



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:08 AM JST

PDB ID : 7W7A / pdb_00007w7a
Title : Heme exporter in complex with Mn-containing protoporphyrin IX, Mn-anomalous data
Authors : Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shirouzu, M.; Shiro, Y.
Deposited on : 2021-12-04
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

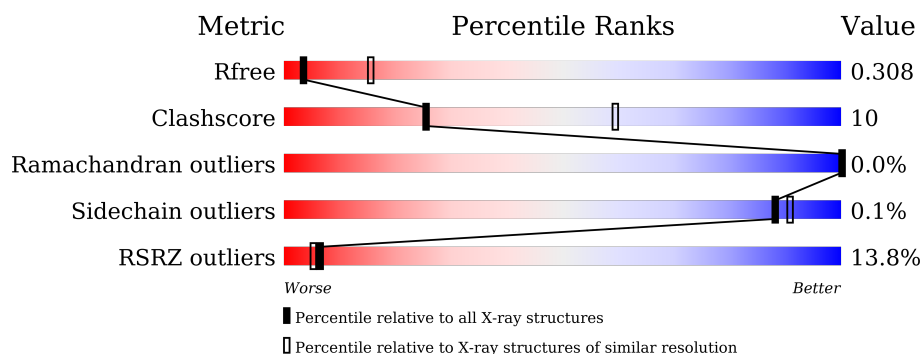
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	231	12% 71% 23% 6%
1	C	231	8% 76% 18% 6%
1	E	231	10% 73% 19% 8%
1	G	231	8% 78% 20% •
1	I	231	10% 65% 31% •
1	K	231	5% 76% 20% •

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Mol	Chain	Length	Quality of chain
2	B	344	16% 81% 18%
2	D	344	16% 83% 17%
2	F	344	18% 82% 18%
2	H	344	19% 80% 20%
2	J	344	15% 76% 24%
2	L	344	16% 82% 18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25102 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	217	Total	C	N	O	S	0	0	0
			1623	1013	294	313	3			
1	E	213	Total	C	N	O	S	0	0	0
			1600	998	290	309	3			
1	G	227	Total	C	N	O	S	0	0	0
			1703	1065	309	326	3			
1	I	222	Total	C	N	O	S	0	0	0
			1657	1034	300	320	3			
1	K	222	Total	C	N	O	S	0	0	0
			1670	1045	302	320	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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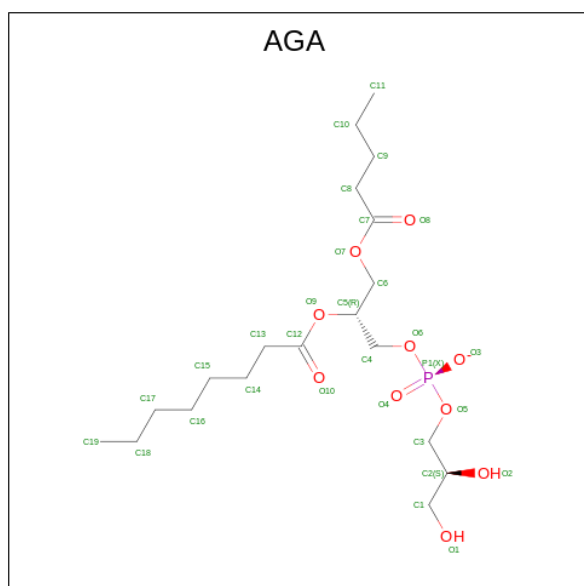
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Chain	Residue	Modelled	Actual	Comment	Reference
K	231	LYS	-	expression tag	UNP Q6NEF2

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

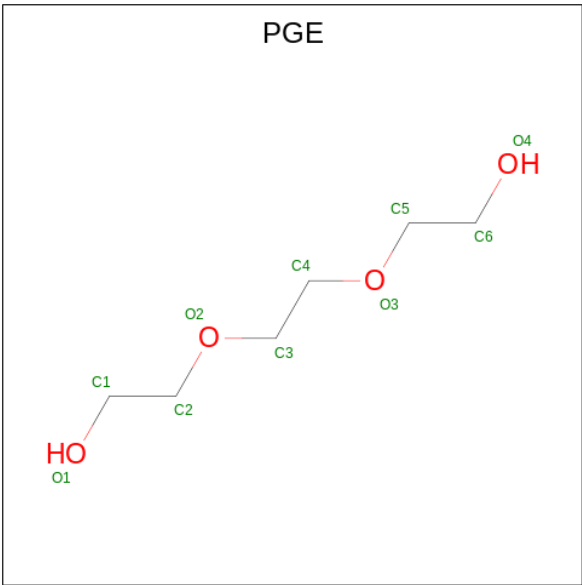
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	341	Total	C	N	O	S	0	0	0
			2510	1612	422	471	5			
2	D	342	Total	C	N	O	S	0	0	0
			2515	1615	423	472	5			
2	F	342	Total	C	N	O	S	0	0	0
			2515	1615	423	472	5			
2	H	342	Total	C	N	O	S	0	0	0
			2515	1615	423	472	5			
2	J	343	Total	C	N	O	S	0	0	0
			2522	1619	424	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).



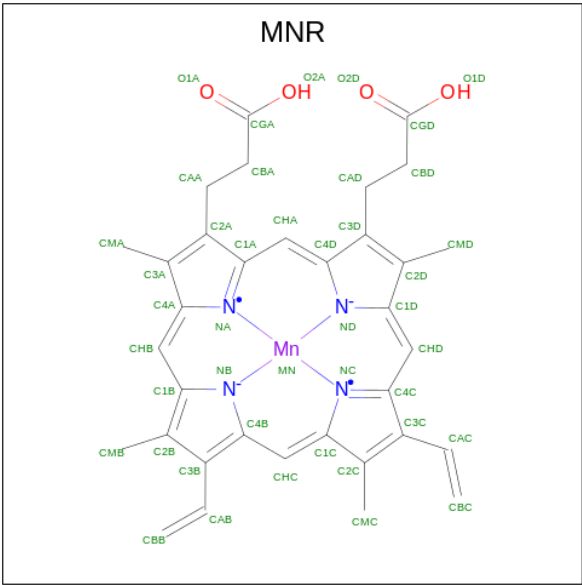
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			25	16	8	1		

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



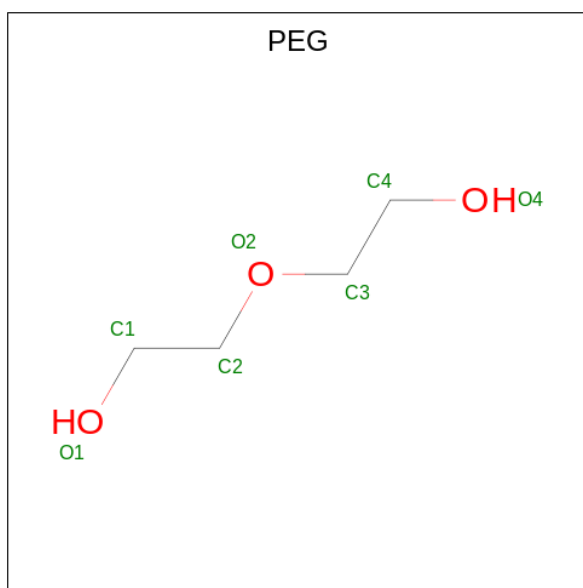
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		

- 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).



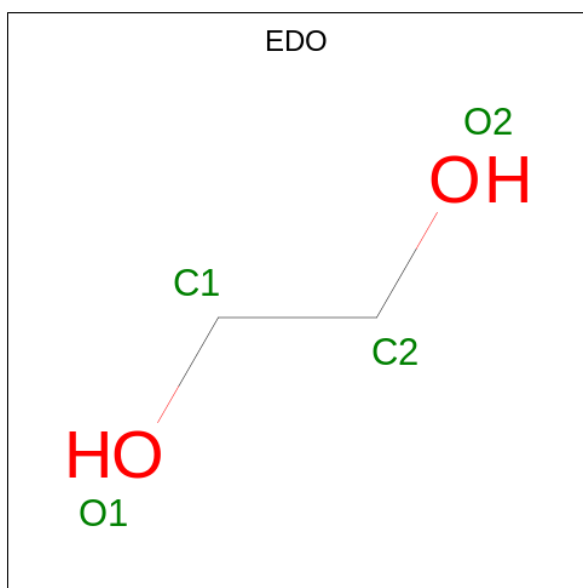
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Mn	N	O	0
			43	34	1	4	4	
5	H	1	Total	C	Mn	N	O	0
			43	34	1	4	4	

- 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		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

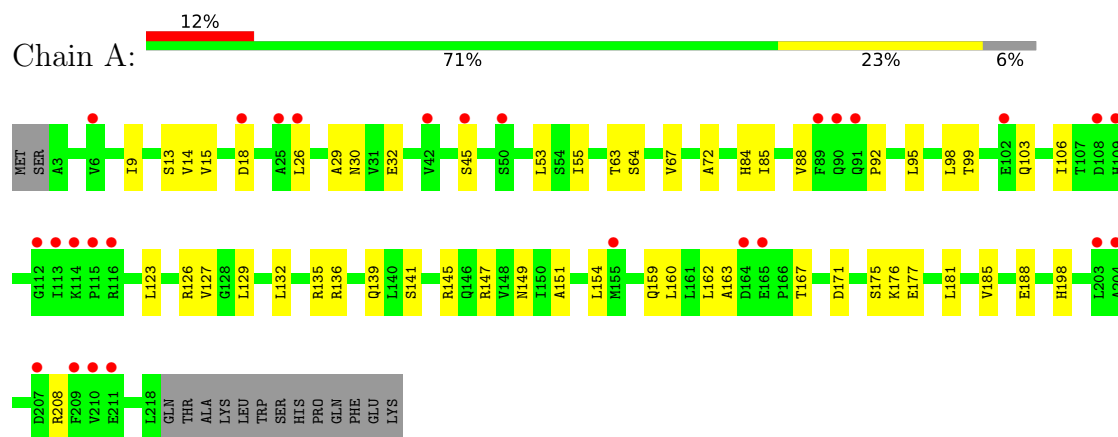


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			4	2	2		

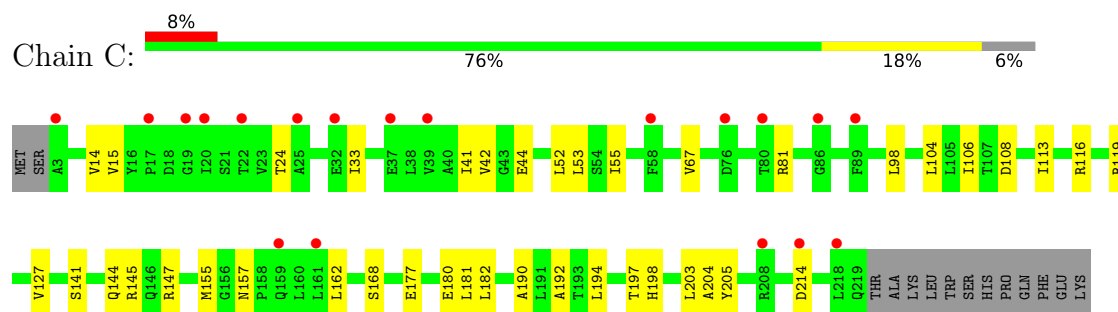
3 Residue-property plots [i](#)

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.

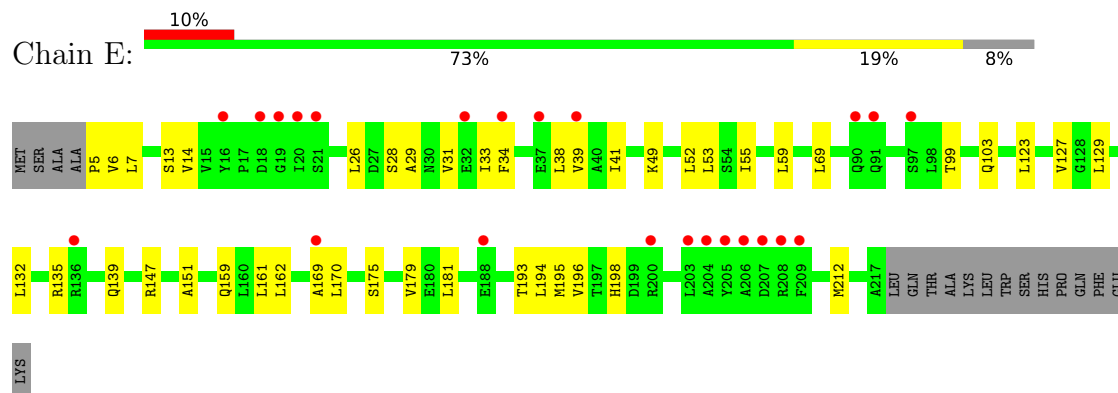
- Molecule 1: Putative ABC transport system, ATP-binding protein



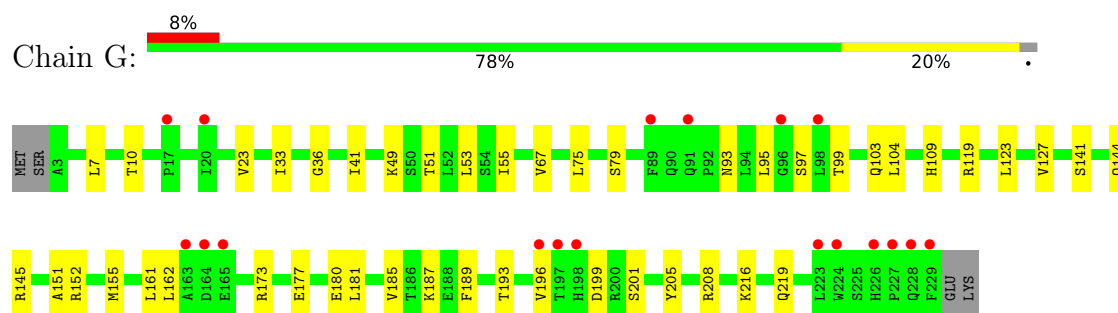
- Molecule 1: Putative ABC transport system, ATP-binding protein



