45
1:K:167:THR:HB	1:K:175:SER:HB3	1.99	0.45
2:D:26:THR:O	2:D:30:VAL:HG23	2.16	0.45
2:D:106:GLY:HA2	2:D:169:VAL:O	2.17	0.45
2:D:85:PRO:HD2	2:D:108:PRO:HG3	1.99	0.44
2:D:156:VAL:HG12	2:D:157:LYS:N	2.30	0.44
1:K:185:VAL:HG13	1:K:189:PHE:CD2	2.52	0.44
2:B:26:THR:HG22	2:B:316:ILE:HG21	2.00	0.44
1:K:169:ALA:O	1:K:170:LEU:HD23	2.17	0.44
2:B:156:VAL:HG12	2:B:157:LYS:H	1.83	0.44
1:G:75:LEU:HD22	1:G:79:SER:HB2	1.99	0.44
1:G:132:LEU:HD23	1:G:135:ARG:HE	1.81	0.44
1:G:173:ARG:O	1:G:177:GLU:HG3	2.17	0.44
1:I:14:VAL:HG21	1:I:55:ILE:HD11	1.99	0.44
2:J:26:THR:OG1	2:J:285:GLY:HA3	2.17	0.44
1:C:6:VAL:HG23	1:C:35:PRO:HG3	1.99	0.44
1:E:209:PHE:CE1	1:E:221:ALA:HB3	2.53	0.44
2:F:95:SER:HB2	2:F:135:LEU:HB3	2.00	0.44
2:H:233:ILE:O	2:H:237:VAL:HG23	2.18	0.44
2:L:43:ASN:HD22	2:L:216:TYR:HA	1.83	0.44
2:D:107:LEU:HB3	2:D:108:PRO:HD2	1.98	0.44
1:K:132:LEU:HD22	1:K:135:ARG:NE	2.27	0.44
2:L:278:LEU:HD13	2:L:320:GLY:HA3	1.99	0.44
2:B:15:PHE:CD1	2:B:277:ILE:HG13	2.53	0.44
2:B:141:ASP:O	2:B:152:VAL:HG23	2.18	0.44
2:D:214:PRO:HG2	5:D:401:MNR:O1D	2.18	0.44
2:F:288:ILE:O	2:F:292:LEU:HB2	2.18	0.44
2:D:1:MET:HE1	2:D:272:GLY:HA3	1.99	0.44
1:G:170:LEU:HD22	1:G:174:LEU:HD13	1.98	0.44
2:H:331:VAL:O	2:H:334:VAL:HG12	2.17	0.44
1:C:42:VAL:HG21	1:C:203:LEU:HD11	1.99	0.44
2:H:169:VAL:CG2	2:H:174:TRP:HB2	2.48	0.44
1:I:44:GLU:HA	1:I:44:GLU:OE1	2.17	0.44
2:D:270:ALA:HB3	2:D:328:VAL:HG11	1.99	0.43
2:D:293:GLY:HA3	2:D:302:PHE:CE2	2.53	0.43
2:L:173:THR:O	2:L:177:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLY:HA2	2:B:169:VAL:O	2.18	0.43
2:F:60:ALA:HB1	2:H:97:GLN:O	2.18	0.43
2:F:233:ILE:O	2:F:237:VAL:HG23	2.18	0.43
2:F:302:PHE:CE2	2:F:304:LEU:HB2	2.53	0.43
2:H:85:PRO:HD2	2:H:108:PRO:CG	2.47	0.43
2:H:192:GLU:HG2	2:H:193:PRO:HD2	2.00	0.43
2:J:36:THR:CG2	2:J:223:LEU:HB3	2.48	0.43
2:J:185:THR:HG23	2:J:186:VAL:HG23	2.00	0.43
2:B:15:PHE:HA	2:B:18:ILE:HG22	2.01	0.43
1:E:132:LEU:HD22	1:E:135:ARG:NE	2.33	0.43
1:I:82:ARG:HB2	2:J:260:GLY:HA3	2.00	0.43
2:J:277:ILE:HD13	2:J:277:ILE:HA	1.84	0.43
2:B:293:GLY:HA2	2:B:296:ILE:HG22	2.00	0.43
2:D:219:GLU:HB2	5:D:401:MNR:C3A	2.48	0.43
2:J:76:GLN:NE2	2:J:201:GLU:HG2	2.33	0.43
2:J:290:ALA:HB2	2:J:309:VAL:HG21	2.01	0.43
2:L:86:LEU:O	2:L:185:THR:HG22	2.18	0.43
1:C:15:VAL:HA	1:C:23:VAL:O	2.18	0.43
2:D:52:PRO:HG3	2:D:188:LEU:HD22	2.00	0.43
1:E:6:VAL:HG23	1:E:35:PRO:HG3	1.99	0.43
1:E:78:THR:HA	1:E:81:ARG:CZ	2.49	0.43
2:F:113:LEU:HD21	2:F:121:ILE:HD11	2.00	0.43
2:H:215:ALA:HB2	5:H:401:MNR:O1D	2.18	0.43
1:K:59:LEU:HD13	2:L:340:LEU:HD11	2.00	0.43
2:L:233:ILE:O	2:L:237:VAL:HG23	2.19	0.43
1:E:167:THR:HB	1:E:175:SER:HB2	2.00	0.43
1:G:15:VAL:H	1:G:63:THR:CG2	2.31	0.43
1:G:220:THR:HG21	1:G:224:TRP:CD1	2.54	0.43
1:I:127:VAL:HG21	1:I:151:ALA:HB2	2.00	0.43
2:B:278:LEU:HD13	2:B:320:GLY:HA3	2.00	0.43
2:H:46:ALA:HB2	2:H:166:VAL:HG21	2.01	0.43
2:J:26:THR:HG22	2:J:316:ILE:CD1	2.48	0.43
2:D:246:THR:HG21	2:D:328:VAL:HG22	2.01	0.43
2:J:197:PRO:HB2	2:J:201:GLU:HB2	2.01	0.43
1:A:18:ASP:HB2	1:A:23:VAL:HG12	2.01	0.43
2:B:156:VAL:CG1	2:B:157:LYS:N	2.80	0.43
2:B:244:VAL:HG11	2:D:244:VAL:HG13	2.00	0.43
1:C:171:ASP:OD1	1:C:174:LEU:HD12	2.18	0.43
1:E:212:MET:HE2	1:E:212:MET:HB3	1.84	0.43
1:I:160:LEU:HD12	1:I:192:ALA:O	2.19	0.43
2:L:277:ILE:HD13	2:L:277:ILE:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ILE:HG12	2:D:105:MET:HE1	2.00	0.42
2:F:215:ALA:HB2	5:H:401:MNR:HMD2	2.01	0.42
