Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 09:02 PM 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:

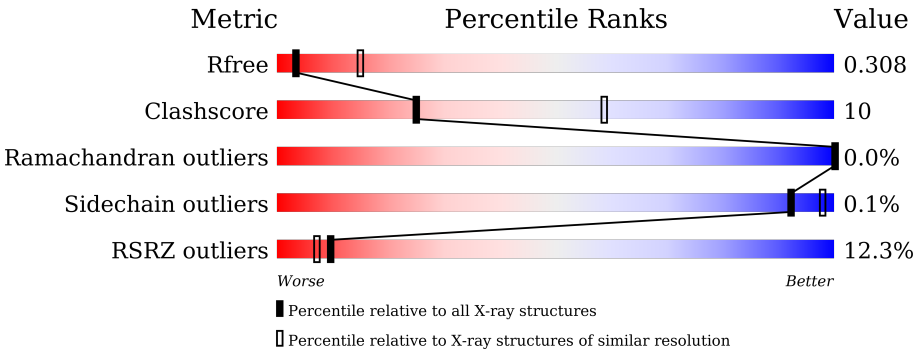
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (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 <=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	10% 71% 23% 6%
1	C	231	6% 76% 18% 6%
1	E	231	9% 73% 19% 8%
1	G	231	8% 78% 20% .
1	I	231	9% 65% 31% .
1	K	231	5% 76% 20% .

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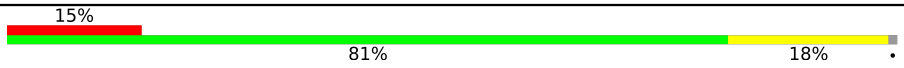
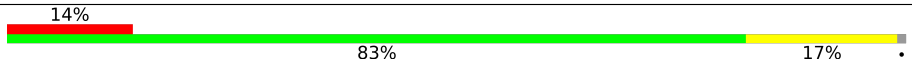
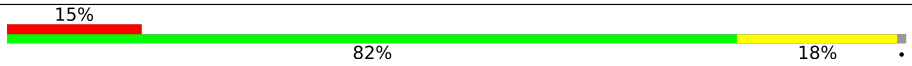
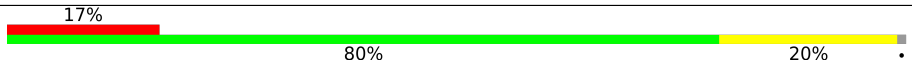
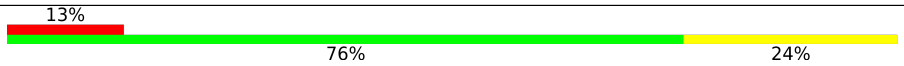
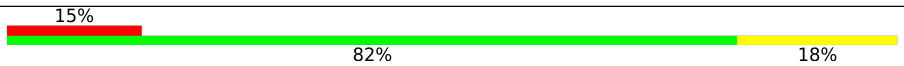
Mol	Chain	Length	Quality of chain
2	B	344	
2	D	344	
2	F	344	
2	H	344	
2	J	344	
2	L	344	

2 Entry composition (i)

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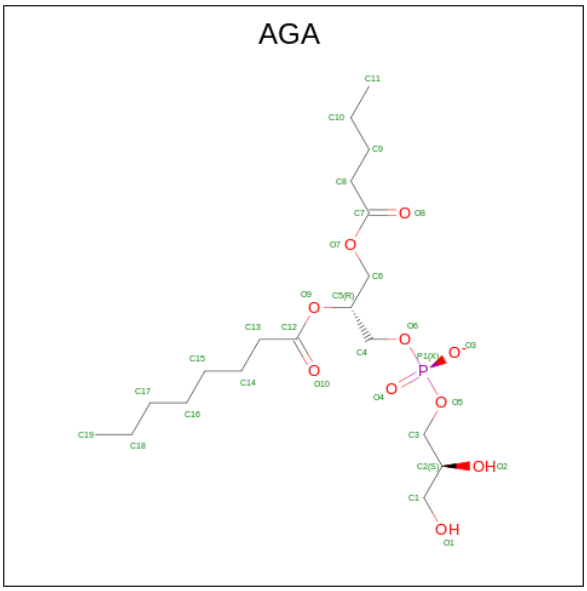
Chain	Residue	Modelled	Actual	Comment	Reference
K	231	LYS	-	expression tag	UNP Q6NEF2