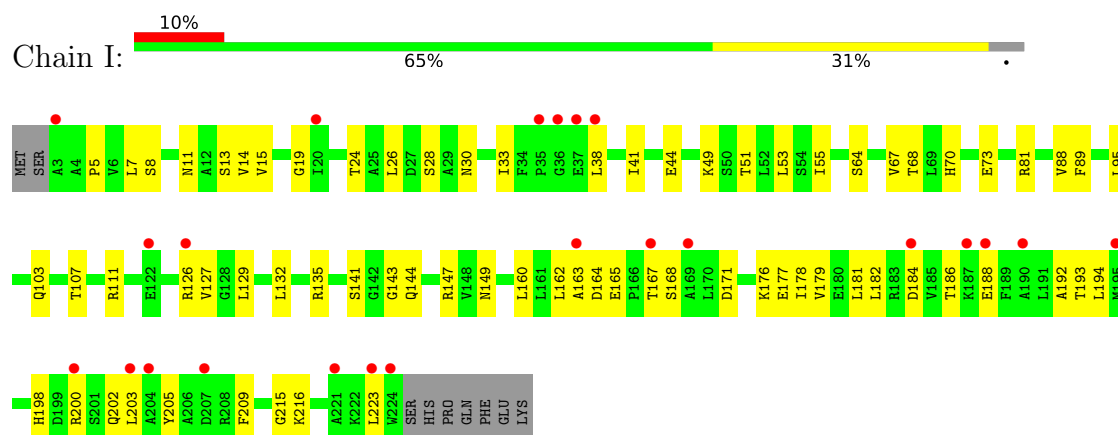
- Molecule 1: Putative ABC transport system, ATP-binding protein



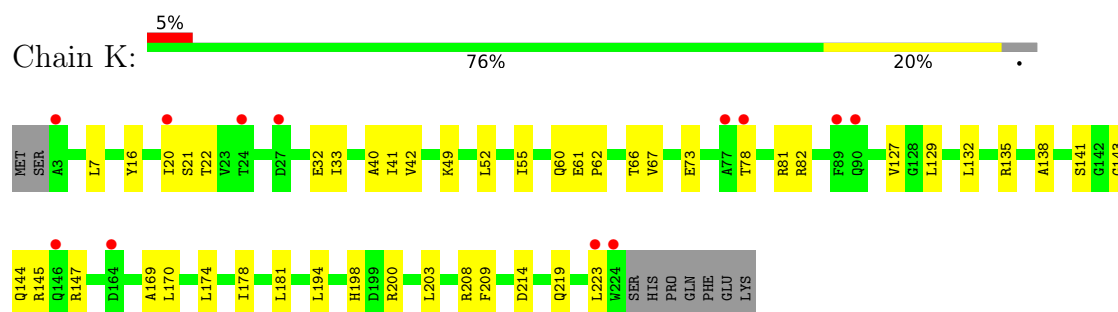
- Molecule 1: Putative ABC transport system, ATP-binding protein



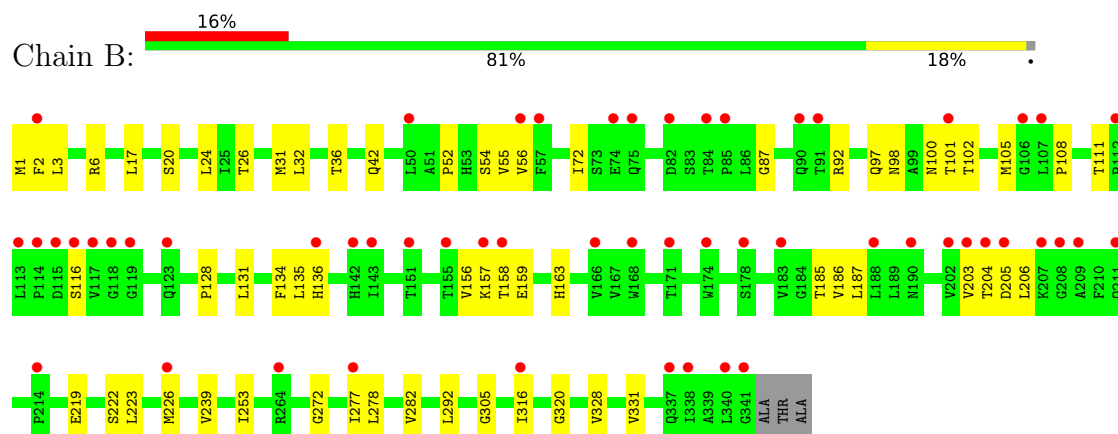
- Molecule 1: Putative ABC transport system, ATP-binding protein



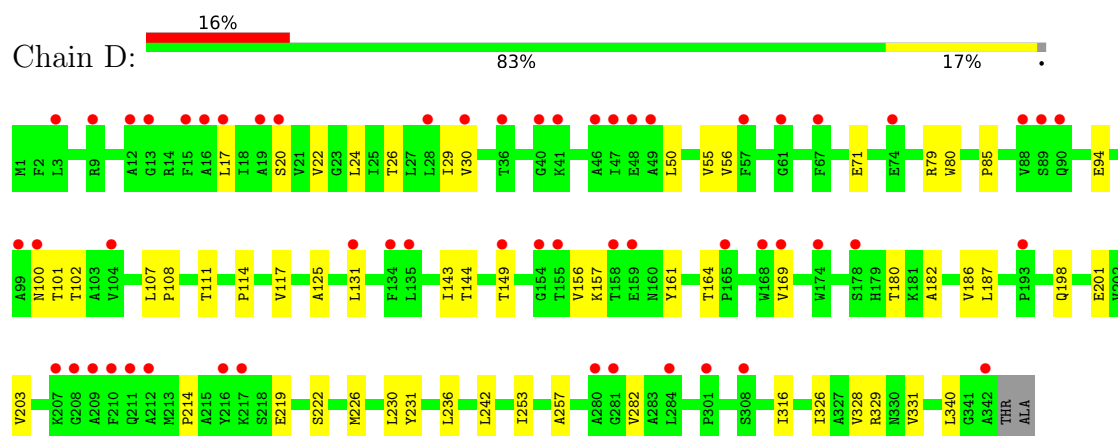
- Molecule 1: Putative ABC transport system, ATP-binding protein



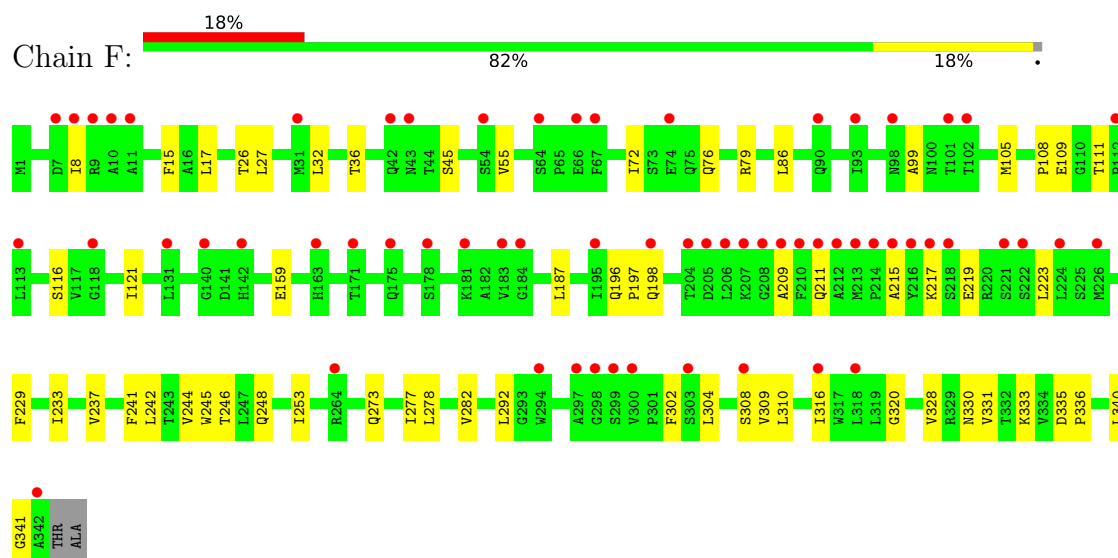
- Molecule 2: Putative ABC transport system integral membrane protein



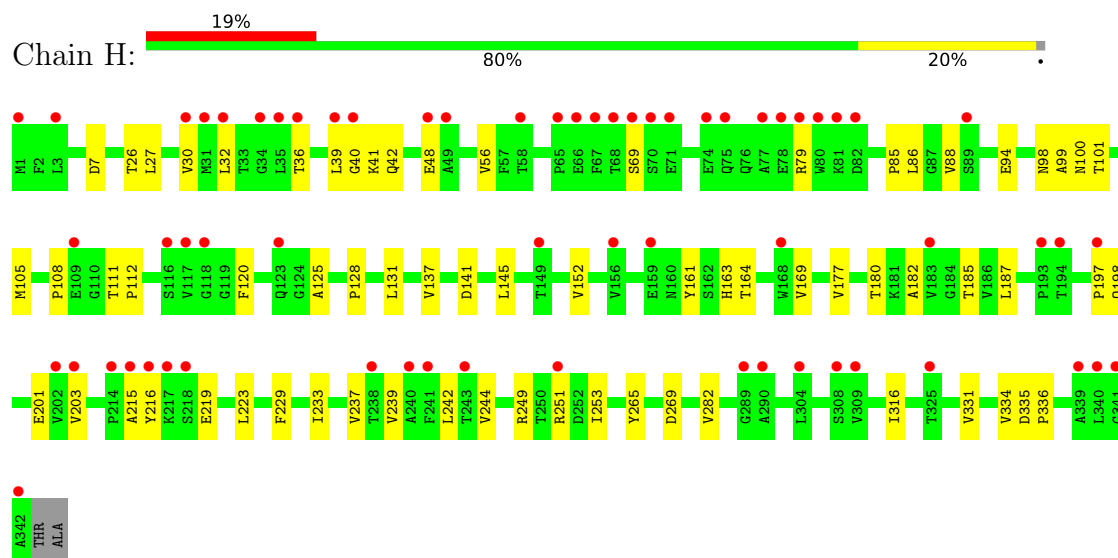
• Molecule 2: Putative ABC transport system integral membrane protein



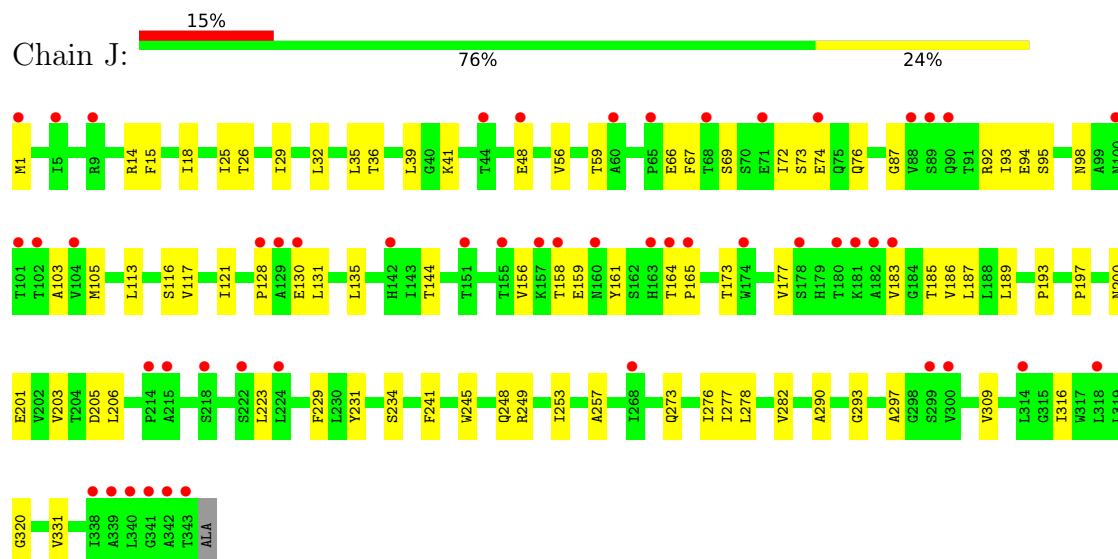
• Molecule 2: Putative ABC transport system integral membrane protein



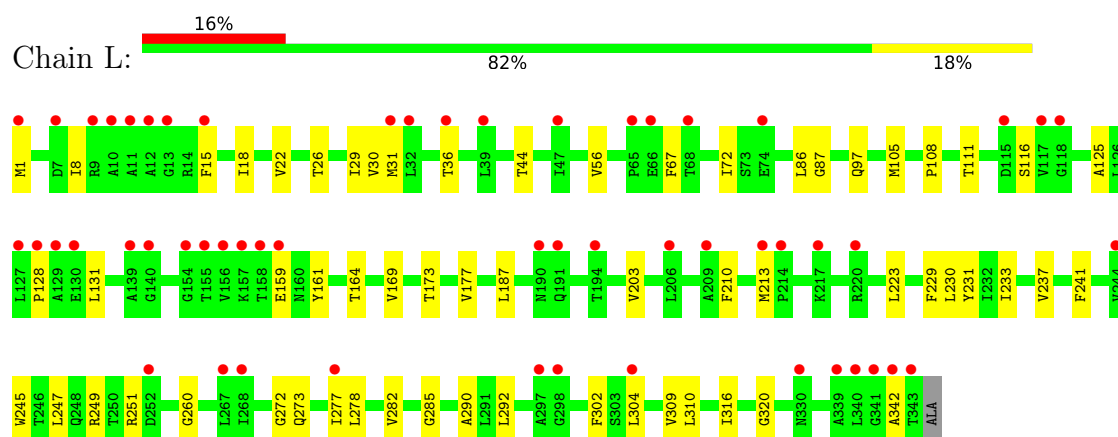
• Molecule 2: Putative ABC transport system integral membrane protein



● Molecule 2: Putative ABC transport system integral membrane protein



● Molecule 2: Putative ABC transport system integral membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.49Å 133.67Å 159.84Å 111.81° 99.83° 94.43°	Depositor
Resolution (Å)	48.82 – 3.20 48.82 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.82-3.20) 83.1 (48.82-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.264 , 0.303 0.267 , 0.308	Depositor DCC
R_{free} test set	4667 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	25102	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: AGA, PGE, MNR, PEG, EDO

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	0.16	0/1637	0.45	0/2216
1	C	0.17	0/1642	0.44	0/2223
1	E	0.14	0/1619	0.43	0/2190
1	G	0.17	0/1726	0.43	0/2339
1	I	0.17	0/1676	0.44	0/2270
1	K	0.16	0/1691	0.44	0/2290
2	B	0.15	0/2556	0.42	0/3495
2	D	0.14	0/2561	0.42	0/3502
2	F	0.15	0/2561	0.40	0/3502
2	H	0.17	0/2561	0.42	0/3502
2	J	0.15	0/2568	0.41	0/3512
2	L	0.13	0/2568	0.40	0/3512
All	All	0.15	0/25366	0.42	0/34553

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

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	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	1666	33	0
1	E	1600	0	1644	29	0
1	G	1703	0	1741	30	0
1	I	1657	0	1699	54	1
1	K	1670	0	1718	40	0
2	B	2510	0	2588	45	0
2	D	2515	0	2593	51	0
2	F	2515	0	2593	51	0
2	H	2515	0	2593	50	0
2	J	2522	0	2600	54	0
2	L	2522	0	2600	45	0
3	B	25	0	29	0	0
4	B	10	0	14	1	0
5	D	43	0	30	6	0
5	H	43	0	30	10	0
6	D	7	0	10	0	0
7	H	4	0	6	0	0
All	All	25102	0	25818	489	1

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 10.