2:H:72:ILE:O	2:H:182:ALA:HB1	2.19	0.42
2:J:22:VAL:O	2:J:26:THR:HG23	2.18	0.42
2:B:255:VAL:O	2:B:259:LEU:HG	2.19	0.42
2:F:278:LEU:HD23	2:F:278:LEU:HA	1.89	0.42
2:H:270:ALA:HB3	2:H:328:VAL:HG11	2.00	0.42
2:F:26:THR:O	2:F:30:VAL:HG23	2.18	0.42
1:I:147:ARG:NH2	1:I:177:GLU:OE1	2.53	0.42
1:K:161:LEU:O	1:K:193:THR:HA	2.19	0.42
2:B:26:THR:HG22	2:B:316:ILE:HD13	1.99	0.42
2:D:230:LEU:HD23	2:D:230:LEU:HA	1.83	0.42
2:H:143:ILE:O	2:H:149:THR:HA	2.19	0.42
1:E:200:ARG:NH2	1:E:211:GLU:OE2	2.53	0.42
1:G:49:LYS:HE3	1:G:49:LYS:HB2	1.74	0.42
1:K:42:VAL:HG11	1:K:200:ARG:NE	2.32	0.42
2:L:22:VAL:O	2:L:26:THR:HG23	2.20	0.42
1:I:19:GLY:HA2	1:K:138:ALA:O	2.20	0.42
2:J:173:THR:O	2:J:177:VAL:HG23	2.19	0.42
1:K:37:GLU:HA	1:K:207:ASP:OD2	2.19	0.42
1:K:210:VAL:HG22	1:K:219:GLN:HG2	2.01	0.42
2:B:266:LEU:HB3	2:B:331:VAL:HG22	2.01	0.42
1:G:42:VAL:HG13	1:G:227:PRO:HB3	2.01	0.42
2:J:125:ALA:HA	2:J:169:VAL:HG12	2.01	0.42
2:H:223:LEU:O	2:H:227:GLN:HG3	2.19	0.42
1:A:106:ILE:HD11	2:B:3:LEU:HB2	2.02	0.42
2:B:8:ILE:HD11	2:B:273:GLN:HG3	2.01	0.42
2:F:277:ILE:HD13	2:F:277:ILE:HA	1.91	0.42
1:G:9:ILE:HG23	1:G:67:VAL:HG22	2.02	0.42
2:H:87:GLY:O	2:H:105:MET:HA	2.20	0.42
2:H:229:PHE:O	2:H:233:ILE:HG13	2.19	0.42
2:L:192:GLU:CG	2:L:193:PRO:HD2	2.50	0.42
1:C:38:LEU:HD11	1:C:195:MET:HE2	2.01	0.42
2:F:128:PRO:HG2	2:F:131:LEU:HB3	2.02	0.42
1:G:62:PRO:HB2	1:G:64:SER:O	2.20	0.42
1:G:171:ASP:O	1:G:175:SER:OG	2.24	0.42
2:J:67:PHE:CE1	2:J:186:VAL:HG21	2.55	0.42
2:B:76:GLN:O	2:B:80:TRP:HD1	2.03	0.41
2:F:330:ASN:OD1	2:F:333:LYS:HD2	2.21	0.41
1:G:182:LEU:HD23	1:G:182:LEU:HA	1.93	0.41
2:B:54:SER:HB3	2:B:203:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:VAL:O	2:F:26:THR:HG23	2.20	0.41
2:F:87:GLY:O	2:F:105:MET:HA	2.19	0.41
2:L:1:MET:HE1	2:L:276:ILE:HD11	2.02	0.41
2:B:98:ASN:OD1	2:D:60:ALA:HB3	2.20	0.41
1:C:199:ASP:OD2	1:C:201:SER:HB3	2.19	0.41
2:D:215:ALA:HB2	5:D:401:MNR:CGD	2.50	0.41
2:D:315:GLY:O	2:D:319:LEU:HD23	2.19	0.41
1:E:98:LEU:HB3	1:E:102:GLU:HB2	2.02	0.41
1:G:75:LEU:HD22	1:G:79:SER:CB	2.50	0.41
1:I:186:THR:HG22	1:I:193:THR:OG1	2.20	0.41
2:J:186:VAL:CG1	2:J:187:LEU:N	2.83	0.41
1:A:118:ASP:O	1:A:122:GLU:HG3	2.20	0.41
1:G:55:ILE:HD13	1:G:60:GLN:HG3	2.01	0.41
1:I:53:LEU:HD11	1:I:162:LEU:HB3	2.03	0.41
2:J:253:ILE:HG21	2:J:331:VAL:HG13	2.03	0.41
2:B:102:THR:HG21	2:B:131:LEU:HD21	2.03	0.41
1:C:127:VAL:O	1:C:147:ARG:HD3	2.19	0.41
1:C:180:GLU:HG2	1:C:205:TYR:HE1	1.85	0.41
2:D:47:ILE:HD12	2:D:213:MET:HE3	2.02	0.41
2:H:29:ILE:HG12	2:H:230:LEU:HB3	2.03	0.41
2:H:146:GLY:HA3	2:H:177:VAL:HG13	2.03	0.41
1:I:73:GLU:OE1	1:I:73:GLU:N	2.44	0.41
2:J:302:PHE:CD2	2:J:302:PHE:C	2.99	0.41
2:L:229:PHE:O	2:L:233:ILE:HG13	2.20	0.41
1:C:41:ILE:HD12	1:C:194:LEU:HD11	2.01	0.41
2:D:50:LEU:HA	2:D:114:PRO:HG3	2.02	0.41
2:D:233:ILE:O	2:D:237:VAL:HG23	2.21	0.41
2:D:242:LEU:HD23	2:D:242:LEU:HA	1.86	0.41
1:K:174:LEU:O	1:K:178:ILE:HG12	2.20	0.41
1:C:55:ILE:CG2	1:C:67:VAL:HG21	2.47	0.41
2:F:56:VAL:HB	2:F:187:LEU:HB2	2.03	0.41
2:F:88:VAL:HB	2:F:185:THR:HG21	2.03	0.41
2:F:321:LEU:HD12	2:F:321:LEU:HA	1.81	0.41
1:G:203:LEU:HD23	1:G:223:LEU:HD11	2.03	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.83	0.41
1:E:8:SER:HA	1:E:32:GLU:HG3	2.02	0.41
2:J:26:THR:O	2:J:30:VAL:HG23	2.20	0.41
2:J:53:HIS:HB2	2:J:190:ASN:O	2.21	0.41
1:A:33:ILE:HD11	1:A:194:LEU:CG	2.46	0.41
1:A:82:ARG:HB2	2:B:260:GLY:HA3	2.03	0.41