All (489) 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:D:55:VAL:CG1	2:D:186:VAL:HG11	1.90	1.01
2:D:55:VAL:CG1	2:D:186:VAL:CG1	2.51	0.89
1:A:53:LEU:HD11	1:A:162:LEU:HB3	1.54	0.88
1:I:132:LEU:HB3	1:I:135:ARG:HD3	1.58	0.85
2:F:304:LEU:HD21	2:F:309:VAL:HG23	1.58	0.85
1:E:127:VAL:HG13	1:E:181:LEU:HD21	1.60	0.83
1:A:72:ALA:HB2	1:A:84:HIS:HD2	1.42	0.83
1:E:53:LEU:HD11	1:E:162:LEU:HB3	1.64	0.80
2:H:180:THR:HG22	2:H:182:ALA:H	1.48	0.79
1:G:127:VAL:HG13	1:G:181:LEU:HD21	1.65	0.79
1:I:127:VAL:HG13	1:I:181:LEU:HD21	1.66	0.77
2:D:108:PRO:HG2	2:D:111:THR:HG21	1.67	0.76
2:D:186:VAL:HG12	2:D:187:LEU:N	1.98	0.76
1:I:95:LEU:O	1:I:103:GLN:NE2	2.20	0.75
2:D:253:ILE:HD13	2:D:331:VAL:HG23	1.69	0.74
2:H:86:LEU:HD21	2:H:105:MET:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:VAL:HG13	2:D:186:VAL:CG1	2.17	0.74
2:B:305:GLY:HA2	4:B:502:PGE:H2	1.70	0.72
2:F:116:SER:OG	2:F:159:GLU:OE2	2.05	0.72
1:C:53:LEU:HD11	1:C:162:LEU:HB3	1.71	0.71
2:D:326:ILE:O	2:D:329:ARG:NH1	2.23	0.71
1:K:55:ILE:HD11	1:K:62:PRO:HG3	1.73	0.70
1:I:198:HIS:HB3	1:K:198:HIS:CE1	2.27	0.69
1:C:104:LEU:HB3	1:C:155:MET:HG3	1.74	0.69
1:C:55:ILE:HG23	1:C:67:VAL:HG21	1.75	0.69
1:A:127:VAL:HG13	1:A:181:LEU:HD21	1.75	0.69
1:E:13:SER:HB3	1:E:28:SER:H	1.58	0.69
2:L:251:ARG:HH12	2:L:342:ALA:HA	1.58	0.69
2:F:79:ARG:NH2	2:F:198:GLN:OE1	2.26	0.68
2:D:55:VAL:HG11	2:D:186:VAL:HG11	1.74	0.68
2:D:180:THR:HG22	2:D:182:ALA:H	1.60	0.67
1:E:7:LEU:HD23	1:E:33:ILE:HD13	1.77	0.66
2:J:253:ILE:HD13	2:J:331:VAL:HG13	1.78	0.66
1:K:127:VAL:HG13	1:K:181:LEU:HD21	1.78	0.66
2:J:245:TRP:NE1	2:J:273:GLN:OE1	2.28	0.66
1:C:127:VAL:HG13	1:C:181:LEU:HD21	1.77	0.66
2:F:196:GLN:HG3	2:F:197:PRO:HD2	1.78	0.65
2:B:26:THR:HG21	2:B:282:VAL:HG22	1.76	0.65
1:G:7:LEU:HB3	1:G:33:ILE:HG22	1.78	0.65
2:F:17:LEU:HD21	2:H:239:VAL:HG12	1.77	0.65
2:B:72:ILE:HG12	2:B:187:LEU:HG	1.78	0.65
2:L:72:ILE:HG12	2:L:187:LEU:HG	1.78	0.65
1:I:8:SER:OG	1:I:68:THR:OG1	2.15	0.64
2:B:253:ILE:HD13	2:B:331:VAL:HG23	1.78	0.64
1:I:147:ARG:NH2	1:I:177:GLU:OE1	2.31	0.64
2:D:186:VAL:CG1	2:D:187:LEU:N	2.60	0.64
2:B:128:PRO:HB3	2:B:158:THR:HG22	1.80	0.63
2:D:56:VAL:HG22	2:D:203:VAL:HG22	1.80	0.63
2:J:116:SER:OG	2:J:159:GLU:OE2	2.08	0.63
1:G:51:THR:O	1:G:55:ILE:HG12	1.99	0.63
2:J:92:ARG:NH1	2:J:94:GLU:OE1	2.30	0.62
1:E:135:ARG:NH2	1:E:139:GLN:O	2.31	0.62
1:I:182:LEU:O	1:I:186:THR:HG23	1.98	0.62
1:K:78:THR:HG22	1:K:81:ARG:HH22	1.65	0.62
1:K:41:ILE:HD11	1:K:194:LEU:HD22	1.81	0.62
1:E:59:LEU:HD13	2:F:340:LEU:HD11	1.82	0.62
2:B:116:SER:OG	2:B:159:GLU:OE2	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:72:ILE:HG12	2:J:187:LEU:HG	1.80	0.61
1:A:72:ALA:HB2	1:A:84:HIS:CD2	2.29	0.61
2:J:32:LEU:O	2:J:36:THR:HG23	2.00	0.61
2:B:36:THR:HG22	2:B:223:LEU:HB3	1.83	0.61
2:D:156:VAL:HG12	2:D:157:LYS:H	1.66	0.61
1:C:14:VAL:HG23	1:C:55:ILE:HD11	1.83	0.60
1:K:132:LEU:HD22	1:K:135:ARG:HE	1.65	0.60
2:B:31:MET:HE1	2:B:292:LEU:HB2	1.84	0.60
2:L:245:TRP:NE1	2:L:273:GLN:OE1	2.34	0.60
1:G:53:LEU:HD11	1:G:162:LEU:HB3	1.82	0.60
2:J:290:ALA:HB2	2:J:309:VAL:HG21	1.84	0.60
1:A:32:GLU:O	1:A:208:ARG:NH2	2.35	0.60
1:E:14:VAL:HG23	1:E:55:ILE:HD11	1.84	0.60
1:C:81:ARG:NH1	2:D:257:ALA:O	2.30	0.60
2:F:245:TRP:NE1	2:F:273:GLN:OE1	2.35	0.59
2:F:304:LEU:CD2	2:F:309:VAL:HG23	2.32	0.59
1:I:7:LEU:HB3	1:I:33:ILE:HG22	1.85	0.59
2:L:31:MET:HE1	2:L:292:LEU:HD23	1.82	0.59
2:D:85:PRO:HD2	2:D:108:PRO:HG3	1.85	0.59
2:H:26:THR:HG21	2:H:282:VAL:HG22	1.83	0.59
2:L:56:VAL:HG22	2:L:203:VAL:HG22	1.83	0.59
2:H:197:PRO:HB2	2:H:201:GLU:HB2	1.85	0.59
1:G:10:THR:HG21	1:K:73:GLU:HG2	1.85	0.58
2:F:211:GLN:HG3	2:F:217:LYS:HD2	1.85	0.58
1:K:208:ARG:NH1	1:K:219:GLN:OE1	2.35	0.58
2:J:1:MET:HE1	2:J:276:ILE:HD11	1.85	0.58
2:J:117:VAL:HG13	2:J:156:VAL:HB	1.86	0.58
2:L:29:ILE:HD11	2:L:230:LEU:HB2	1.84	0.58
2:D:94:GLU:HB3	2:D:144:THR:HB	1.85	0.58
2:F:32:LEU:O	2:F:36:THR:HG23	2.02	0.58
2:H:32:LEU:O	2:H:36:THR:HG23	2.03	0.58
2:B:42:GLN:HG3	2:B:163:HIS:HA	1.86	0.58
2:B:156:VAL:HG12	2:B:157:LYS:N	2.19	0.58
2:F:302:PHE:CE2	2:F:304:LEU:HD12	2.38	0.58
2:J:130:GLU:OE1	2:J:158:THR:OG1	2.13	0.58
1:G:55:ILE:HG22	1:G:67:VAL:HG21	1.85	0.58
2:J:205:ASP:OD1	2:J:206:LEU:N	2.34	0.58
1:K:42:VAL:HG11	1:K:200:ARG:NH2	2.20	0.57
2:F:27:LEU:HD23	2:H:229:PHE:HE1	1.69	0.57
1:E:31:VAL:HG21	1:E:52:LEU:HD21	1.84	0.57
2:D:186:VAL:CG1	2:D:187:LEU:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:LEU:HB3	1:I:209:PHE:CE1	2.40	0.57
2:D:186:VAL:HG12	2:D:187:LEU:H	1.70	0.57
1:I:179:VAL:HG21	1:I:202:GLN:HG2	1.87	0.57
2:J:59:THR:N	2:J:200:ASN:O	2.29	0.57
1:K:55:ILE:HG12	1:K:67:VAL:HG21	1.86	0.57
2:L:245:TRP:NE1	2:L:249:ARG:HD2	2.20	0.57
1:E:49:LYS:HD2	1:E:196:VAL:HG13	1.85	0.57
2:D:102:THR:HG21	2:D:131:LEU:HD22	1.87	0.56
1:E:49:LYS:HZ1	1:E:198:HIS:CE1	2.23	0.56
1:A:26:LEU:HD21	1:A:29:ALA:HB2	1.86	0.56
2:D:219:GLU:HB2	5:D:401:MNR:C3A	2.35	0.56
2:D:26:THR:HG21	2:D:282:VAL:HG22	1.86	0.56
1:I:200:ARG:HA	1:I:203:LEU:HG	1.86	0.56
1:G:141:SER:O	1:G:145:ARG:HG3	2.05	0.55
2:H:94:GLU:HG3	2:H:99:ALA:HB2	1.88	0.55
2:J:26:THR:HG21	2:J:282:VAL:HG22	1.88	0.55
2:L:302:PHE:HE1	2:L:304:LEU:HD13	1.69	0.55
2:B:223:LEU:HD21	5:D:401:MNR:HMB3	1.89	0.55
1:K:42:VAL:HG21	1:K:203:LEU:HD21	1.87	0.55
1:G:208:ARG:NH2	1:G:219:GLN:OE1	2.39	0.55
1:I:49:LYS:HE3	1:I:198:HIS:CD2	2.41	0.55
1:K:61:GLU:N	1:K:61:GLU:OE1	2.39	0.55
2:L:302:PHE:CE1	2:L:304:LEU:HD13	2.42	0.55
1:C:147:ARG:NH2	1:C:177:GLU:OE1	2.36	0.55
1:K:82:ARG:HB2	2:L:260:GLY:HA3	1.88	0.55
1:G:104:LEU:HD23	1:G:152:ARG:HA	1.89	0.55
2:L:116:SER:OG	2:L:159:GLU:OE2	2.22	0.55
1:G:41:ILE:HB	1:G:196:VAL:HG22	1.89	0.55
1:A:123:LEU:O	1:A:127:VAL:HG23	2.06	0.54
1:I:126:ARG:NH2	1:I:188:GLU:OE1	2.39	0.54
2:H:335:ASP:OD1	2:H:336:PRO:HD2	2.08	0.54
2:D:100:ASN:OD1	2:D:101:THR:N	2.40	0.54
2:F:229:PHE:HE1	2:H:27:LEU:HD23	1.71	0.54
1:I:127:VAL:HG12	1:I:147:ARG:HB3	1.90	0.54
1:C:141:SER:OG	1:C:144:GLN:HG3	2.07	0.54
2:D:55:VAL:HG12	2:D:186:VAL:CG1	2.34	0.54
1:E:129:LEU:HD22	1:E:132:LEU:HD12	1.88	0.54
2:B:219:GLU:HB2	5:D:401:MNR:C1C	2.38	0.54
1:E:38:LEU:HD21	1:E:195:MET:HE2	1.90	0.54
2:J:14:ARG:NH1	2:J:248:GLN:OE1	2.36	0.53
2:B:219:GLU:HB2	5:D:401:MNR:C2C	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:VAL:HG12	2:D:17:LEU:HD21	1.91	0.53
1:I:51:THR:O	1:I:55:ILE:HG12	2.07	0.53
2:D:161:TYR:O	2:D:164:THR:OG1	2.25	0.53
1:A:99:THR:HG22	1:A:136:ARG:HG2	1.89	0.53
1:E:127:VAL:HG21	1:E:151:ALA:HB2	1.90	0.53
2:H:42:GLN:HG3	2:H:163:HIS:HA	1.90	0.53
1:K:40:ALA:HB3	1:K:209:PHE:HB3	1.88	0.53
1:A:171:ASP:HB2	1:C:214:ASP:OD1	2.08	0.53
2:B:128:PRO:HD2	2:B:131:LEU:HD23	1.91	0.53
1:K:52:LEU:O	1:K:55:ILE:HG22	2.08	0.53
2:B:32:LEU:O	2:B:36:THR:HG23	2.09	0.53
1:G:36:GLY:O	1:G:187:LYS:NZ	2.30	0.53
2:J:25:ILE:HG21	2:J:234:SER:HB3	1.91	0.53
1:G:173:ARG:O	1:G:177:GLU:HG3	2.09	0.53
2:H:41:LYS:NZ	2:H:48:GLU:OE1	2.35	0.53
1:A:167:THR:HB	1:A:175:SER:HB2	1.91	0.53
2:H:108:PRO:HD2	2:H:111:THR:HG21	1.90	0.53
2:H:249:ARG:NH2	2:H:269:ASP:OD2	2.29	0.53
2:H:137:VAL:HG13	2:H:141:ASP:HB2	1.91	0.52
2:B:55:VAL:O	2:B:204:THR:HG22	2.09	0.52
2:B:1:MET:HE1	2:B:272:GLY:HA3	1.91	0.52
2:L:125:ALA:HA	2:L:169:VAL:HG12	1.91	0.52
1:C:42:VAL:CG2	1:C:203:LEU:HD21	2.39	0.52
2:J:128:PRO:HG3	2:J:165:PRO:HB2	1.92	0.52
2:L:108:PRO:HD2	2:L:111:THR:HG21	1.92	0.52
1:A:127:VAL:O	1:A:147:ARG:HD3	2.10	0.52
2:H:161:TYR:O	2:H:164:THR:OG1	2.25	0.52
1:C:44:GLU:OE2	1:C:198:HIS:NE2	2.42	0.52
2:J:26:THR:HG22	2:J:316:ILE:HD13	1.91	0.52
2:L:161:TYR:O	2:L:164:THR:OG1	2.26	0.52
1:I:73:GLU:H	1:I:73:GLU:CD	2.16	0.52
2:J:161:TYR:O	2:J:164:THR:OG1	2.24	0.52
2:J:186:VAL:HG12	2:J:187:LEU:N	2.25	0.52
1:C:41:ILE:HD13	1:C:52:LEU:HD23	1.92	0.52
1:A:92:PRO:O	1:A:149:ASN:ND2	2.37	0.51
2:F:246:THR:HG21	2:F:328:VAL:HG22	1.92	0.51
1:A:14:VAL:HG23	1:A:55:ILE:HD11	1.91	0.51
1:C:119:ARG:NH1	1:C:155:MET:O	2.43	0.51
2:D:26:THR:HG22	2:D:316:ILE:HD13	1.93	0.51
2:L:278:LEU:HD13	2:L:320:GLY:HA3	1.92	0.51
1:A:95:LEU:HD13	2:B:3:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ARG:NH1	2:D:71:GLU:OE2	2.43	0.51
2:F:108:PRO:HG2	2:F:111:THR:HG21	1.93	0.51
1:C:15:VAL:HG22	1:C:24:THR:HA	1.93	0.51
2:H:88:VAL:HG22	2:H:105:MET:HG2	1.93	0.51
2:H:125:ALA:HA	2:H:169:VAL:HG12	1.92	0.51
1:E:6:VAL:HG11	1:E:159:GLN:O	2.11	0.51
2:L:29:ILE:HD12	2:L:231:TYR:CE1	2.46	0.51
1:C:42:VAL:HG21	1:C:203:LEU:HD21	1.93	0.51
1:G:97:SER:OG	2:H:7:ASP:OD1	2.24	0.51
2:F:72:ILE:HG12	2:F:187:LEU:HG	1.93	0.51
1:K:127:VAL:HG12	1:K:147:ARG:HB3	1.93	0.51
2:H:128:PRO:HG2	2:H:131:LEU:HB3	1.93	0.51
2:J:29:ILE:HD13	2:J:231:TYR:CD2	2.46	0.51
1:K:21:SER:OG	1:K:22:THR:N	2.44	0.51
1:A:147:ARG:NH2	1:A:177:GLU:OE1	2.44	0.50
1:K:141:SER:OG	1:K:144:GLN:HG3	2.11	0.50
2:F:26:THR:HG22	2:F:316:ILE:HD13	1.93	0.50
1:I:126:ARG:HH22	1:I:184:ASP:CG	2.19	0.50
1:K:32:GLU:O	1:K:208:ARG:NH2	2.20	0.50
2:L:26:THR:HG21	2:L:282:VAL:HA	1.93	0.50
1:A:13:SER:OG	1:A:64:SER:OG	2.28	0.50
1:A:126:ARG:NH2	1:A:188:GLU:OE1	2.39	0.50
2:H:253:ILE:HD13	2:H:331:VAL:HG13	1.93	0.50
2:D:125:ALA:HA	2:D:169:VAL:HG12	1.93	0.50
1:I:176:LYS:HZ3	1:I:205:TYR:HH	1.51	0.50
1:C:141:SER:O	1:C:145:ARG:HG3	2.12	0.50
2:H:145:LEU:HG	2:H:177:VAL:HG11	1.93	0.50
1:I:55:ILE:HG22	1:I:67:VAL:HG21	1.94	0.50
2:H:56:VAL:HB	2:H:187:LEU:HB2	1.93	0.50
1:I:143:GLY:O	1:I:147:ARG:HG3	2.11	0.50
2:F:241:PHE:HD2	2:F:242:LEU:HD22	1.75	0.49
1:I:167:THR:O	1:I:167:THR:OG1	2.28	0.49
1:A:45:SER:HB3	1:C:168:SER:O	2.12	0.49
1:C:198:HIS:O	1:C:198:HIS:ND1	2.34	0.49
2:J:66:GLU:HB2	2:J:69:SER:OG	2.12	0.49
1:A:135:ARG:HD2	1:A:139:GLN:HB3	1.95	0.49
2:H:39:LEU:HD11	5:H:401:MNR:HHC	1.95	0.49
1:C:127:VAL:HG11	1:C:147:ARG:O	2.13	0.49
1:A:127:VAL:HG21	1:A:151:ALA:HB2	1.93	0.49
2:F:244:VAL:HG12	2:H:244:VAL:HG12	1.94	0.49
1:I:15:VAL:HG22	1:I:24:THR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:135:ARG:HH22	1:K:20:ILE:HG13	1.78	0.49
1:E:26:LEU:HD11	1:E:29:ALA:HB2	1.94	0.49
1:E:41:ILE:HG22	1:E:49:LYS:HB3	1.93	0.49
2:H:219:GLU:HB2	5:H:401:MNR:C3A	2.41	0.49
2:J:128:PRO:HG2	2:J:131:LEU:HB3	1.94	0.49
1:I:55:ILE:CG2	1:I:67:VAL:HG21	2.43	0.49
2:L:44:THR:HA	2:L:213:MET:HE1	1.94	0.49
1:G:180:GLU:HG2	1:G:205:TYR:CE1	2.48	0.48
2:B:278:LEU:HD13	2:B:320:GLY:HA3	1.96	0.48
1:G:127:VAL:HG21	1:G:151:ALA:HB2	1.95	0.48
1:I:19:GLY:HA2	1:K:138:ALA:O	2.14	0.48
1:G:199:ASP:OD2	1:G:201:SER:OG	2.18	0.48
2:H:26:THR:HG22	2:H:316:ILE:HD13	1.95	0.48
1:I:176:LYS:NZ	1:I:205:TYR:OH	2.30	0.48
2:B:98:ASN:HB2	2:B:135:LEU:HA	1.94	0.48
1:A:14:VAL:CG2	1:A:55:ILE:HD11	2.43	0.48
1:A:198:HIS:O	1:A:198:HIS:ND1	2.46	0.48
2:D:17:LEU:O	2:D:20:SER:OG	2.26	0.48
5:H:401:MNR:HMB1	5:H:401:MNR:HBB1	1.94	0.48
2:B:2:PHE:O	2:B:6:ARG:NH1	2.45	0.48
2:D:108:PRO:HG2	2:D:111:THR:CG2	2.40	0.48
1:I:203:LEU:HB3	1:I:209:PHE:HE1	1.78	0.48
1:K:132:LEU:HD13	1:K:135:ARG:HE	1.78	0.48
1:K:16:TYR:OH	1:K:60:GLN:NE2	2.34	0.48
2:F:253:ILE:HD13	2:F:331:VAL:HG23	1.96	0.48
2:J:14:ARG:O	2:J:18:ILE:HG13	2.14	0.48
1:E:175:SER:O	1:E:179:VAL:HG23	2.14	0.47
2:B:26:THR:HG22	2:B:316:ILE:HD13	1.96	0.47
1:E:39:VAL:HB	1:E:194:LEU:HD23	1.97	0.47
1:A:88:VAL:HA	1:A:149:ASN:OD1	2.15	0.47
2:H:26:THR:O	2:H:30:VAL:HG23	2.14	0.47
1:C:41:ILE:HG13	1:C:194:LEU:HD11	1.97	0.47
1:G:185:VAL:HG13	1:G:189:PHE:CD2	2.50	0.47
2:J:93:ILE:HA	2:J:144:THR:O	2.15	0.47
2:L:1:MET:SD	2:L:272:GLY:HA3	2.54	0.47
1:A:129:LEU:HD22	1:A:132:LEU:HD12	1.96	0.47
2:B:185:THR:HG23	2:B:186:VAL:HG22	1.97	0.47
2:B:328:VAL:O	2:B:331:VAL:HG12	2.15	0.47
2:F:223:LEU:HD21	5:H:401:MNR:HMB2	1.96	0.47
2:J:56:VAL:HG22	2:J:203:VAL:HG22	1.97	0.47
2:J:98:ASN:HB3	2:J:135:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:LEU:HD22	1:K:135:ARG:NE	2.30	0.47
1:C:108:ASP:OD2	1:C:116:ARG:HG2	2.15	0.47
2:J:36:THR:CG2	2:J:223:LEU:HB3	2.44	0.47
2:L:173:THR:O	2:L:177:VAL:HG23	2.15	0.47
2:B:97:GLN:HG3	2:B:136:HIS:HB2	1.97	0.47
1:C:180:GLU:HG2	1:C:205:TYR:CE1	2.50	0.47
2:F:8:ILE:HA	2:F:15:PHE:CD2	2.49	0.47
2:J:87:GLY:O	2:J:105:MET:HA	2.15	0.47
2:B:56:VAL:HB	2:B:187:LEU:HB2	1.97	0.46
1:C:190:ALA:HB1	1:K:66:THR:HG23	1.96	0.46
2:D:214:PRO:HG2	5:D:401:MNR:O1D	2.14	0.46
2:F:27:LEU:HD23	2:H:229:PHE:CE1	2.50	0.46
2:F:309:VAL:HG12	2:F:310:LEU:HD23	1.96	0.46
2:J:113:LEU:HD21	2:J:121:ILE:HD11	1.97	0.46
2:J:293:GLY:O	2:J:297:ALA:N	2.49	0.46
2:B:24:LEU:HD12	2:D:236:LEU:HD12	1.97	0.46
2:B:205:ASP:OD1	2:B:206:LEU:N	2.42	0.46
2:F:335:ASP:OD1	2:F:336:PRO:HD2	2.16	0.46
2:J:36:THR:HG22	2:J:223:LEU:HB3	1.96	0.46
2:L:86:LEU:HD21	2:L:105:MET:HE2	1.98	0.46
1:A:9:ILE:O	1:A:30:ASN:HA	2.15	0.46
2:B:100:ASN:OD1	2:B:101:THR:N	2.48	0.46
2:D:79:ARG:HH12	2:D:198:GLN:HB2	1.81	0.46
2:H:145:LEU:HD23	2:H:177:VAL:HG21	1.97	0.46
2:D:328:VAL:HG12	2:D:328:VAL:O	2.16	0.46
2:F:241:PHE:CE1	2:H:244:VAL:HG21	2.50	0.46
2:L:128:PRO:HG2	2:L:131:LEU:HB3	1.97	0.46
1:E:212:MET:HE2	1:E:212:MET:HB3	1.80	0.46
1:G:119:ARG:HD3	1:G:155:MET:HE3	1.98	0.46
2:J:245:TRP:NE1	2:J:249:ARG:HD2	2.31	0.46
1:G:109:HIS:HD1	2:H:265:TYR:HE1	1.63	0.46
1:I:44:GLU:HA	1:I:44:GLU:OE1	2.16	0.46
2:L:87:GLY:O	2:L:105:MET:HA	2.16	0.46
2:B:52:PRO:HD2	2:B:206:LEU:HD13	1.97	0.45
2:B:222:SER:O	2:B:226:MET:HG3	2.16	0.45
1:K:203:LEU:HD12	1:K:223:LEU:HD22	1.97	0.45
2:L:26:THR:HG21	2:L:282:VAL:HG22	1.97	0.45
2:F:215:ALA:HB1	5:H:401:MNR:HHD	1.99	0.45
2:L:29:ILE:HD11	2:L:230:LEU:CB	2.46	0.45
2:F:86:LEU:HD21	2:F:105:MET:HE2	1.98	0.45
2:F:219:GLU:HB2	5:H:401:MNR:C2C	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:229:PHE:O	2:F:233:ILE:HG13	2.17	0.45
2:F:233:ILE:O	2:F:237:VAL:HG23	2.16	0.45
2:F:304:LEU:HD23	2:F:308:SER:HB3	1.98	0.45
1:I:53:LEU:HD21	1:I:164:ASP:HB2	1.98	0.45
2:J:185:THR:HG23	2:J:186:VAL:HG23	1.98	0.45
2:B:156:VAL:HG12	2:B:157:LYS:H	1.82	0.45
1:A:88:VAL:HB	1:A:163:ALA:HA	1.99	0.45
1:I:53:LEU:HD11	1:I:162:LEU:HB3	1.99	0.45
1:I:141:SER:OG	1:I:144:GLN:HG3	2.17	0.45
1:I:216:LYS:HE2	1:I:216:LYS:HB2	1.77	0.45
2:B:108:PRO:HD2	2:B:111:THR:HG21	1.99	0.45
2:F:302:PHE:HE2	2:F:304:LEU:HD12	1.79	0.45
2:J:73:SER:OG	2:J:76:GLN:HB2	2.17	0.45
1:E:6:VAL:O	1:E:69:LEU:HD12	2.17	0.45
2:F:36:THR:HG22	2:F:223:LEU:HB3	1.99	0.45
2:F:278:LEU:HD13	2:F:320:GLY:HA3	1.99	0.45
2:H:56:VAL:HG22	2:H:203:VAL:HG22	1.99	0.45
2:H:86:LEU:O	2:H:185:THR:HG22	2.17	0.45
2:J:173:THR:O	2:J:177:VAL:HG23	2.17	0.45
1:G:55:ILE:CG2	1:G:67:VAL:HG21	2.48	0.44
2:L:229:PHE:O	2:L:233:ILE:HG13	2.17	0.44
1:C:41:ILE:CD1	1:C:194:LEU:HD11	2.47	0.44
2:D:26:THR:O	2:D:30:VAL:HG23	2.17	0.44
2:F:79:ARG:HH12	2:F:198:GLN:HG3	1.80	0.44
2:J:15:PHE:CD1	2:J:277:ILE:HG13	2.52	0.44
1:K:41:ILE:HG22	1:K:49:LYS:HG2	1.97	0.44
1:C:203:LEU:HD23	1:C:203:LEU:HA	1.71	0.44
1:I:200:ARG:HD3	1:I:223:LEU:HD21	1.99	0.44
2:J:74:GLU:HG2	2:J:183:VAL:HG13	1.99	0.44
1:K:7:LEU:HD23	1:K:33:ILE:HD12	2.00	0.44
1:G:141:SER:OG	1:G:144:GLN:HG3	2.18	0.44
2:H:233:ILE:O	2:H:237:VAL:HG23	2.18	0.44
2:B:87:GLY:O	2:B:105:MET:HA	2.18	0.44
1:G:75:LEU:HD22	1:G:79:SER:HB2	2.00	0.44
2:H:98:ASN:OD1	2:H:99:ALA:N	2.46	0.44
1:I:26:LEU:HD12	1:I:215:GLY:O	2.18	0.44
2:J:277:ILE:HD13	2:J:277:ILE:HA	1.87	0.44
2:L:26:THR:HG22	2:L:316:ILE:HD13	1.98	0.44
2:B:156:VAL:CG1	2:B:157:LYS:N	2.81	0.44
1:E:161:LEU:O	1:E:193:THR:HA	2.18	0.44
2:F:245:TRP:O	2:F:248:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:CG2	1:A:67:VAL:HG21	2.48	0.43
2:H:215:ALA:HB1	5:H:401:MNR:HHA	2.00	0.43
1:I:107:THR:O	1:I:111:ARG:HG3	2.18	0.43
2:J:95:SER:HB3	2:J:135:LEU:HD13	2.00	0.43
2:L:15:PHE:HB3	2:L:277:ILE:HD11	1.98	0.43
2:L:245:TRP:O	2:L:249:ARG:HG3	2.18	0.43
1:A:15:VAL:H	1:A:63:THR:HG21	1.83	0.43
1:I:88:VAL:HB	1:I:163:ALA:HA	2.00	0.43
2:J:29:ILE:HD13	2:J:231:TYR:HD2	1.82	0.43
2:L:309:VAL:HG12	2:L:310:LEU:HD23	2.00	0.43
1:A:141:SER:O	1:A:145:ARG:HG3	2.17	0.43
2:F:109:GLU:HA	2:F:121:ILE:HG22	1.99	0.43
2:D:55:VAL:HG13	2:D:186:VAL:HG12	1.99	0.43
1:I:160:LEU:HD12	1:I:192:ALA:O	2.18	0.43
1:K:42:VAL:CG2	1:K:203:LEU:HD21	2.47	0.43
1:K:209:PHE:CZ	1:K:223:LEU:HB2	2.53	0.43
2:J:231:TYR:O	2:J:234:SER:OG	2.28	0.43
2:L:247:LEU:HD23	2:L:247:LEU:HA	1.80	0.43
2:B:98:ASN:ND2	2:B:134:PHE:O	2.50	0.43
1:E:5:PRO:HA	1:E:34:PHE:HA	2.00	0.43
1:I:13:SER:HB3	1:I:28:SER:H	1.83	0.43
1:I:171:ASP:HB2	1:K:214:ASP:OD1	2.19	0.43
2:J:18:ILE:HG12	2:J:241:PHE:CD1	2.53	0.43
2:J:41:LYS:NZ	2:J:48:GLU:OE1	2.49	0.43
2:B:36:THR:CG2	2:B:223:LEU:HB3	2.47	0.43
2:H:40:GLY:HA2	2:H:216:TYR:HE1	1.84	0.43
2:H:112:PRO:HA	2:H:120:PHE:HD1	1.84	0.43
1:I:198:HIS:O	1:K:198:HIS:HE1	2.02	0.43
1:K:41:ILE:HD13	1:K:52:LEU:HD23	2.01	0.43
1:C:98:LEU:HD11	1:C:106:ILE:HD12	2.01	0.43
2:F:99:ALA:O	2:H:69:SER:OG	2.24	0.43
2:F:108:PRO:HG2	2:F:111:THR:CG2	2.49	0.43
1:I:186:THR:HG22	1:I:193:THR:OG1	2.19	0.43
1:A:18:ASP:CG	1:C:141:SER:HB2	2.43	0.43
2:H:86:LEU:HD11	2:H:105:MET:HB3	2.01	0.43
1:A:85:ILE:HG12	1:A:160:LEU:HB3	2.01	0.42
2:F:277:ILE:HD13	2:F:277:ILE:HA	1.89	0.42
2:J:67:PHE:HD2	2:J:161:TYR:OH	2.02	0.42
1:K:127:VAL:HG11	1:K:147:ARG:O	2.18	0.42
2:L:36:THR:HA	2:L:223:LEU:HD13	2.01	0.42
2:L:278:LEU:HD23	2:L:278:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:340:LEU:HD12	2:D:340:LEU:HA	1.86	0.42
1:G:161:LEU:O	1:G:193:THR:HA	2.20	0.42
5:H:401:MNR:HMD1	5:H:401:MNR:HBD1	2.02	0.42
2:J:103:ALA:HB2	2:J:164:THR:OG1	2.19	0.42
2:L:22:VAL:O	2:L:26:THR:HG23	2.20	0.42
2:F:26:THR:HG21	2:F:282:VAL:HG22	2.01	0.42
1:I:41:ILE:HD11	1:I:194:LEU:HD22	2.01	0.42
1:K:174:LEU:O	1:K:178:ILE:HG12	2.19	0.42
2:J:197:PRO:HB2	2:J:201:GLU:HB2	2.01	0.42
2:L:26:THR:O	2:L:30:VAL:HG23	2.19	0.42
2:D:242:LEU:HD23	2:D:242:LEU:HA	1.85	0.42
2:J:29:ILE:HG21	2:J:231:TYR:HE2	1.85	0.42
2:J:189:LEU:HD13	2:J:193:PRO:HB3	2.01	0.42
2:L:290:ALA:HB2	2:L:309:VAL:HG21	2.01	0.42
1:I:38:LEU:HD23	1:I:205:TYR:O	2.19	0.42
1:K:129:LEU:HD11	1:K:147:ARG:HB2	2.01	0.42
1:K:169:ALA:O	1:K:170:LEU:HD23	2.20	0.42
2:L:44:THR:HB	2:L:210:PHE:CE1	2.55	0.42
2:B:277:ILE:HD13	2:B:277:ILE:HA	1.86	0.42
2:H:79:ARG:HH22	2:H:198:GLN:CD	2.28	0.42
2:L:15:PHE:CD1	2:L:277:ILE:HG13	2.55	0.42
2:L:18:ILE:HG12	2:L:241:PHE:CD1	2.55	0.42
1:A:106:ILE:HD11	2:B:3:LEU:HB2	2.02	0.42
2:J:245:TRP:O	2:J:249:ARG:HG3	2.20	0.42
2:L:97:GLN:HG2	2:L:97:GLN:O	2.19	0.42
1:A:167:THR:HB	1:A:175:SER:CB	2.50	0.41
2:D:143:ILE:O	2:D:149:THR:HA	2.20	0.41
2:F:223:LEU:HD21	5:H:401:MNR:CMB	2.50	0.41
1:G:123:LEU:O	1:G:127:VAL:HG23	2.20	0.41
1:I:89:PHE:N	1:I:149:ASN:HD21	2.18	0.41
1:A:84:HIS:CG	1:A:159:GLN:HE21	2.37	0.41
2:B:54:SER:HB3	2:B:203:VAL:HG13	2.01	0.41
1:E:169:ALA:O	1:E:170:LEU:HD23	2.20	0.41
2:F:196:GLN:HG3	2:F:197:PRO:CD	2.49	0.41
1:I:5:PRO:O	1:I:70:HIS:ND1	2.53	0.41
2:B:32:LEU:HD13	2:D:226:MET:HE1	2.01	0.41
2:B:102:THR:HG21	2:B:131:LEU:CD2	2.50	0.41
1:E:123:LEU:O	1:E:127:VAL:HG23	2.20	0.41
2:H:85:PRO:HD2	2:H:108:PRO:CG	2.50	0.41
2:L:8:ILE:HD11	2:L:273:GLN:HG3	2.01	0.41
1:A:95:LEU:O	1:A:103:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:PRO:O	2:D:117:VAL:N	2.50	0.41
2:D:222:SER:O	2:D:226:MET:HG3	2.21	0.41
2:H:36:THR:HG22	2:H:223:LEU:HB3	2.03	0.41
2:J:278:LEU:HD13	2:J:320:GLY:HA3	2.02	0.41
1:C:108:ASP:OD1	1:C:113:ILE:HD11	2.21	0.41
1:C:204:ALA:HB1	1:G:216:LYS:HB3	2.03	0.41
2:D:156:VAL:HG12	2:D:157:LYS:N	2.33	0.41
2:F:72:ILE:HG23	2:F:76:GLN:HB3	2.03	0.41
1:A:98:LEU:HD11	1:A:106:ILE:HD12	2.02	0.41
1:E:127:VAL:HG12	1:E:147:ARG:HB3	2.02	0.41
2:F:278:LEU:HD23	2:F:278:LEU:HA	1.91	0.41
1:I:81:ARG:NH1	2:J:257:ALA:O	2.53	0.41
1:C:157:ASN:O	1:C:157:ASN:ND2	2.54	0.41
2:D:230:LEU:HD23	2:D:230:LEU:HA	1.82	0.41
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.89	0.41
1:G:23:VAL:O	1:G:23:VAL:HG13	2.21	0.41
1:C:33:ILE:HG22	1:C:192:ALA:HB1	2.03	0.41
2:D:24:LEU:HD23	2:D:24:LEU:HA	1.82	0.41
2:D:50:LEU:HD23	2:D:114:PRO:HD3	2.02	0.41
2:D:79:ARG:NH1	2:D:201:GLU:OE2	2.53	0.41
2:D:219:GLU:HB2	5:D:401:MNR:C4A	2.50	0.41
1:E:99:THR:O	1:E:103:GLN:HG2	2.21	0.41
2:F:45:SER:HB2	2:F:159:GLU:OE1	2.21	0.41
1:G:93:ASN:OD1	2:H:251:ARG:NH2	2.50	0.41
1:G:95:LEU:N	1:G:103:GLN:HE22	2.18	0.41
2:H:39:LEU:HD11	5:H:401:MNR:CHC	2.50	0.41
1:I:11:ASN:N	1:I:30:ASN:OD1	2.47	0.41
2:J:229:PHE:HD1	2:L:229:PHE:HB3	1.85	0.41
1:K:143:GLY:O	1:K:147:ARG:HG3	2.21	0.41
2:L:277:ILE:HD13	2:L:277:ILE:HA	1.83	0.41
2:D:107:LEU:HB3	2:D:108:PRO:HD2	2.01	0.41
1:E:41:ILE:HD13	1:E:52:LEU:HD23	2.03	0.41
1:E:127:VAL:O	1:E:147:ARG:HD3	2.21	0.41
1:I:13:SER:OG	1:I:64:SER:HB2	2.21	0.41
2:J:186:VAL:CG1	2:J:187:LEU:N	2.84	0.41
1:K:141:SER:O	1:K:145:ARG:HG3	2.21	0.41
2:D:22:VAL:O	2:D:26:THR:HG23	2.21	0.40
2:H:137:VAL:HG11	2:H:152:VAL:HG21	2.02	0.40
1:I:14:VAL:HG21	1:I:55:ILE:HD11	2.04	0.40
1:I:127:VAL:CG1	1:I:147:ARG:HB3	2.50	0.40
2:D:29:ILE:HG21	2:D:231:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:ARG:HG2	1:I:203:LEU:HD11	2.02	0.40
2:L:233:ILE:O	2:L:237:VAL:HG23	2.22	0.40
1:A:154:LEU:HD11	1:A:185:VAL:HG11	2.03	0.40
2:B:17:LEU:O	2:B:20:SER:OG	2.38	0.40
2:D:80:TRP:H	2:D:80:TRP:CD1	2.39	0.40
1:I:178:ILE:HD13	1:I:178:ILE:HA	1.94	0.40
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.87	0.40
2:F:302:PHE:CE2	2:F:304:LEU:HB2	2.57	0.40
2:F:330:ASN:OD1	2:F:333:LYS:HD2	2.21	0.40
1:G:49:LYS:HE3	1:G:49:LYS:HB2	1.84	0.40
1:G:99:THR:O	1:G:103:GLN:HG2	2.21	0.40
2:H:253:ILE:HG22	2:H:334:VAL:HG11	2.02	0.40
1:I:129:LEU:HD11	1:I:147:ARG:HB2	2.04	0.40
1:I:165:GLU:HB3	1:I:168:SER:OG	2.22	0.40
1:K:55:ILE:HD13	1:K:55:ILE:HG21	1.80	0.40
2:L:26:THR:OG1	2:L:285:GLY:HA3	2.22	0.40
1:C:127:VAL:HG12	1:C:127:VAL:O	2.22	0.40
2:F:55:VAL:HG11	2:F:209:ALA:HB2	2.04	0.40
2:F:292:LEU:HD12	2:F:292:LEU:HA	1.96	0.40
2:H:100:ASN:OD1	2:H:101:THR:N	2.49	0.40
2:H:242:LEU:HD23	2:H:242:LEU:HA	1.83	0.40
2:J:35:LEU:O	2:J:39:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:NZ	1:I:184:ASP:OD1[1_655]	2.13	0.07