1:A:110:LEU:HA	2:B:265:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ALA:HB1	2:D:97:GLN:O	2.20	0.41
1:C:161:LEU:O	1:C:193:THR:HG23	2.21	0.41
2:F:219:GLU:HB2	5:H:401:MNR:C1C	2.50	0.41
1:G:161:LEU:O	1:G:193:THR:HA	2.20	0.41
2:H:137:VAL:CG1	2:H:152:VAL:HG21	2.51	0.41
2:J:21:VAL:CG1	2:J:237:VAL:HG11	2.50	0.41
2:J:223:LEU:O	2:J:227:GLN:HG3	2.20	0.41
2:J:337:GLN:O	2:J:337:GLN:HG3	2.21	0.41
1:K:141:SER:O	1:K:145:ARG:HG3	2.21	0.41
2:B:277:ILE:HD13	2:B:277:ILE:HA	1.87	0.41
2:B:278:LEU:HD23	2:B:278:LEU:HA	1.87	0.41
1:E:13:SER:HB2	1:E:64:SER:OG	2.21	0.41
1:E:49:LYS:HZ1	1:E:198:HIS:CE1	2.38	0.41
2:F:117:VAL:HG13	2:F:156:VAL:HB	2.02	0.41
1:I:81:ARG:HG2	1:I:87:PHE:CZ	2.56	0.41
1:K:171:ASP:OD1	1:K:174:LEU:HB2	2.21	0.41
2:L:32:LEU:HD23	2:L:32:LEU:HA	1.85	0.41
2:L:88:VAL:HB	2:L:185:THR:HG21	2.02	0.41
2:B:2:PHE:O	2:B:6:ARG:NH1	2.54	0.40
1:C:100:ALA:HB3	1:C:133:GLY:HA2	2.04	0.40
2:D:95:SER:HB2	2:D:137:VAL:CG1	2.51	0.40
1:G:78:THR:HA	1:G:81:ARG:CZ	2.51	0.40
2:J:35:LEU:O	2:J:39:LEU:HG	2.21	0.40
2:L:26:THR:O	2:L:30:VAL:HG23	2.21	0.40
2:J:66:GLU:HB2	2:J:69:SER:OG	2.21	0.40
2:L:278:LEU:HA	2:L:278:LEU:HD23	1.88	0.40
1:A:33:ILE:CD1	1:A:194:LEU:HG	2.47	0.40
1:A:141:SER:OG	1:A:142:GLY:N	2.54	0.40
2:B:145:LEU:HD23	2:B:177:VAL:HG21	2.02	0.40
1:C:5:PRO:HB3	1:C:32:GLU:HG2	2.03	0.40
1:C:127:VAL:O	1:C:127:VAL:HG12	2.22	0.40
2:H:45:SER:HB2	2:H:159:GLU:OE1	2.22	0.40
2:H:156:VAL:HG23	2:H:157:LYS:O	2.21	0.40
2:J:55:VAL:HB	2:J:204:THR:CG2	2.52	0.40
2:B:192:GLU:HG2	2:B:193:PRO:HD2	2.03	0.40
2:D:95:SER:HB3	2:D:135:LEU:HB3	2.04	0.40
2:H:100:ASN:OD1	2:H:101:THR:N	2.51	0.40
1:I:135:ARG:NH2	1:I:139:GLN:O	2.53	0.40
1:I:171:ASP:OD1	1:I:174:LEU:HB2	2.22	0.40
2:J:145:LEU:HD12	2:J:150:VAL:HG21	2.04	0.40
2:B:24:LEU:HD23	2:B:24:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:THR:HB	2:D:210:PHE:CE1	2.55	0.40
1:G:185:VAL:HG13	1:G:189:PHE:HD2	1.86	0.40
2:J:100:ASN:HB2	2:J:134:PHE:HE2	1.85	0.40
2:L:109:GLU:HA	2:L:121:ILE:HG22	2.03	0.40
2:L:128:PRO:HG2	2:L:131:LEU:HB3	2.03	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	214/231 (93%)	208 (97%)	6 (3%)	0	100	100
1	C	216/231 (94%)	210 (97%)	6 (3%)	0	100	100
1	E	215/231 (93%)	208 (97%)	7 (3%)	0	100	100
1	G	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
1	I	219/231 (95%)	211 (96%)	8 (4%)	0	100	100
1	K	217/231 (94%)	210 (97%)	7 (3%)	0	100	100
2	B	340/344 (99%)	334 (98%)	6 (2%)	0	100	100
2	D	342/344 (99%)	336 (98%)	6 (2%)	0	100	100
2	F	341/344 (99%)	331 (97%)	10 (3%)	0	100	100
2	H	339/344 (98%)	331 (98%)	8 (2%)	0	100	100
2	J	342/344 (99%)	332 (97%)	10 (3%)	0	100	100
2	L	341/344 (99%)	335 (98%)	6 (2%)	0	100	100
All	All	3349/3450 (97%)	3262 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	172/186 (92%)	172 (100%)	0	100	100
1	C	174/186 (94%)	173 (99%)	1 (1%)	78	88
1	E	174/186 (94%)	174 (100%)	0	100	100
1	G	180/186 (97%)	180 (100%)	0	100	100
1	I	175/186 (94%)	173 (99%)	2 (1%)	65	83
1	K	174/186 (94%)	173 (99%)	1 (1%)	78	88
2	B	265/265 (100%)	265 (100%)	0	100	100
2	D	266/265 (100%)	266 (100%)	0	100	100
2	F	265/265 (100%)	264 (100%)	1 (0%)	84	90
2	H	264/265 (100%)	264 (100%)	0	100	100
2	J	266/265 (100%)	265 (100%)	1 (0%)	84	90
2	L	265/265 (100%)	264 (100%)	1 (0%)	84	90
All	All	2640/2706 (98%)	2633 (100%)	7 (0%)	86	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	197	THR
2	F	55	VAL
1	I	167	THR
1	I	219	GLN