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	214/231 (93%)	207 (97%)	7 (3%)	0	100	100
1	C	215/231 (93%)	211 (98%)	4 (2%)	0	100	100
1	E	211/231 (91%)	205 (97%)	6 (3%)	0	100	100
1	G	225/231 (97%)	218 (97%)	7 (3%)	0	100	100
1	I	220/231 (95%)	211 (96%)	9 (4%)	0	100	100
1	K	220/231 (95%)	215 (98%)	5 (2%)	0	100	100
2	B	339/344 (98%)	334 (98%)	5 (2%)	0	100	100
2	D	340/344 (99%)	335 (98%)	5 (2%)	0	100	100
2	F	340/344 (99%)	330 (97%)	9 (3%)	1 (0%)	36	68
2	H	340/344 (99%)	332 (98%)	8 (2%)	0	100	100
2	J	341/344 (99%)	333 (98%)	8 (2%)	0	100	100
2	L	341/344 (99%)	336 (98%)	5 (2%)	0	100	100
All	All	3346/3450 (97%)	3267 (98%)	78 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	341	GLY

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	172/186 (92%)	171 (99%)	1 (1%)	78	84
1	E	171/186 (92%)	171 (100%)	0	100	100
1	G	180/186 (97%)	180 (100%)	0	100	100
1	I	175/186 (94%)	175 (100%)	0	100	100
1	K	177/186 (95%)	177 (100%)	0	100	100
2	B	264/265 (100%)	264 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	264/265 (100%)	264 (100%)	0	100	100
2	F	264/265 (100%)	264 (100%)	0	100	100
2	H	264/265 (100%)	264 (100%)	0	100	100
2	J	265/265 (100%)	265 (100%)	0	100	100
2	L	265/265 (100%)	264 (100%)	1 (0%)	84	86
All	All	2633/2706 (97%)	2631 (100%)	2 (0%)	88	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	197	THR
2	L	67	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	159	GLN
2	B	90	GLN
2	B	97	GLN
2	B	136	HIS
2	B	337	GLN
2	D	90	GLN
2	D	175	GLN
1	E	146	GLN
1	E	149	ASN
1	E	198	HIS
2	F	160	ASN
2	F	248	GLN
2	H	136	HIS
2	J	90	GLN
2	J	160	ASN
2	J	163	HIS
2	J	211	GLN
2	J	227	GLN
1	K	84	HIS
1	K	198	HIS
2	L	160	ASN
2	L	163	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 ⓘ

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	$\# Z > 2$
7	EDO	H	402	-	3,3,3	0.07	0	2,2,2	0.17	0
3	AGA	B	501	-	24,24,29	0.48	0	28,29,35	0.72	1 (3%)
5	MNR	D	401	2	46,50,50	2.65	24 (52%)	59,82,82	2.18	19 (32%)
5	MNR	H	401	2	46,50,50	2.59	22 (47%)	59,82,82	1.95	15 (25%)
4	PGE	B	502	-	9,9,9	0.16	0	8,8,8	0.11	0
6	PEG	D	402	-	6,6,6	0.12	0	5,5,5	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	H	402	-	-	0/1/1/1	-
3	AGA	B	501	-	-	3/26/26/34	-
5	MNR	D	401	2	-	2/14/94/94	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MNR	H	401	2	-	6/14/94/94	-
4	PGE	B	502	-	-	2/7/7/7	-
6	PEG	D	402	-	-	0/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	MNR	C3D-C2D	5.71	1.48	1.36
5	H	401	MNR	C3D-C2D	5.61	1.48	1.36
5	D	401	MNR	C3C-C2C	5.55	1.48	1.37
5	D	401	MNR	C2A-C3A	5.50	1.48	1.36
5	H	401	MNR	C2A-C3A	5.48	1.48	1.36
5	H	401	MNR	C3C-C2C	5.18	1.47	1.37
5	H	401	MNR	CHA-C4D	4.50	1.47	1.38
5	D	401	MNR	CHC-C1C	4.46	1.47	1.38
5	H	401	MNR	CHB-C4A	4.45	1.47	1.38
5	D	401	MNR	CHA-C4D	4.36	1.46	1.38
5	D	401	MNR	CHD-C1D	4.25	1.46	1.38
5	H	401	MNR	CHD-C1D	4.25	1.46	1.38
5	H	401	MNR	CHC-C1C	4.22	1.47	1.38
5	D	401	MNR	CHB-C4A	4.17	1.47	1.38
5	D	401	MNR	C1B-NB	3.71	1.45	1.39
5	H	401	MNR	CHA-C1A	3.53	1.47	1.39
5	D	401	MNR	C4B-NB	3.52	1.45	1.39
5	H	401	MNR	C1B-NB	3.44	1.44	1.39
5	D	401	MNR	CHA-C1A	3.44	1.47	1.39
5	D	401	MNR	CHD-C4C	3.40	1.47	1.39
5	H	401	MNR	CHB-C1B	3.38	1.47	1.39
5	D	401	MNR	CHC-C4B	3.37	1.47	1.39
5	H	401	MNR	CHD-C4C	3.29	1.46	1.39
5	D	401	MNR	CHB-C1B	3.20	1.46	1.39
5	H	401	MNR	CHC-C4B	3.19	1.46	1.39
5	H	401	MNR	C4B-NB	3.16	1.44	1.39
5	D	401	MNR	C3B-C4B	2.93	1.49	1.42
5	D	401	MNR	C3B-C2B	2.86	1.50	1.41
5	H	401	MNR	C1B-C2B	2.77	1.49	1.43
5	H	401	MNR	C3B-C2B	2.70	1.50	1.41
5	D	401	MNR	C4A-C3A	2.67	1.49	1.44
5	D	401	MNR	C1B-C2B	2.66	1.49	1.43
5	D	401	MNR	C1C-C2C	2.65	1.49	1.44
5	H	401	MNR	C1C-C2C	2.61	1.49	1.44
5	D	401	MNR	C4D-C3D	2.60	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	MNR	C4D-C3D	2.59	1.49	1.45
5	H	401	MNR	C3B-C4B	2.57	1.48	1.42
5	H	401	MNR	C1D-ND	-2.56	1.34	1.39
5	H	401	MNR	C1A-C2A	2.56	1.49	1.45
5	H	401	MNR	C4D-ND	-2.50	1.34	1.39
5	D	401	MNR	C1A-C2A	2.49	1.49	1.45
5	H	401	MNR	C4A-C3A	2.35	1.49	1.44
5	D	401	MNR	C1D-ND	-2.26	1.35	1.39
5	D	401	MNR	C3C-C4C	2.23	1.49	1.44
5	D	401	MNR	C4D-ND	-2.23	1.35	1.39
5	D	401	MNR	C1D-C2D	2.14	1.49	1.45

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	401	MNR	C3C-C2C-C1C	-6.61	101.58	106.49
5	D	401	MNR	C3C-C2C-C1C	-6.36	101.77	106.49
5	D	401	MNR	C2A-C1A-NA	4.97	113.62	109.79
5	D	401	MNR	C2D-C1D-ND	4.97	114.16	109.94
5	D	401	MNR	C3D-C4D-ND	4.50	113.43	110.02
5	D	401	MNR	C2C-C1C-NC	4.35	114.01	109.84
5	D	401	MNR	C3A-C4A-NA	4.29	113.96	109.84
5	D	401	MNR	C4A-C3A-C2A	-4.17	102.57	106.96
5	H	401	MNR	C2A-C1A-NA	3.83	112.74	109.79
5	H	401	MNR	C2C-C1C-NC	3.82	113.50	109.84
5	H	401	MNR	C3D-C4D-ND	3.75	112.86	110.02
5	H	401	MNR	C2D-C1D-ND	3.72	113.10	109.94
5	D	401	MNR	C3B-C2B-C1B	-3.32	103.15	107.16
5	H	401	MNR	C4A-C3A-C2A	-3.15	103.65	106.96
5	H	401	MNR	C4D-C3D-C2D	-3.07	103.13	107.13
5	D	401	MNR	C1D-C2D-C3D	-2.97	102.60	106.94
5	D	401	MNR	C2B-C1B-NB	2.88	113.53	109.89
5	H	401	MNR	C3A-C4A-NA	2.86	112.59	109.84
5	D	401	MNR	C4D-C3D-C2D	-2.85	103.42	107.13
5	H	401	MNR	CMC-C2C-C1C	2.79	129.29	125.04
5	H	401	MNR	C3B-C2B-C1B	-2.73	103.87	107.16
5	H	401	MNR	CAA-C2A-C1A	2.62	129.24	124.66
5	D	401	MNR	CMB-C2B-C3B	2.59	132.87	126.59
5	H	401	MNR	C1D-C2D-C3D	-2.47	103.34	106.94
5	H	401	MNR	C1A-C2A-C3A	-2.41	103.39	106.90
3	B	501	AGA	O3-P1-O4	2.36	119.90	110.68
5	D	401	MNR	CHC-C1C-C2C	-2.32	120.28	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	MNR	C4C-C3C-C2C	-2.28	105.31	107.11
5	D	401	MNR	CAA-CBA-CGA	-2.15	108.97	113.60
5	D	401	MNR	CMA-C3A-C4A	2.11	128.25	125.04
5	D	401	MNR	C1A-C2A-C3A	-2.10	103.84	106.90
5	D	401	MNR	CHA-C1A-C2A	-2.08	121.79	124.84
5	D	401	MNR	CHB-C4A-C3A	-2.07	120.97	126.73
5	H	401	MNR	CMA-C3A-C4A	2.03	128.13	125.04
5	H	401	MNR	CAD-CBD-CGD	-2.02	109.26	113.60

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	401	MNR	C2C-C3C-CAC-CBC
5	H	401	MNR	C4C-C3C-CAC-CBC
5	D	401	MNR	C4D-C3D-CAD-CBD
5	D	401	MNR	C2D-C3D-CAD-CBD
5	H	401	MNR	C4D-C3D-CAD-CBD
5	H	401	MNR	C2D-C3D-CAD-CBD
4	B	502	PGE	C4-C3-O2-C2
5	H	401	MNR	CAA-CBA-CGA-O2A
3	B	501	AGA	C12-C13-C14-C15
5	H	401	MNR	CAA-CBA-CGA-O1A
3	B	501	AGA	C13-C12-O9-C5
3	B	501	AGA	O7-C7-C8-C9
4	B	502	PGE	O2-C3-C4-O3

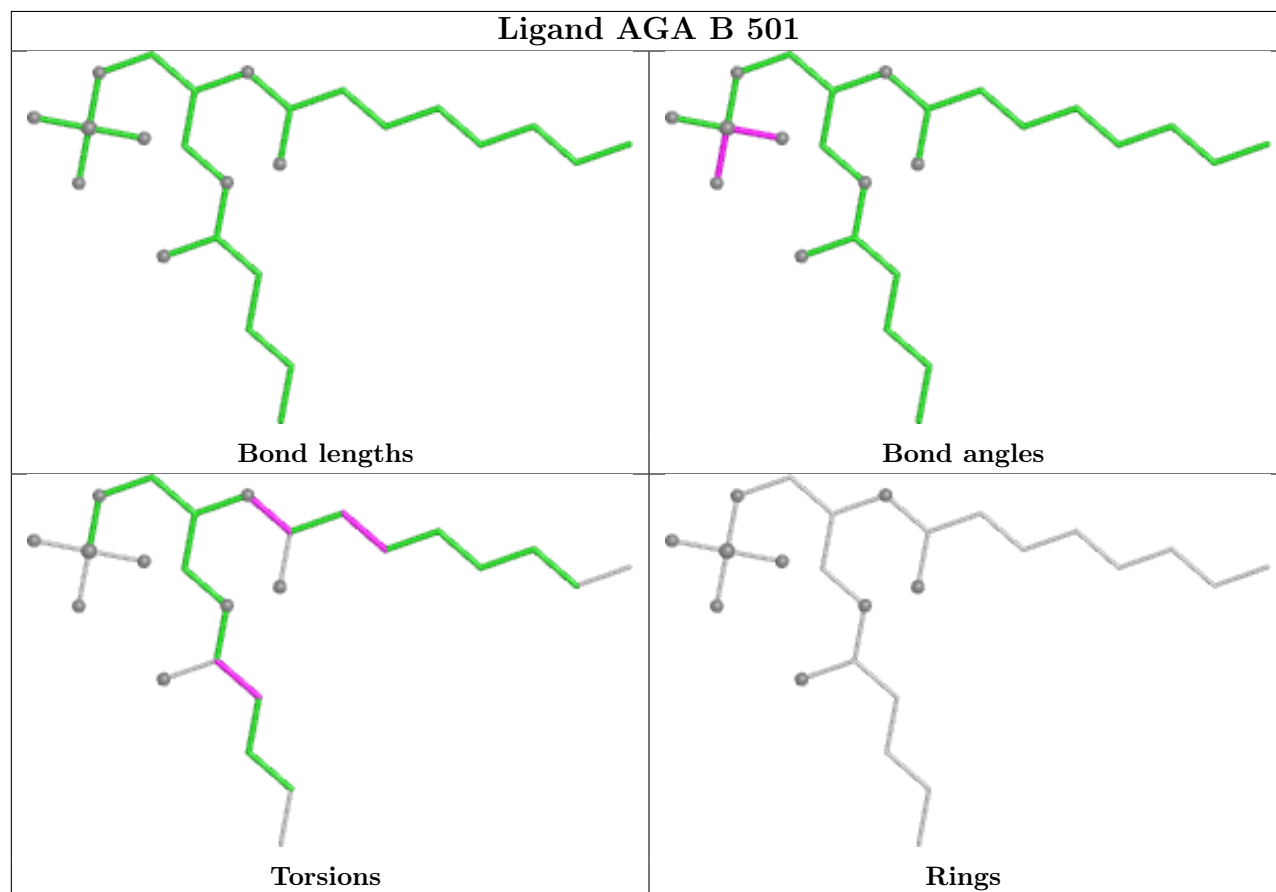
There are no ring outliers.

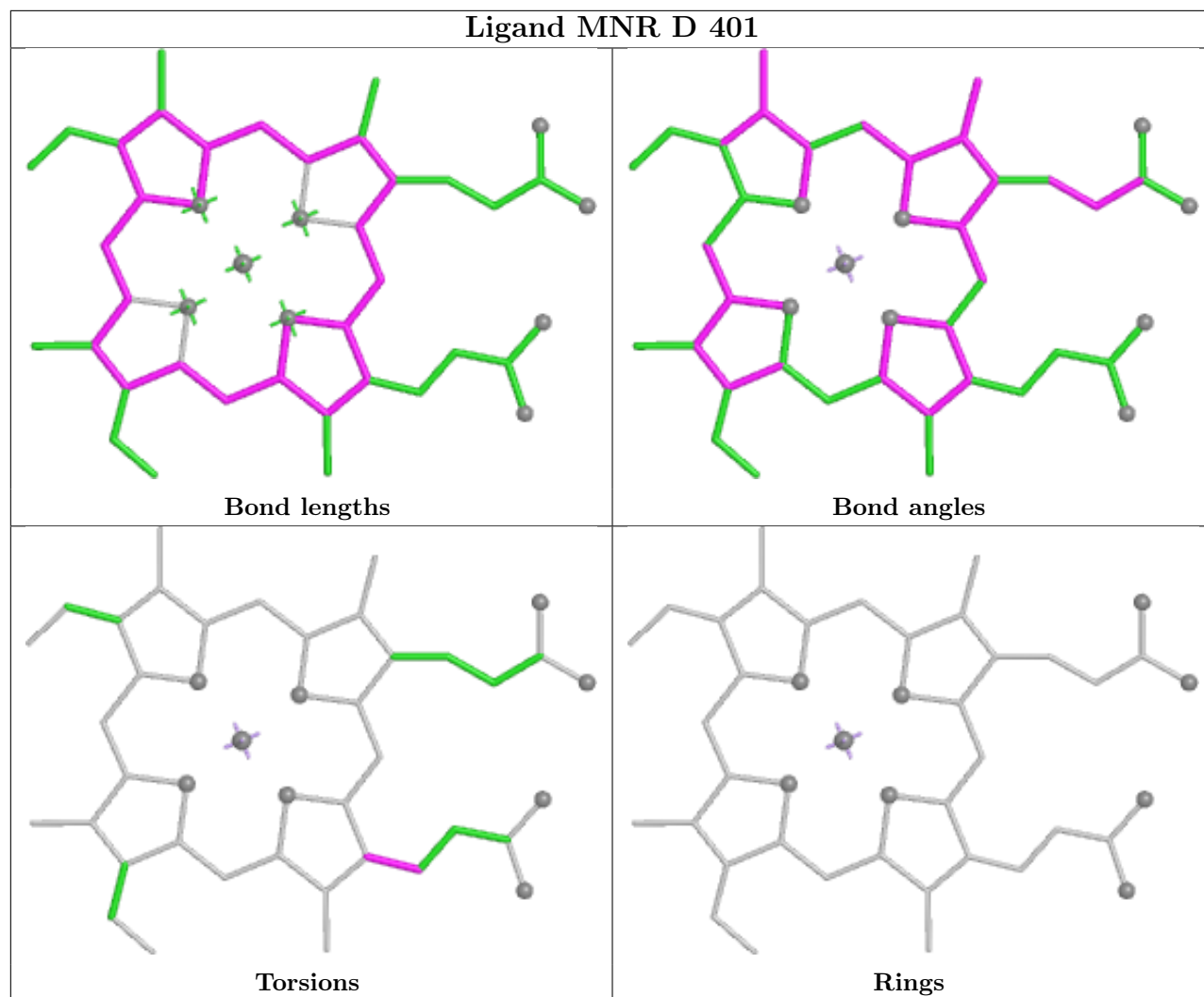
3 monomers are involved in 17 short contacts:

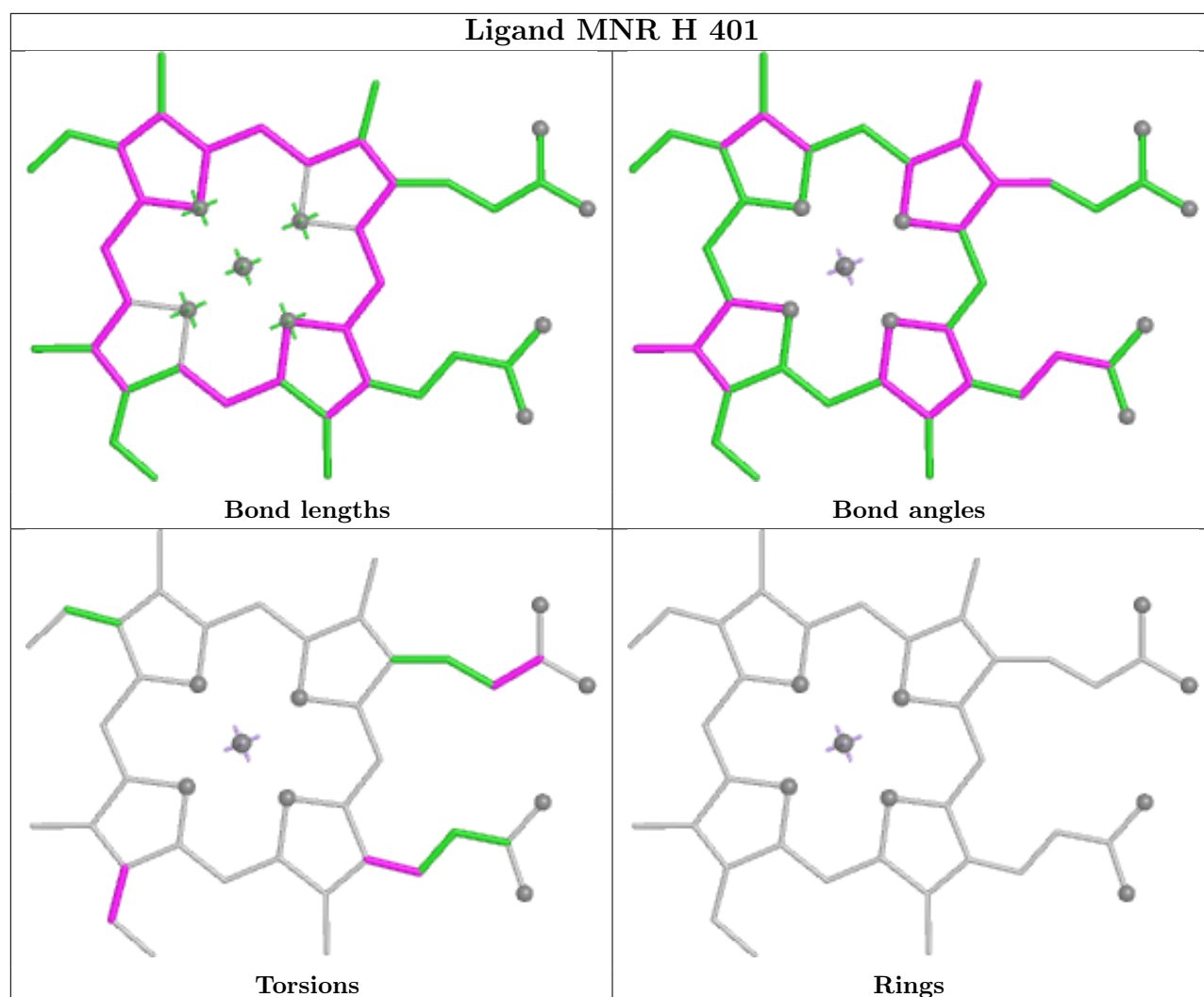
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	MNR	6	0
5	H	401	MNR	10	0
4	B	502	PGE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/231 (93%)	0.87	27 (12%) 8 6	89, 109, 128, 145	0
1	C	217/231 (93%)	0.61	19 (8%) 15 10	74, 99, 118, 127	0
1	E	213/231 (92%)	0.70	23 (10%) 11 7	101, 136, 163, 220	0
1	G	227/231 (98%)	0.52	18 (7%) 18 12	81, 106, 144, 166	0
1	I	222/231 (96%)	0.60	23 (10%) 11 8	77, 98, 115, 133	0
1	K	222/231 (96%)	0.45	12 (5%) 31 20	70, 91, 122, 172	0
2	B	341/344 (99%)	0.99	55 (16%) 4 3	96, 116, 167, 210	0
2	D	342/344 (99%)	1.00	56 (16%) 4 3	88, 162, 220, 249	0
2	F	342/344 (99%)	1.07	63 (18%) 3 3	109, 129, 168, 202	0
2	H	342/344 (99%)	1.00	64 (18%) 3 2	109, 169, 214, 254	0
2	J	343/344 (99%)	0.98	51 (14%) 5 4	91, 149, 185, 213	0
2	L	343/344 (99%)	1.03	55 (16%) 5 3	82, 142, 185, 211	0
All	All	3370/3450 (97%)	0.86	466 (13%) 6 5	70, 124, 194, 254	0

All (466) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	158	THR	10.8
2	F	211	GLN	9.6
2	L	155	THR	9.5
1	E	208	ARG	8.2
2	B	207	LYS	7.9
2	F	298	GLY	7.7
2	F	210	PHE	7.5
2	J	163	HIS	7.5
1	E	204	ALA	7.5
2	B	118	GLY	7.4
2	L	156	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
2	J	101	THR	7.0
1	E	19	GLY	7.0
2	L	154	GLY	7.0
1	G	164	ASP	6.9
1	E	203	LEU	6.9
1	E	206	ALA	6.8
2	D	48	GLU	6.6
2	L	157	LYS	6.6
2	J	90	GLN	6.5
1	K	224	TRP	6.3
1	A	114	LYS	6.2
2	L	12	ALA	6.2
2	F	299	SER	6.2
2	B	115	ASP	6.1
1	G	229	PHE	6.1
1	A	164	ASP	6.1
2	B	190	ASN	5.9
2	J	215	ALA	5.9
2	D	209	ALA	5.8
2	L	297	ALA	5.7
2	L	191	GLN	5.7
2	F	215	ALA	5.7
2	H	341	GLY	5.7
2	F	10	ALA	5.7
2	H	241	PHE	5.7
2	F	163	HIS	5.6
2	H	215	ALA	5.6
1	A	210	VAL	5.5
1	A	209	PHE	5.5
1	I	204	ALA	5.4
2	B	112	PRO	5.3
2	B	205	ASP	5.3
2	F	209	ALA	5.3
2	B	117	VAL	5.1
2	J	342	ALA	5.1
2	H	214	PRO	5.1
2	H	217	LYS	5.1
2	L	118	GLY	5.1
1	A	211	GLU	5.0
1	A	18	ASP	5.0
2	H	77	ALA	5.0
1	I	224	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
2	D	90	GLN	4.9
2	H	342	ALA	4.9
2	L	117	VAL	4.8
2	F	342	ALA	4.8
1	I	188	GLU	4.8
1	A	90	GLN	4.8
2	L	342	ALA	4.7
1	E	37	GLU	4.7
2	F	207	LYS	4.7
2	F	297	ALA	4.7
1	C	20	ILE	4.7
2	F	216	TYR	4.6
1	E	34	PHE	4.6
2	F	9	ARG	4.6
2	F	206	LEU	4.6
1	G	165	GLU	4.6
1	I	223	LEU	4.5
1	A	115	PRO	4.5
2	B	188	LEU	4.5
2	B	113	LEU	4.4
2	F	204	THR	4.4
2	F	205	ASP	4.4
1	I	190	ALA	4.4
2	H	80	TRP	4.4
2	D	16	ALA	4.3
2	J	5	ILE	4.3
1	K	89	PHE	4.3
1	A	112	GLY	4.3
2	B	174	TRP	4.2
2	B	183	VAL	4.2
2	B	341	GLY	4.2
2	J	9	ARG	4.2
2	B	340	LEU	4.2
2	H	74	GLU	4.1
1	G	228	GLN	4.1
2	B	116	SER	4.1
2	D	174	TRP	4.1
2	H	339	ALA	4.1
2	J	339	ALA	4.1
2	F	93	ILE	4.1
2	J	100	ASN	4.1
2	J	341	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	48	GLU	4.1
2	L	129	ALA	4.1
2	H	218	SER	4.0
1	G	91	GLN	4.0
2	L	127	LEU	4.0
2	H	68	THR	4.0
1	E	32	GLU	4.0
2	B	157	LYS	3.9
2	L	267	LEU	3.9
2	F	208	GLY	3.9
1	E	97	SER	3.9
2	J	165	PRO	3.9
2	F	217	LYS	3.9
2	J	60	ALA	3.9
2	H	78	GLU	3.9
2	F	175	GLN	3.9
2	J	48	GLU	3.8
2	F	183	VAL	3.8
1	E	91	GLN	3.8
2	H	123	GLN	3.8
2	J	314	LEU	3.8
1	K	27	ASP	3.8
2	L	10	ALA	3.7
1	E	207	ASP	3.7
2	D	47	ILE	3.7
2	B	85	PRO	3.7
2	D	88	VAL	3.7
2	H	82	ASP	3.7
1	E	21	SER	3.7
1	G	89	PHE	3.6
2	H	69	SER	3.6
2	H	1	MET	3.6
2	L	343	THR	3.6
1	K	164	ASP	3.6
2	B	204	THR	3.6
1	G	227	PRO	3.6
2	F	112	PRO	3.6
2	J	71	GLU	3.6
2	F	195	ILE	3.6
1	E	136	ARG	3.5
2	F	222	SER	3.5
2	L	194	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	181	LYS	3.5
1	G	20	ILE	3.5
2	L	268	ILE	3.5
2	H	109	GLU	3.5
2	H	116	SER	3.5
2	B	84	THR	3.5
2	B	166	VAL	3.5
1	I	36	GLY	3.4
2	D	342	ALA	3.4
2	F	113	LEU	3.4
2	H	39	LEU	3.4
2	D	207	LYS	3.4
2	B	74	GLU	3.4
2	D	28	LEU	3.4
1	A	116	ARG	3.4
2	D	134	PHE	3.3
2	B	211	GLN	3.3
2	H	36	THR	3.3
2	J	158	THR	3.3
2	L	47	ILE	3.3
1	G	198	HIS	3.3
2	D	67	PHE	3.3
2	H	340	LEU	3.3
2	L	115	ASP	3.2
1	G	224	TRP	3.2
2	D	19	ALA	3.2
2	L	13	GLY	3.2
2	J	164	THR	3.2
1	C	3	ALA	3.2
2	B	50	LEU	3.2
2	F	213	MET	3.2
1	E	16	TYR	3.2
2	J	222	SER	3.2
1	A	25	ALA	3.2
2	L	209	ALA	3.2
1	A	165	GLU	3.2
2	L	206	LEU	3.2
1	E	188	GLU	3.1
1	A	203	LEU	3.1
2	D	281	GLY	3.1
2	L	341	GLY	3.1
2	F	300	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	280	ALA	3.1
2	B	91	THR	3.1
2	D	89	SER	3.1
2	J	174	TRP	3.1
2	F	90	GLN	3.1
2	D	308	SER	3.1
1	E	18	ASP	3.1
2	H	183	VAL	3.1
2	D	41	LYS	3.1
2	B	316	ILE	3.1
2	F	214	PRO	3.1
2	J	214	PRO	3.1
2	L	190	ASN	3.0
2	B	208	GLY	3.0
2	D	208	GLY	3.0
2	F	221	SER	3.0
2	H	159	GLU	3.0
2	H	308	SER	3.0
2	F	316	ILE	3.0
2	L	304	LEU	3.0
1	I	187	LYS	3.0
2	H	30	VAL	3.0
2	D	3	LEU	3.0
2	L	130	GLU	3.0
2	B	155	THR	3.0
2	B	214	PRO	2.9
2	L	66	GLU	2.9
2	H	65	PRO	2.9
1	G	163	ALA	2.9
2	B	56	VAL	2.9
2	L	139	ALA	2.9
1	E	205	TYR	2.9
1	A	89	PHE	2.9
2	D	154	GLY	2.9
2	J	183	VAL	2.9
2	D	15	PHE	2.9
2	B	107	LEU	2.9
1	I	207	ASP	2.8
1	I	167	THR	2.8
2	H	194	THR	2.8
2	L	68	THR	2.8
1	I	200	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	109	HIS	2.8
2	B	178	SER	2.8
2	H	243	THR	2.8
1	C	58	PHE	2.8
2	L	32	LEU	2.8
2	L	339	ALA	2.8
2	L	128	PRO	2.8
1	C	39	VAL	2.8
1	K	78	THR	2.8
2	D	159	GLU	2.8
2	F	101	THR	2.8
2	J	44	THR	2.8
2	F	98	ASN	2.8
2	L	298	GLY	2.8
2	H	240	ALA	2.8
2	B	203	VAL	2.8
2	H	203	VAL	2.8
2	J	151	THR	2.8
2	L	340	LEU	2.8
1	E	20	ILE	2.8
1	K	20	ILE	2.8
1	K	3	ALA	2.8
2	J	182	ALA	2.8
2	B	114	PRO	2.8
2	D	165	PRO	2.8
2	F	218	SER	2.8
2	J	1	MET	2.7
2	L	220	ARG	2.7
2	D	135	LEU	2.7
1	C	214	ASP	2.7
2	B	82	ASP	2.7
2	L	7	ASP	2.7
2	D	193	PRO	2.7
2	H	193	PRO	2.7
2	L	159	GLU	2.7
2	B	264	ARG	2.7
2	B	123	GLN	2.7
1	I	20	ILE	2.7
1	I	122	GLU	2.7
2	D	12	ALA	2.7
2	D	99	ALA	2.7
2	D	17	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	131	LEU	2.7
2	H	35	LEU	2.7
2	D	9	ARG	2.7
2	J	155	THR	2.7
2	H	70	SER	2.7
1	C	25	ALA	2.7
1	C	89	PHE	2.6
1	E	209	PHE	2.6
2	B	119	GLY	2.6
1	A	26	LEU	2.6
1	I	163	ALA	2.6
2	J	218	SER	2.6
2	B	338	ILE	2.6
1	A	155	MET	2.6
1	K	146	GLN	2.6
2	B	75	GLN	2.6
2	H	118	GLY	2.6
2	J	65	PRO	2.6
2	L	15	PHE	2.6
2	D	100	ASN	2.6
2	J	160	ASN	2.6
2	J	102	THR	2.6
2	L	36	THR	2.6
1	I	195	MET	2.6
2	H	31	MET	2.6
2	D	46	ALA	2.6
2	H	49	ALA	2.6
2	J	299	SER	2.6
1	C	32	GLU	2.6
2	D	49	ALA	2.6
2	F	264	ARG	2.6
2	J	129	ALA	2.6
2	J	142	HIS	2.5
2	H	75	GLN	2.5
1	A	42	VAL	2.5
2	H	156	VAL	2.5
2	J	157	LYS	2.5
2	F	212	ALA	2.5
2	D	155	THR	2.5
2	F	118	GLY	2.5
1	A	113	ILE	2.5
2	H	67	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	337	GLN	2.5
2	F	303	SER	2.5
1	G	196	VAL	2.5
1	A	204	ALA	2.5
1	C	80	THR	2.5
2	D	168	TRP	2.5
1	I	203	LEU	2.5
2	B	158	THR	2.5
2	H	79	ARG	2.5
2	H	309	VAL	2.5
2	F	178	SER	2.4
2	L	277	ILE	2.4
2	D	36	THR	2.4
2	F	318	LEU	2.4
2	F	142	HIS	2.4
2	F	140	GLY	2.4
1	C	218	LEU	2.4
2	F	224	LEU	2.4
1	K	24	THR	2.4
1	C	17	PRO	2.4
1	A	6	VAL	2.4
2	L	140	GLY	2.4
1	K	77	ALA	2.4
1	A	91	GLN	2.4
2	B	90	GLN	2.4
2	J	178	SER	2.4
1	A	108	ASP	2.4
2	D	30	VAL	2.4
2	J	181	LYS	2.4
2	L	213	MET	2.4
2	J	318	LEU	2.4
2	F	64	SER	2.4
2	J	89	SER	2.4
2	H	168	TRP	2.4
2	B	171	THR	2.4
2	H	58	THR	2.4
2	J	343	THR	2.4
2	L	65	PRO	2.4
2	B	226	MET	2.4
2	B	2	PHE	2.4
2	J	74	GLU	2.4
2	L	244	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	226	HIS	2.3
2	B	277	ILE	2.3
2	F	226	MET	2.3
1	C	159	GLN	2.3
2	F	66	GLU	2.3
2	H	81	LYS	2.3
2	J	180	THR	2.3
2	L	217	LYS	2.3
1	E	200	ARG	2.3
1	I	221	ALA	2.3
1	I	38	LEU	2.3
1	K	90	GLN	2.3
1	G	17	PRO	2.3
2	B	143	ILE	2.3
2	D	61	GLY	2.3
2	B	101	THR	2.3
2	F	308	SER	2.3
2	H	238	THR	2.3
1	K	223	LEU	2.3
2	F	67	PHE	2.3
2	L	74	GLU	2.3
2	L	1	MET	2.3
1	G	98	LEU	2.3
2	H	216	TYR	2.3
2	L	9	ARG	2.3
2	F	102	THR	2.3
2	H	304	LEU	2.3
2	D	178	SER	2.3
1	C	208	ARG	2.3
1	A	102	GLU	2.2
2	H	289	GLY	2.2
2	J	224	LEU	2.2
1	G	197	THR	2.2
2	B	57	PHE	2.2
2	F	171	THR	2.2
2	D	20	SER	2.2
2	H	89	SER	2.2
2	H	117	VAL	2.2
1	I	37	GLU	2.2
2	D	74	GLU	2.2
2	H	66	GLU	2.2
1	C	161	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	3	ALA	2.2
2	L	39	LEU	2.2
2	D	210	PHE	2.2
2	D	149	THR	2.2
2	B	202	VAL	2.2
2	D	104	VAL	2.2
2	F	43	ASN	2.2
2	B	209	ALA	2.2
2	H	3	LEU	2.2
2	H	32	LEU	2.2
2	D	169	VAL	2.2
2	J	88	VAL	2.2
2	J	338	ILE	2.2
2	L	330	ASN	2.2
1	G	223	LEU	2.2
1	G	96	GLY	2.2
2	H	290	ALA	2.2
2	D	217	LYS	2.2
2	H	149	THR	2.2
2	H	202	VAL	2.2
2	D	211	GLN	2.2
1	C	37	GLU	2.2
2	B	136	HIS	2.2
1	E	90	GLN	2.1
2	D	284	LEU	2.1
2	F	131	LEU	2.1
2	J	340	LEU	2.1
1	A	45	SER	2.1
2	H	34	GLY	2.1
2	H	251	ARG	2.1
2	B	168	TRP	2.1
1	C	22	THR	2.1
2	D	216	TYR	2.1
2	L	31	MET	2.1
1	I	126	ARG	2.1
2	B	106	GLY	2.1
2	H	40	GLY	2.1
2	D	57	PHE	2.1
1	A	207	ASP	2.1
2	J	104	VAL	2.1
2	B	142	HIS	2.1
2	J	68	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	11	ALA	2.1
2	L	11	ALA	2.1
1	I	35	PRO	2.1
2	F	184	GLY	2.1
1	A	50	SER	2.1
1	C	76	ASP	2.1
2	J	268	ILE	2.1
2	B	151	THR	2.1
2	H	325	THR	2.1
2	F	31	MET	2.1
1	E	169	ALA	2.1
1	I	169	ALA	2.1
2	D	13	GLY	2.1
2	H	71	GLU	2.1
2	L	214	PRO	2.1
1	I	184	ASP	2.1
2	F	7	ASP	2.1
2	L	252	ASP	2.1
1	C	19	GLY	2.1
2	D	40	GLY	2.1
2	F	42	GLN	2.1
2	F	198	GLN	2.1
2	F	294	TRP	2.0
1	C	86	GLY	2.0
2	J	300	VAL	2.0
2	F	8	ILE	2.0
2	F	54	SER	2.0
2	D	158	THR	2.0
2	D	212	ALA	2.0
2	D	301	PRO	2.0
2	H	197	PRO	2.0
2	J	128	PRO	2.0
1	E	39	VAL	2.0
2	F	74	GLU	2.0
2	J	130	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