2	J	67	PHE
1	K	197	THR
2	L	67	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	97	GLN
2	B	337	GLN

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Mol	Chain	Res	Type
2	D	43	ASN
2	D	53	HIS
2	D	97	GLN
2	D	163	HIS
2	D	175	GLN
2	D	191	GLN
2	D	198	GLN
1	E	202	GLN
2	F	37	GLN
2	F	227	GLN
1	G	60	GLN
2	H	53	HIS
2	H	90	GLN
1	I	60	GLN
1	I	91	GLN
1	I	149	ASN
2	J	76	GLN
2	J	98	ASN
2	J	160	ASN
2	J	200	ASN
2	J	227	GLN
1	K	84	HIS
1	K	198	HIS
2	L	90	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
5	MNR	H	401	2	37,50,50	2.32	8 (21%)	34,82,82	1.91	10 (29%)
4	PGE	B	502	-	9,9,9	0.16	0	8,8,8	0.10	0
3	AGA	B	501	-	22,22,29	0.50	0	25,27,35	0.73	1 (4%)
5	MNR	D	401	2	37,50,50	2.30	8 (21%)	34,82,82	1.82	10 (29%)
6	PEG	H	402	-	6,6,6	0.12	0	5,5,5	0.06	0
6	PEG	D	402	-	6,6,6	0.13	0	5,5,5	0.07	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
5	MNR	H	401	2	-	6/12/94/94	-
4	PGE	B	502	-	-	1/7/7/7	-
3	AGA	B	501	-	-	2/24/24/34	-
5	MNR	D	401	2	-	5/12/94/94	-
6	PEG	H	402	-	-	2/4/4/4	-
6	PEG	D	402	-	-	1/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	MNR	C3B-C4B	6.86	1.48	1.41
5	D	401	MNR	C3B-C4B	6.83	1.48	1.41
5	H	401	MNR	C1D-C2D	5.79	1.46	1.39
5	D	401	MNR	C1B-C2B	5.60	1.45	1.39
5	H	401	MNR	CAC-C3C	-5.52	1.41	1.47
5	D	401	MNR	C1D-C2D	5.50	1.45	1.39
5	D	401	MNR	CAC-C3C	-5.38	1.41	1.47
5	H	401	MNR	C1B-C2B	5.37	1.45	1.39
5	H	401	MNR	CAA-C2A	3.51	1.56	1.51
5	D	401	MNR	CAA-C2A	3.36	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	MNR	CMC-C2C	2.62	1.54	1.50
5	D	401	MNR	CMC-C2C	2.55	1.54	1.50
5	D	401	MNR	C4A-NA	2.26	1.41	1.37
5	D	401	MNR	CHB-C4A	2.22	1.43	1.39
5	H	401	MNR	CHB-C4A	2.20	1.43	1.39
5	H	401	MNR	C4A-NA	2.16	1.40	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	401	MNR	CBD-CAD-C3D	4.36	119.87	112.54
5	H	401	MNR	CHD-C4C-NC	3.68	124.50	120.60
5	D	401	MNR	CHD-C4C-NC	3.66	124.48	120.60
5	H	401	MNR	CHA-C1A-NA	3.37	124.17	120.60
5	H	401	MNR	C1C-CHC-C4B	3.19	127.49	116.07
5	D	401	MNR	CHA-C1A-NA	3.17	123.97	120.60
5	D	401	MNR	C1C-CHC-C4B	3.16	127.37	116.07
5	D	401	MNR	CBD-CAD-C3D	3.03	117.64	112.54
5	H	401	MNR	C4C-CHD-C1D	2.97	126.69	116.07
5	D	401	MNR	C4A-CHB-C1B	2.96	126.67	116.07
5	H	401	MNR	C4A-CHB-C1B	2.96	126.65	116.07
5	D	401	MNR	C4C-CHD-C1D	2.95	126.62	116.07
5	H	401	MNR	CHC-C1C-NC	2.88	123.66	120.60
5	H	401	MNR	C1A-CHA-C4D	2.87	126.34	116.07
5	D	401	MNR	C1A-CHA-C4D	2.81	126.11	116.07
5	D	401	MNR	CHB-C4A-NA	2.75	123.52	120.60
5	H	401	MNR	CHB-C4A-NA	2.66	123.42	120.60
5	D	401	MNR	CHC-C1C-NC	2.62	123.38	120.60
3	B	501	AGA	O3-P1-O4	2.39	120.13	110.83
5	H	401	MNR	C1A-C2A-C3A	-2.17	104.79	113.37
5	D	401	MNR	C1A-C2A-C3A	-2.11	105.05	113.37

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	401	MNR	C2D-C3D-CAD-CBD
5	D	401	MNR	C4D-C3D-CAD-CBD
5	H	401	MNR	C1A-C2A-CAA-CBA
5	H	401	MNR	C4D-C3D-CAD-CBD
5	H	401	MNR	C2D-C3D-CAD-CBD
3	B	501	AGA	C13-C12-O9-C5

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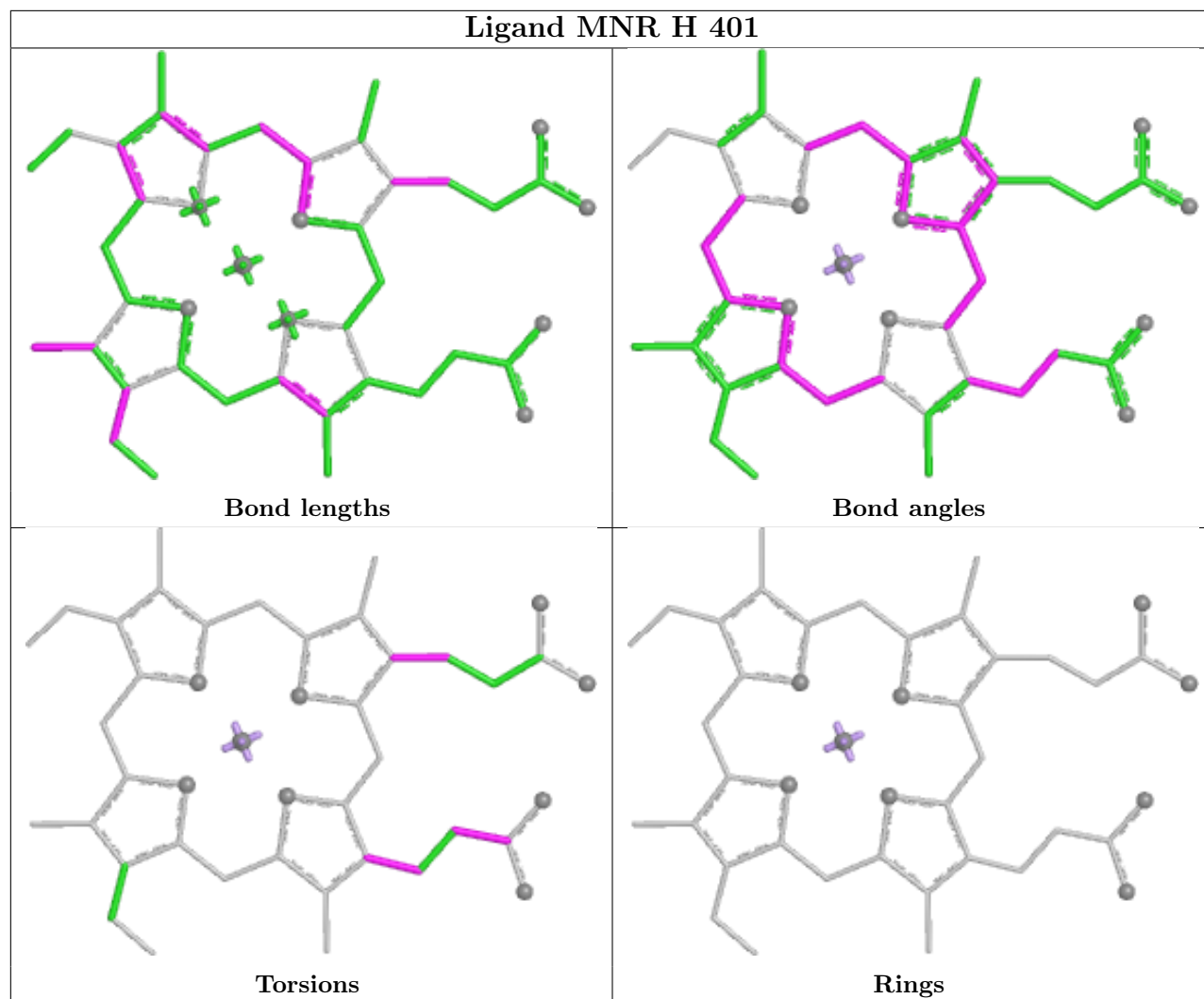
Mol	Chain	Res	Type	Atoms
6	H	402	PEG	C1-C2-O2-C3
5	H	401	MNR	C3A-C2A-CAA-CBA
3	B	501	AGA	O10-C12-O9-C5
6	H	402	PEG	C4-C3-O2-C2
4	B	502	PGE	O2-C3-C4-O3
5	H	401	MNR	CAD-CBD-CGD-O1D
5	H	401	MNR	CAD-CBD-CGD-O2D
5	D	401	MNR	C3D-CAD-CBD-CGD
5	D	401	MNR	CAD-CBD-CGD-O1D
5	D	401	MNR	CAD-CBD-CGD-O2D
6	D	402	PEG	C4-C3-O2-C2

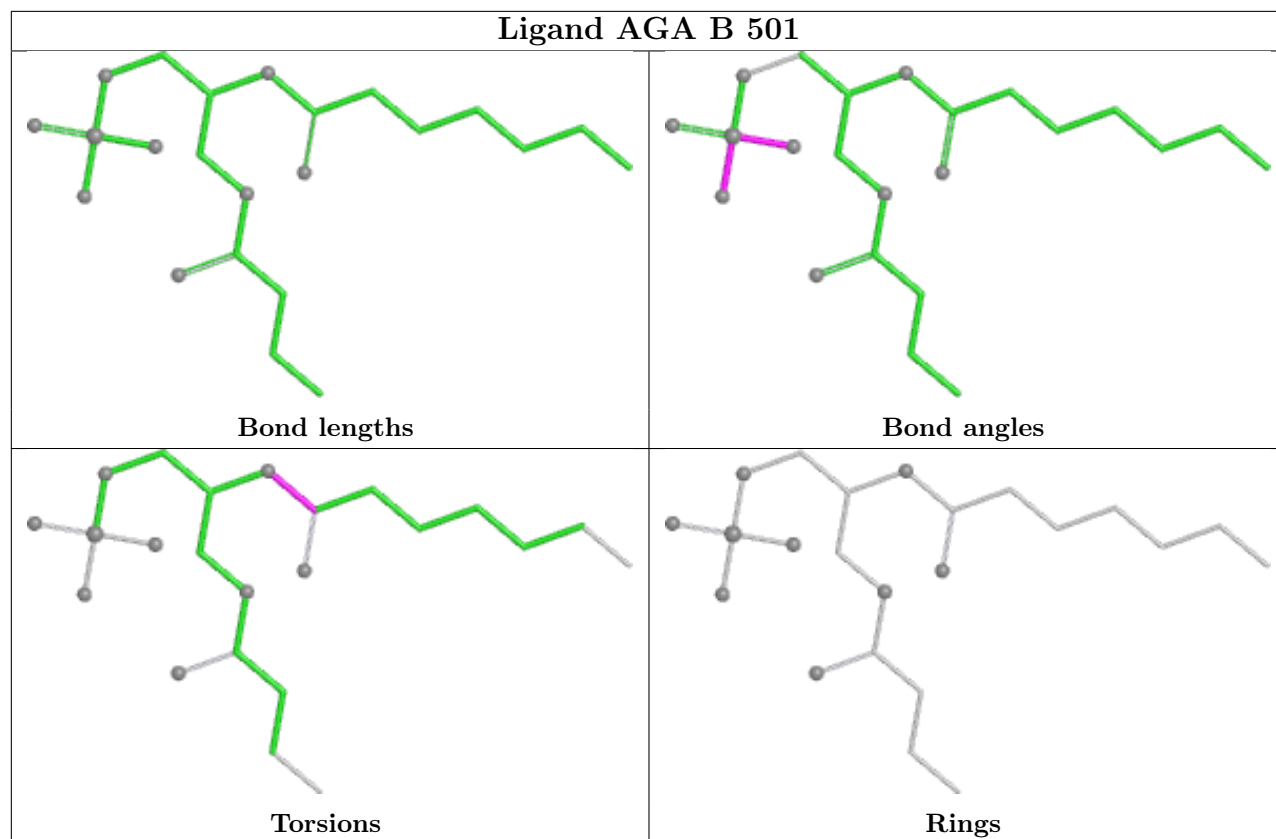
There are no ring outliers.

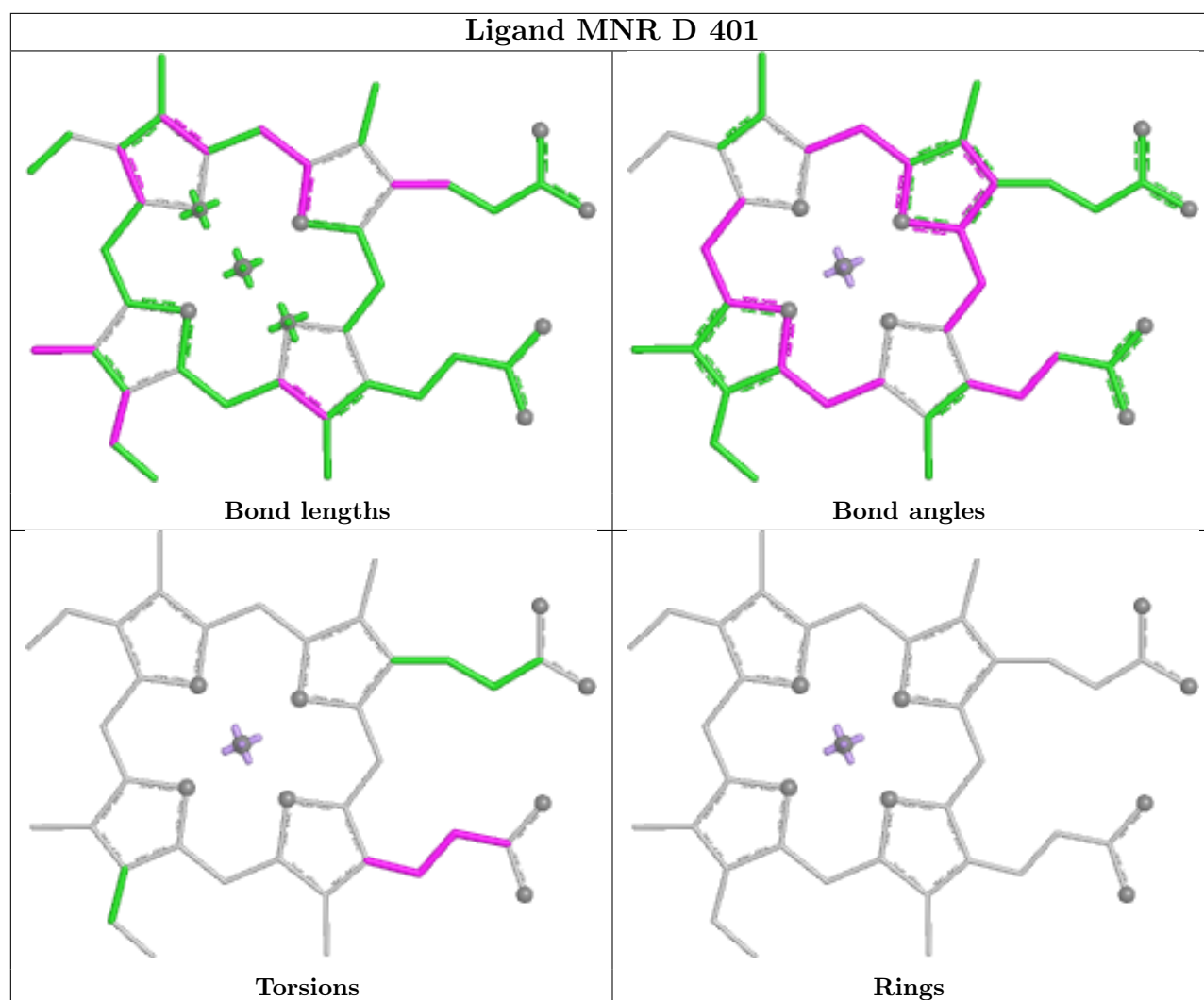
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	401	MNR	6	0
4	B	502	PGE	1	0
3	B	501	AGA	2	0
5	D	401	MNR	6	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	216/231 (93%)	0.97	32 (14%) 5 3	94, 115, 134, 152	0
1	C	218/231 (94%)	0.79	27 (12%) 8 5	75, 100, 120, 134	0
1	E	217/231 (93%)	1.04	33 (15%) 5 3	110, 147, 192, 290	0
1	G	225/231 (97%)	0.53	18 (8%) 18 9	82, 108, 145, 171	0
1	I	221/231 (95%)	0.54	17 (7%) 19 10	79, 99, 117, 130	0
1	K	219/231 (94%)	0.55	14 (6%) 25 13	77, 92, 114, 151	0
2	B	341/344 (99%)	1.32	72 (21%) 2 1	68, 120, 183, 228	1 (0%)
2	D	343/344 (99%)	1.27	62 (18%) 3 2	85, 160, 220, 246	1 (0%)
2	F	342/344 (99%)	1.22	60 (17%) 4 3	75, 133, 173, 202	1 (0%)
2	H	341/344 (99%)	1.49	102 (29%) 1 1	109, 176, 221, 267	0
2	J	343/344 (99%)	1.57	98 (28%) 1 1	94, 149, 187, 241	1 (0%)
2	L	343/344 (99%)	1.35	76 (22%) 2 1	86, 144, 191, 215	0
All	All	3369/3450 (97%)	1.12	611 (18%) 3 2	68, 128, 195, 290	4 (0%)

All (611) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	211	GLN	10.0
2	J	163	HIS	9.7
2	F	298	GLY	9.4
2	J	101	THR	9.1
2	L	156	VAL	8.9
2	L	297	ALA	8.9
2	B	207	LYS	8.7
2	L	158	THR	8.6
2	B	115	ASP	8.3
2	B	157	LYS	8.1
2	L	155	THR	8.1

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Mol	Chain	Res	Type	RSRZ
2	L	343	THR	8.1
2	L	342	ALA	7.8
2	B	205	ASP	7.6
2	F	112	PRO	7.4
2	J	48	GLU	7.2
2	B	118	GLY	7.2
2	J	90	GLN	7.1
1	A	18	ASP	7.1
2	J	342	ALA	7.0
2	F	207	LYS	6.9
2	L	191	GLN	6.9
2	B	341	GLY	6.9
2	B	204	THR	6.8
2	F	299	SER	6.8
1	A	209	PHE	6.7
2	J	216	TYR	6.7
1	E	203	LEU	6.7
2	L	341	GLY	6.6
2	F	210	PHE	6.5
2	H	78	GLU	6.4
2	L	157	LYS	6.2
2	F	178	SER	6.1
2	H	308	SER	6.1
1	E	220	THR	6.0
1	E	206	ALA	6.0
2	F	195	ILE	5.9
2	H	218	SER	5.9
2	L	129	ALA	5.8
2	D	209	ALA	5.8
2	F	206	LEU	5.7
2	J	215	ALA	5.7
2	F	342	ALA	5.6
2	H	77	ALA	5.5
2	H	118	GLY	5.5
2	L	190	ASN	5.5
2	D	48	GLU	5.5
2	B	117	VAL	5.5
2	J	214	PRO	5.4
2	D	308	SER	5.4
2	H	116	SER	5.3
2	D	343	THR	5.3
2	F	208	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
2	F	216	TYR	5.3
2	H	1	MET	5.3
1	E	204	ALA	5.3
2	J	44	THR	5.3
1	C	20	ILE	5.3
2	L	154	GLY	5.2
2	H	215	ALA	5.2
1	E	91	GLN	5.2
2	H	241	PHE	5.2
2	H	157	LYS	5.2
2	J	164	THR	5.2
2	F	10	ALA	5.2
2	D	159	GLU	5.1
2	L	304	LEU	5.1
2	J	100	ASN	5.1
2	L	339	ALA	5.1
2	H	217	LYS	5.1
1	A	210	VAL	5.0
2	B	116	SER	5.0
2	J	341	GLY	5.0
2	J	238	THR	4.9
2	H	214	PRO	4.9
2	J	339	ALA	4.9
2	F	205	ASP	4.9
1	E	21	SER	4.9
2	F	297	ALA	4.9
2	J	205	ASP	4.9
2	H	339	ALA	4.8
2	H	68	THR	4.8
2	D	208	GLY	4.7
2	B	2	PHE	4.7
2	L	251	ARG	4.7
2	L	12	ALA	4.7
2	J	165	PRO	4.6
2	H	238	THR	4.6
1	E	188	GLU	4.5
2	L	101	THR	4.5
2	H	117	VAL	4.5
2	J	31	MET	4.5
2	B	203	VAL	4.5
2	B	211	GLN	4.5
2	B	56	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	20	ILE	4.4
2	J	222	SER	4.4
2	L	117	VAL	4.4
2	B	10	ALA	4.4
2	B	208	GLY	4.4
2	D	154	GLY	4.4
1	G	224	TRP	4.4
2	D	168	TRP	4.3
2	J	60	ALA	4.3
2	H	48	GLU	4.3
2	B	75	GLN	4.3
1	K	89	PHE	4.3
1	C	3	ALA	4.3
2	J	340	LEU	4.3
2	J	5	ILE	4.3
2	H	159	GLU	4.3
2	B	202	VAL	4.3
2	H	235	ALA	4.2
2	F	209	ALA	4.2
1	A	211	GLU	4.2
2	L	298	GLY	4.2
2	H	251	ARG	4.2