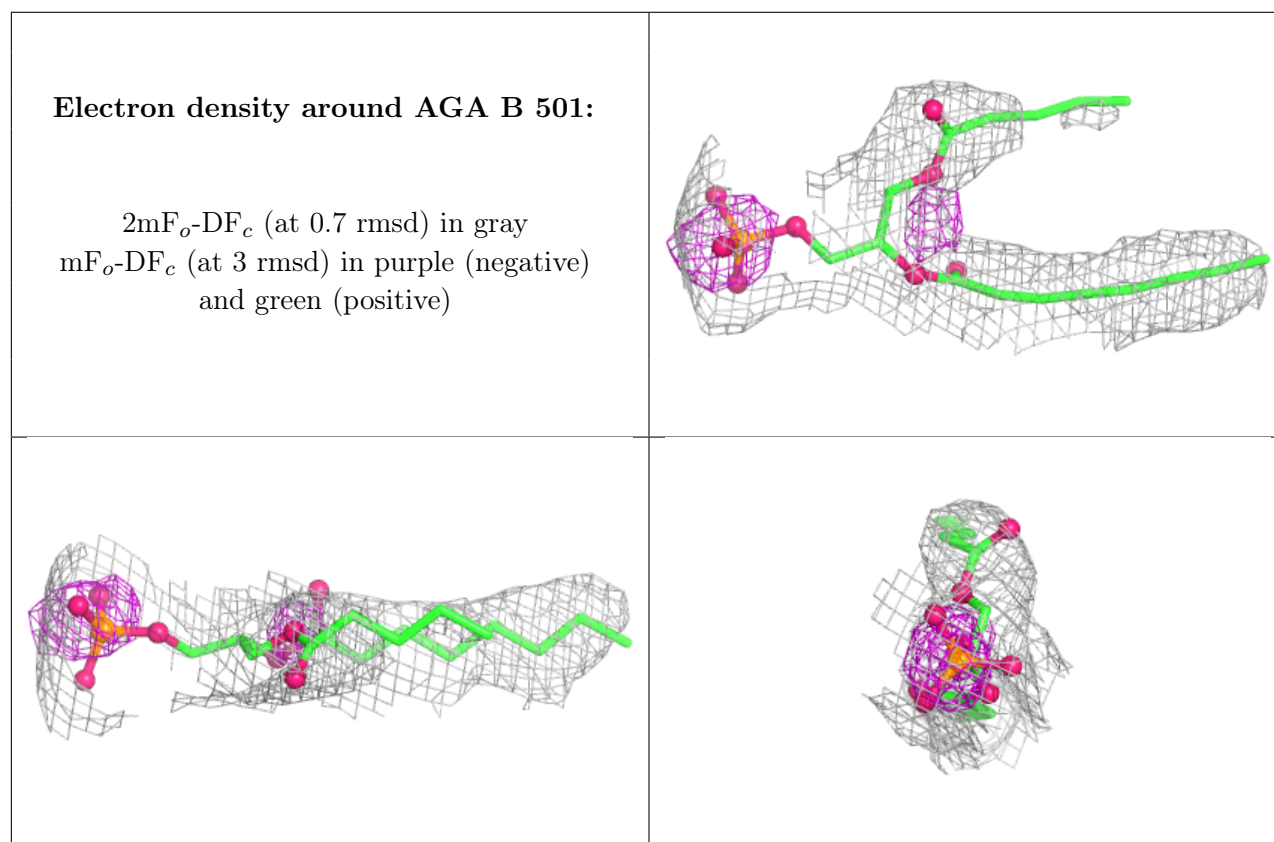
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

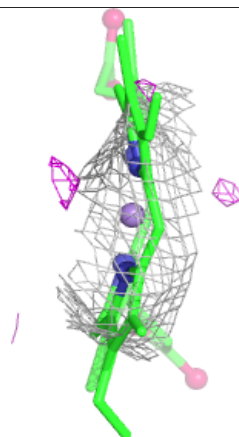
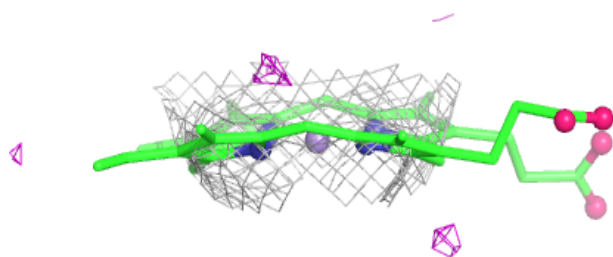
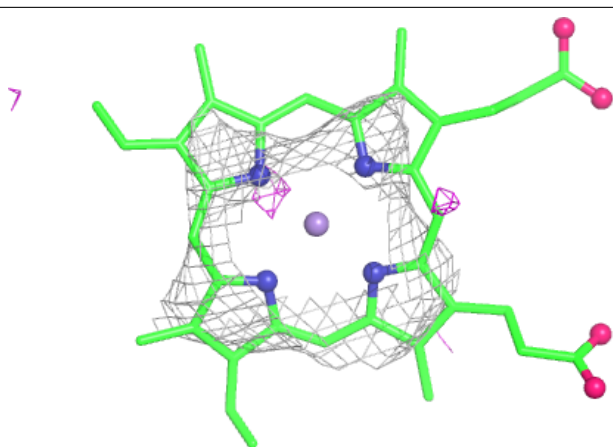
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	H	402	4/4	0.28	0.37	142,142,142,142	0
4	PGE	B	502	10/10	0.59	0.14	102,102,102,102	0
6	PEG	D	402	7/7	0.60	0.24	142,142,142,142	0
3	AGA	B	501	25/30	0.78	0.23	107,107,107,107	0
5	MNR	H	401	43/43	0.86	0.29	477,482,484,485	0
5	MNR	D	401	43/43	0.93	0.24	237,240,244,245	0

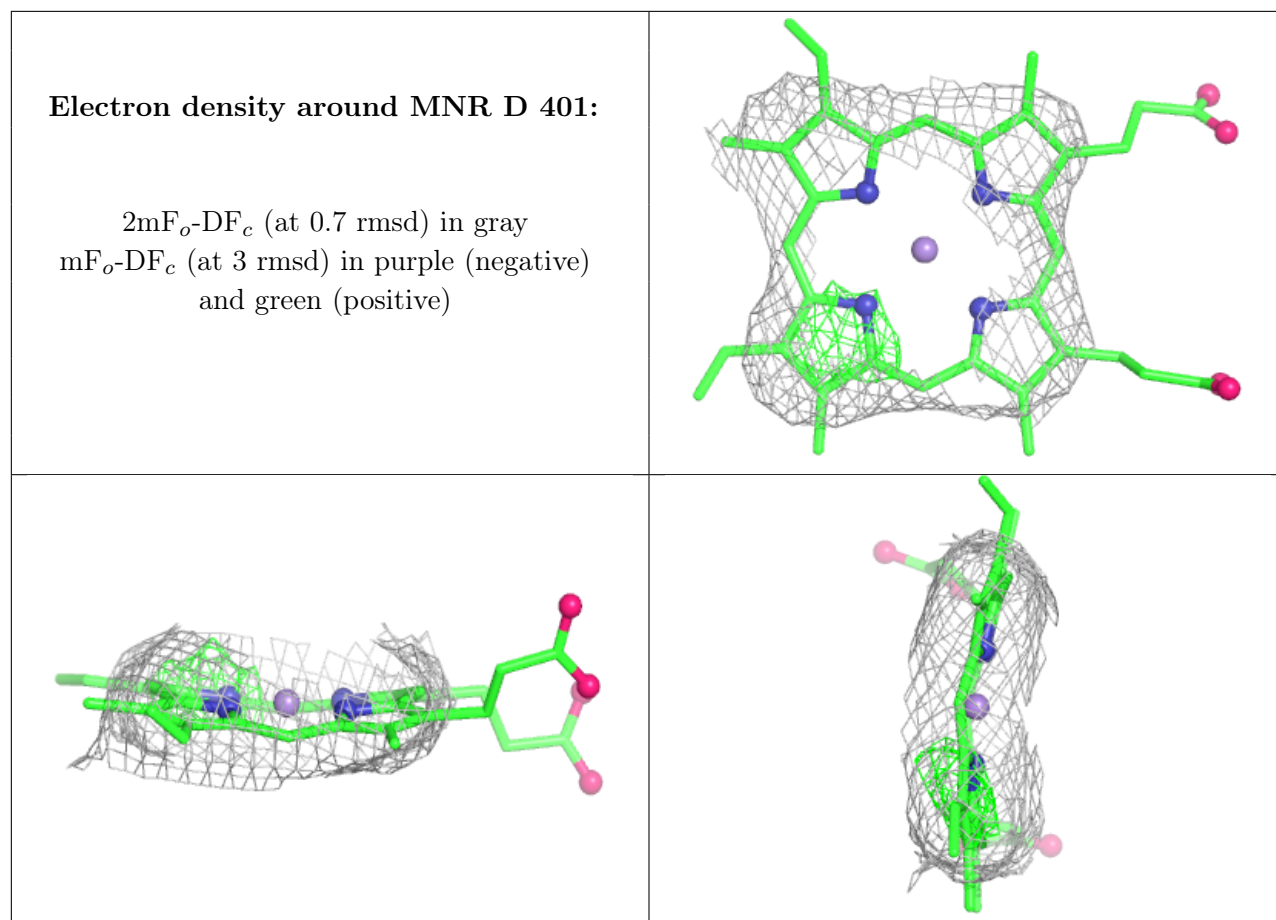
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around 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.