1	A	116	ARG	4.1
2	H	36	THR	4.1
2	B	84	THR	4.1
2	B	190	ASN	4.1
2	B	183	VAL	4.1
1	G	227	PRO	4.1
2	F	9	ARG	4.1
2	H	289	GLY	4.1
2	J	206	LEU	4.0
2	F	215	ALA	4.0
2	J	9	ARG	4.0
2	J	210	PHE	4.0
1	A	115	PRO	4.0
2	B	189	LEU	4.0
2	H	34	GLY	4.0
1	K	93	ASN	4.0
1	A	90	GLN	4.0
2	F	217	LYS	4.0
2	J	160	ASN	3.9
1	E	32	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	130	GLU	3.9
2	J	19	ALA	3.9
1	E	19	GLY	3.9
2	L	118	GLY	3.9
2	F	113	LEU	3.9
2	L	127	LEU	3.9
2	J	68	THR	3.9
2	F	221	SER	3.9
2	H	82	ASP	3.9
1	I	20	ILE	3.9
2	F	175	GLN	3.9
1	I	204	ALA	3.9
2	B	158	THR	3.8
2	H	74	GLU	3.8
2	L	74	GLU	3.8
1	G	91	GLN	3.8
2	D	211	GLN	3.8
2	B	188	LEU	3.8
2	H	39	LEU	3.8
2	J	17	LEU	3.8
1	A	168	SER	3.8
1	I	3	ALA	3.8
2	L	128	PRO	3.8
2	L	115	ASP	3.8
2	H	80	TRP	3.8
2	H	193	PRO	3.8
2	H	240	ALA	3.7
2	D	342	ALA	3.7
2	J	337	GLN	3.7
1	A	48	GLY	3.7
2	D	212	ALA	3.7
2	J	42	GLN	3.7
2	D	204	THR	3.7
2	H	30	VAL	3.7
2	B	101	THR	3.6
2	H	248	GLN	3.6
1	G	198	HIS	3.6
2	B	112	PRO	3.6
2	D	116	SER	3.6
2	J	299	SER	3.6
2	L	181	LYS	3.6
2	F	294	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	69	SER	3.6
2	D	90	GLN	3.6
2	F	198	GLN	3.6
2	L	302	PHE	3.6
2	J	218	SER	3.6
2	H	341	GLY	3.5
1	A	25	ALA	3.5
2	H	70	SER	3.5
2	H	183	VAL	3.5
2	J	35	LEU	3.5
1	E	208	ARG	3.5
2	J	308	SER	3.5
2	B	340	LEU	3.5
1	A	114	LYS	3.5
2	D	207	LYS	3.5
1	C	22	THR	3.5
1	E	18	ASP	3.5
2	J	343	THR	3.4
2	H	123	GLN	3.4
2	H	71	GLU	3.4
2	L	194	THR	3.4
1	G	226	HIS	3.4
2	F	163	HIS	3.4
2	H	303	SER	3.4
2	J	207	LYS	3.4
2	B	82	ASP	3.4
2	H	147	GLY	3.4
2	D	270	ALA	3.4
2	H	340	LEU	3.4
1	C	138	ALA	3.4
2	H	75	GLN	3.4
2	L	68	THR	3.4
2	D	67	PHE	3.4
2	D	241	PHE	3.4
2	L	140	GLY	3.3
1	E	20	ILE	3.3
1	E	221	ALA	3.3
2	H	65	PRO	3.3
1	G	197	THR	3.3
2	H	194	THR	3.3
2	J	33	THR	3.3
2	L	163	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	14	ARG	3.3
1	K	168	SER	3.3
2	F	64	SER	3.2
2	H	221	SER	3.2
2	L	340	LEU	3.2
1	K	90	GLN	3.2
2	D	210	PHE	3.2
2	F	268	ILE	3.2
2	D	41	LYS	3.2
2	D	176	LEU	3.2
2	L	295	LEU	3.2
1	A	89	PHE	3.2
1	A	91	GLN	3.2
2	J	43	ASN	3.2
2	D	340	LEU	3.2
2	D	336	PRO	3.2
2	B	218	SER	3.2
2	H	239	VAL	3.2
2	B	142	HIS	3.2
2	J	174	TRP	3.2
1	E	44	GLU	3.2
2	J	88	VAL	3.2
1	C	64	SER	3.2
2	H	286	ALA	3.2
1	I	89	PHE	3.2
2	B	339	ALA	3.2
2	F	341	GLY	3.1
1	C	58	PHE	3.1
2	J	251	ARG	3.1
2	D	158	THR	3.1
2	L	36	THR	3.1
2	J	12	ALA	3.1
1	E	218	LEU	3.1
2	J	102	THR	3.1
2	H	49	ALA	3.1
2	J	2	PHE	3.1
2	L	159	GLU	3.1
1	A	164	ASP	3.1
2	H	41	LYS	3.0
1	C	37	GLU	3.0
2	J	20	SER	3.0
2	L	64	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	303	SER	3.0
1	A	26	LEU	3.0
2	B	155	THR	3.0
2	H	58	THR	3.0
2	L	82	ASP	3.0
1	A	97	SER	3.0
1	G	89	PHE	3.0
2	H	67	PHE	3.0
2	H	66	GLU	2.9
2	H	46	ALA	2.9
2	D	38	GLY	2.9
2	J	75	GLN	2.9
1	C	80	THR	2.9
1	E	200	ARG	2.9
2	J	103	ALA	2.9
2	L	215	ALA	2.9
2	D	40	GLY	2.9
1	A	203	LEU	2.9
2	F	267	LEU	2.9
1	C	114	LYS	2.9
2	H	246	THR	2.9
2	H	309	VAL	2.9
2	H	89	SER	2.9
2	D	206	LEU	2.9
2	J	213	MET	2.9
2	J	217	LYS	2.9
2	J	91	THR	2.9
2	B	57	PHE	2.9
1	E	97	SER	2.9
2	D	39	LEU	2.9
2	J	89	SER	2.9
1	C	142	GLY	2.9
2	D	57	PHE	2.9
2	B	226	MET	2.9
2	F	181	LYS	2.9
1	I	45	SER	2.8
2	D	73	SER	2.8
2	J	162	SER	2.8
1	A	207	ASP	2.8
2	H	192	GLU	2.8
2	B	100	ASN	2.8
2	B	338	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	337	GLN	2.8
2	L	116	SER	2.8
2	L	214	PRO	2.8
1	C	39	VAL	2.8
1	E	136	ARG	2.8
2	B	264	ARG	2.8
2	F	300	VAL	2.8
2	L	267	LEU	2.8
2	L	308	SER	2.8
2	B	85	PRO	2.8
2	D	36	THR	2.8
2	H	202	VAL	2.8
2	J	158	THR	2.8
2	J	219	GLU	2.8
2	H	168	TRP	2.8
2	J	161	TYR	2.8
2	F	214	PRO	2.8
1	C	59	LEU	2.8
1	E	24	THR	2.8
2	H	38	GLY	2.8
2	B	123	GLN	2.8
2	L	32	LEU	2.8
2	J	36	THR	2.8
1	G	164	ASP	2.7
1	K	164	ASP	2.7
2	H	115	ASP	2.7
1	C	208	ARG	2.7
2	L	112	PRO	2.7
2	B	159	GLU	2.7
2	L	99	ALA	2.7
1	A	113	ILE	2.7
2	L	120	PHE	2.7
2	D	192	GLU	2.7
2	J	181	LYS	2.7
2	F	98	ASN	2.7
1	K	92	PRO	2.7
2	F	316	ILE	2.7
2	H	268	ILE	2.7
2	F	79	ARG	2.7
2	B	178	SER	2.7
1	C	15	VAL	2.7
1	C	202	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	338	ILE	2.7
1	I	221	ALA	2.7
1	K	94	LEU	2.7
2	J	39	LEU	2.7
1	K	20	ILE	2.6
2	B	120	PHE	2.6
2	L	264	ARG	2.6
2	D	305	GLY	2.6
2	H	305	GLY	2.6
2	D	155	THR	2.6
2	J	180	THR	2.6
2	B	306	TRP	2.6
1	G	225	SER	2.6
2	F	247	LEU	2.6
2	H	225	SER	2.6
2	H	271	LEU	2.6
2	L	24	LEU	2.6
2	B	6	ARG	2.6
2	D	333	LYS	2.6
2	F	43	ASN	2.6
1	K	46	GLY	2.6
2	H	109	GLU	2.6
2	H	35	LEU	2.6
2	L	294	TRP	2.6
2	J	46	ALA	2.6
2	J	300	VAL	2.6
2	H	79	ARG	2.6
2	H	322	ILE	2.6
2	J	1	MET	2.6
1	K	91	GLN	2.6
2	D	335	ASP	2.6
2	H	284	LEU	2.6
2	D	19	ALA	2.6
2	L	216	TYR	2.6
2	L	65	PRO	2.6
1	A	112	GLY	2.6
2	B	151	THR	2.6
2	B	209	ALA	2.6
2	J	49	ALA	2.6
2	L	47	ILE	2.6
2	H	272	GLY	2.6
2	L	305	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	288	ILE	2.5
2	F	101	THR	2.5
1	E	34	PHE	2.5
1	C	16	TYR	2.5
2	D	165	PRO	2.5
2	J	110	GLY	2.5
2	B	251	ARG	2.5
1	C	77	ALA	2.5
2	J	159	GLU	2.5
2	J	182	ALA	2.5
2	F	171	THR	2.5
2	F	246	THR	2.5
1	G	17	PRO	2.5
2	D	193	PRO	2.5
1	I	174	LEU	2.5
1	C	21	SER	2.5
1	C	28	SER	2.5
2	F	218	SER	2.5
2	H	90	GLN	2.5
2	D	30	VAL	2.5
2	D	88	VAL	2.5
2	J	78	GLU	2.5
1	C	220	THR	2.5
2	F	204	THR	2.5
2	D	9	ARG	2.5
2	H	181	LYS	2.5
2	J	289	GLY	2.5
2	B	215	ALA	2.5
2	B	225	SER	2.5
2	F	15	PHE	2.5
2	D	149	THR	2.5
2	J	59	THR	2.5
2	J	14	ARG	2.5
2	H	165	PRO	2.5
1	G	97	SER	2.4
2	D	74	GLU	2.4
2	B	113	LEU	2.4
2	B	163	HIS	2.4
1	G	74	GLY	2.4
2	H	156	VAL	2.4
2	J	166	VAL	2.4
1	E	90	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	12	ALA	2.4
2	B	270	ALA	2.4
2	B	195	ILE	2.4
2	D	20	SER	2.4
2	D	281	GLY	2.4
1	A	20	ILE	2.4
1	A	206	ALA	2.4
1	I	169	ALA	2.4
2	D	47	ILE	2.4
2	F	97	GLN	2.4
2	F	333	LYS	2.4
2	H	299	SER	2.4
2	H	291	LEU	2.4
2	B	214	PRO	2.4
2	J	111	THR	2.4
2	F	118	GLY	2.4
2	J	34	GLY	2.4
2	L	147	GLY	2.4
2	L	217	LYS	2.4
2	H	54	SER	2.4
2	L	306	TRP	2.4
1	E	23	VAL	2.4
2	H	203	VAL	2.4
1	K	199	ASP	2.4
2	J	208	GLY	2.4
2	H	93	ILE	2.4
2	H	31	MET	2.4
2	J	71	GLU	2.4
1	A	13	SER	2.4
1	A	21	SER	2.4
2	B	156	VAL	2.4
2	B	331	VAL	2.4
2	H	59	THR	2.3
1	I	136	ARG	2.3
2	H	195	ILE	2.3
2	J	29	ILE	2.3
1	E	209	PHE	2.3
2	B	90	GLN	2.3
2	B	248	GLN	2.3
2	J	211	GLN	2.3
2	J	74	GLU	2.3
2	D	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	217	LYS	2.3
2	B	277	ILE	2.3
2	D	16	ALA	2.3
2	H	290	ALA	2.3
2	L	296	ILE	2.3
2	B	1	MET	2.3
2	L	213	MET	2.3
2	B	11	ALA	2.3
2	F	194	THR	2.3
2	J	144	THR	2.3
2	L	209	ALA	2.3
1	I	198	HIS	2.3
2	L	1	MET	2.3
2	J	203	VAL	2.3
2	J	309	VAL	2.3
2	F	114	PRO	2.3
2	F	338	ILE	2.3
2	D	294	TRP	2.3
1	E	68	THR	2.3
2	F	340	LEU	2.3
2	J	142	HIS	2.3
2	L	126	LEU	2.3
1	K	146	GLN	2.3
2	J	198	GLN	2.3
2	L	9	ARG	2.3
1	C	17	PRO	2.3
2	H	287	GLY	2.3
2	J	187	LEU	2.3
1	E	16	TYR	2.3
2	F	241	PHE	2.3
2	F	90	GLN	2.3
2	H	326	ILE	2.2
1	C	46	GLY	2.2
2	B	50	LEU	2.2
2	B	221	SER	2.2
2	D	162	SER	2.2
1	A	208	ARG	2.2
1	I	199	ASP	2.2
2	B	74	GLU	2.2
1	A	155	MET	2.2
1	G	163	ALA	2.2
2	F	50	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	290	ALA	2.2
2	H	302	PHE	2.2
1	E	66	THR	2.2
2	F	243	THR	2.2
1	G	200	ARG	2.2
2	H	83	SER	2.2
2	F	330	ASN	2.2
2	L	330	ASN	2.2
2	D	78	GLU	2.2
2	J	195	ILE	2.2
2	F	7	ASP	2.2
2	H	126	LEU	2.2
2	J	51	ALA	2.2
2	L	220	ARG	2.2
2	L	268	ILE	2.2
2	H	304	LEU	2.2
2	H	319	LEU	2.2
2	L	192	GLU	2.2
1	I	163	ALA	2.2
2	B	320	GLY	2.2
2	H	40	GLY	2.2
1	E	198	HIS	2.2
2	F	179	HIS	2.2
2	F	234	SER	2.2
2	L	299	SER	2.2
1	C	163	ALA	2.2
1	E	37	GLU	2.2
2	L	10	ALA	2.2
1	I	36	GLY	2.2
2	H	114	PRO	2.2
2	L	207	LYS	2.2
1	G	24	THR	2.1
2	L	161	TYR	2.1
2	B	5	ILE	2.1
2	H	81	LYS	2.1
2	J	56	VAL	2.1
2	J	183	VAL	2.1
2	J	306	TRP	2.1
2	J	151	THR	2.1
2	H	216	TYR	2.1
1	K	61	GLU	2.1
2	B	114	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	130	GLU	2.1
2	L	63	SER	2.1
1	I	164	ASP	2.1
1	A	218	LEU	2.1
1	I	223	LEU	2.1
1	E	153	ALA	2.1
1	G	3	ALA	2.1
2	D	76	GLN	2.1
1	A	102	GLU	2.1
1	C	32	GLU	2.1
2	B	119	GLY	2.1
2	L	66	GLU	2.1
1	A	47	SER	2.1
1	E	50	SER	2.1
1	I	54	SER	2.1
2	J	221	SER	2.1
1	E	205	TYR	2.1
2	D	99	ALA	2.1
1	A	19	GLY	2.1
2	H	85	PRO	2.1
2	L	67	PHE	2.1
2	D	152	VAL	2.1
2	L	88	VAL	2.1
1	A	117	LYS	2.1
2	F	135	LEU	2.1
1	C	24	THR	2.1
2	H	161	TYR	2.1
2	H	243	THR	2.1
1	K	169	ALA	2.1
2	J	305	GLY	2.1
1	E	5	PRO	2.1
2	B	109	GLU	2.1
1	A	105	LEU	2.0
2	D	142	HIS	2.0
2	J	80	TRP	2.0
2	B	274	ALA	2.0
1	C	65	GLY	2.0
1	C	91	GLN	2.0
1	I	91	GLN	2.0
2	J	40	GLY	2.0
2	D	156	VAL	2.0
2	D	167	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	203	VAL	2.0
2	D	49	ALA	2.0
2	H	101	THR	2.0
2	H	149	THR	2.0
2	L	149	THR	2.0
2	D	65	PRO	2.0
2	H	211	GLN	2.0
1	E	15	VAL	2.0
1	G	196	VAL	2.0
2	D	331	VAL	2.0
2	H	176	LEU	2.0
2	J	32	LEU	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](#)

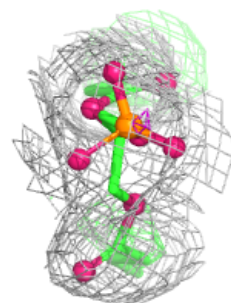
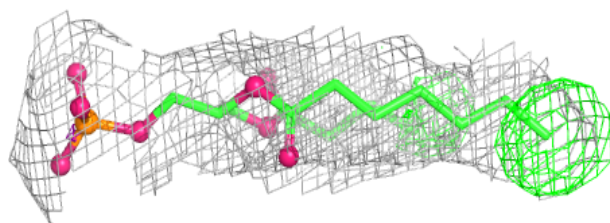
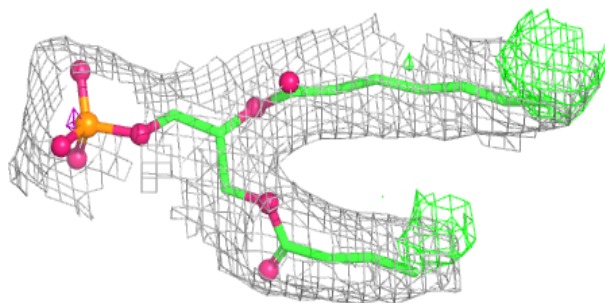
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	D	402	7/7	0.59	0.38	172,172,172,172	0
6	PEG	H	402	7/7	0.61	0.31	172,172,172,172	0
3	AGA	B	501	23/30	0.65	0.29	142,142,142,142	0
4	PGE	B	502	10/10	0.74	0.16	132,132,132,132	0
5	MNR	H	401	43/43	0.87	0.21	179,179,179,179	0
5	MNR	D	401	43/43	0.92	0.16	119,119,119,119	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.

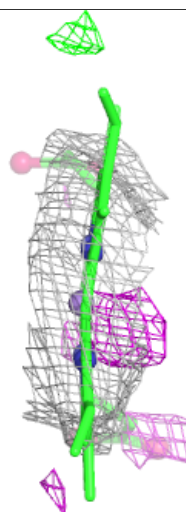
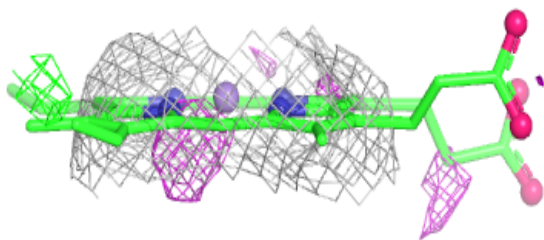
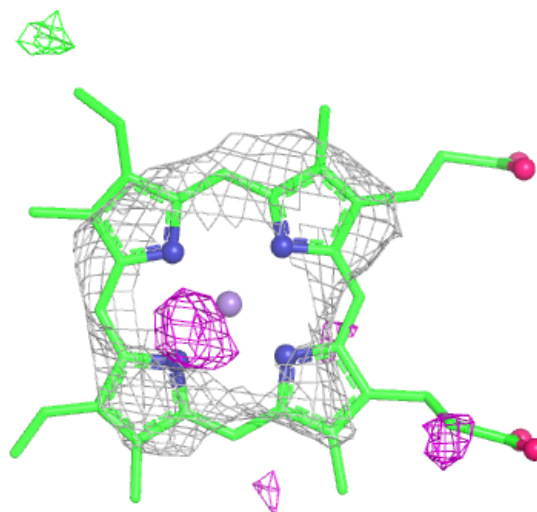
Electron density around AGA B 501:

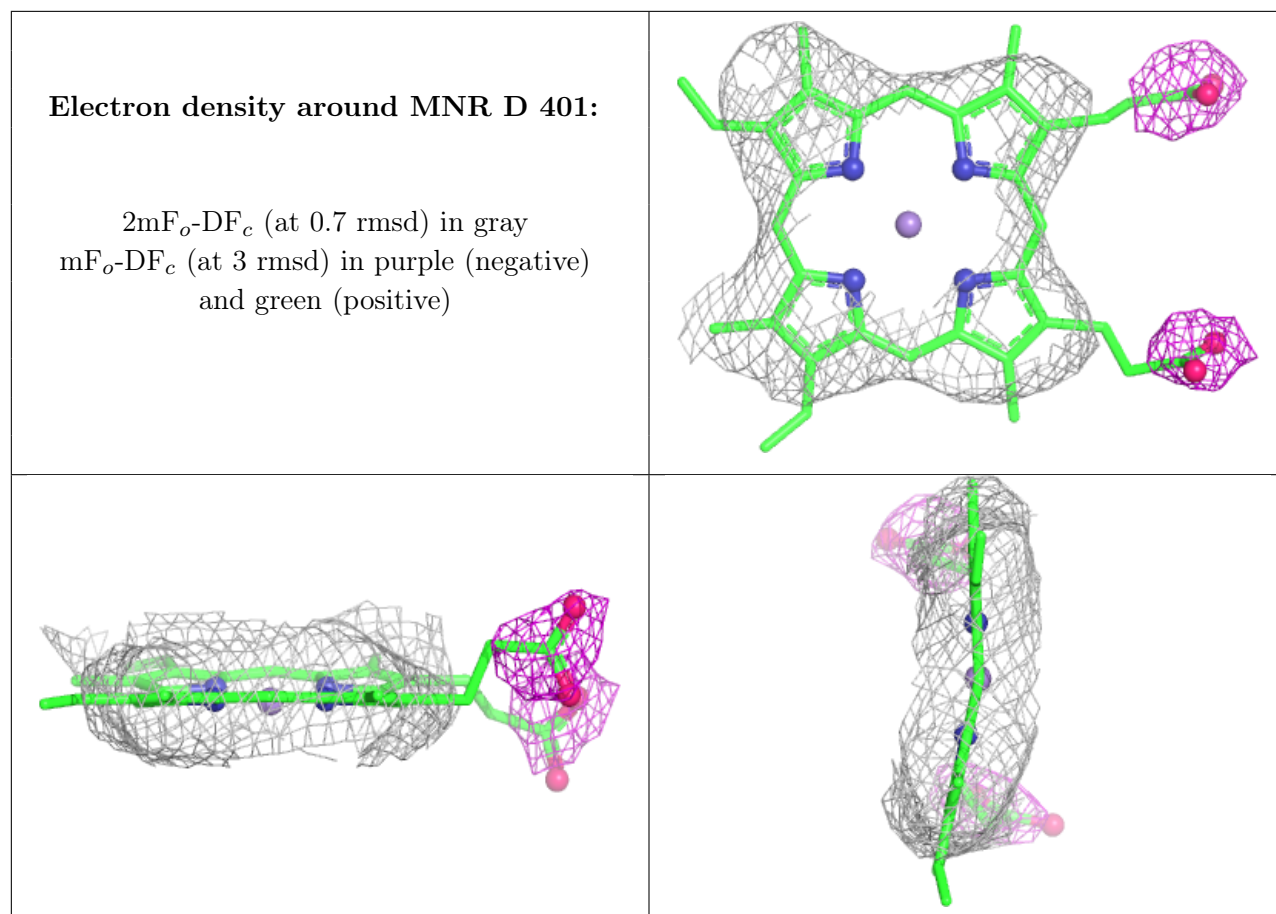
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MNR H 401:

$2mF_o-DF_c$ (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.