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

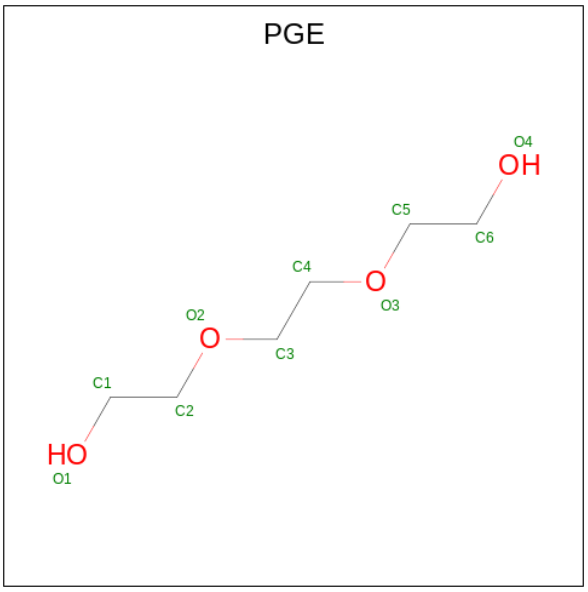
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	341	Total	C	N	O	S	0	0	0
			2510	1612	422	471	5			
2	D	342	Total	C	N	O	S	0	0	0
			2515	1615	423	472	5			
2	F	342	Total	C	N	O	S	0	0	0
			2515	1615	423	472	5			
2	H	342	Total	C	N	O	S	0	0	0
			2515	1615	423	472	5			
2	J	343	Total	C	N	O	S	0	0	0
			2522	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: $C_{19}H_{36}O_{10}P$).



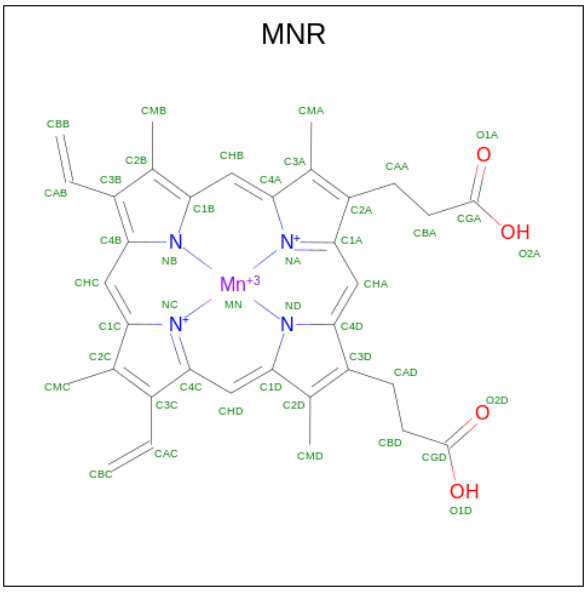
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			25	16	8	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



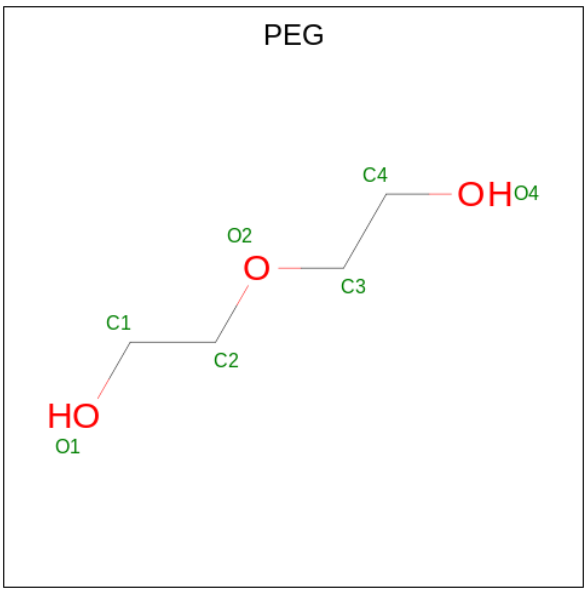
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 10 6 4	0	0

- 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).



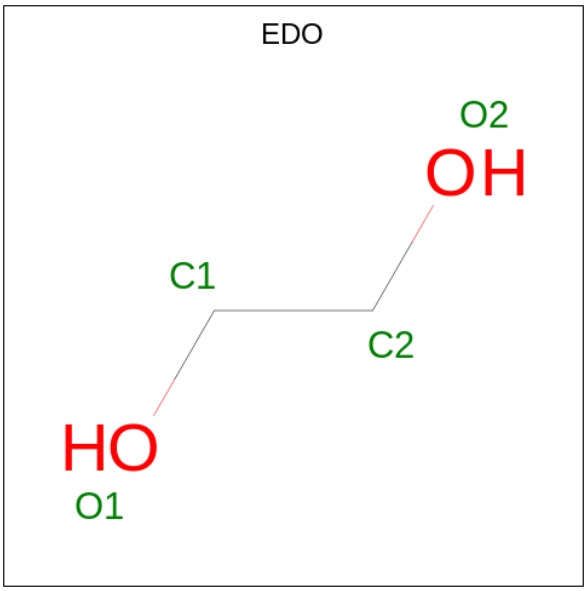
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C Mn N O 43 34 1 4 4	0	0
5	H	1	Total C Mn N O 43 34 1 4 4	0	0

- 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 7 4 3	0	0

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



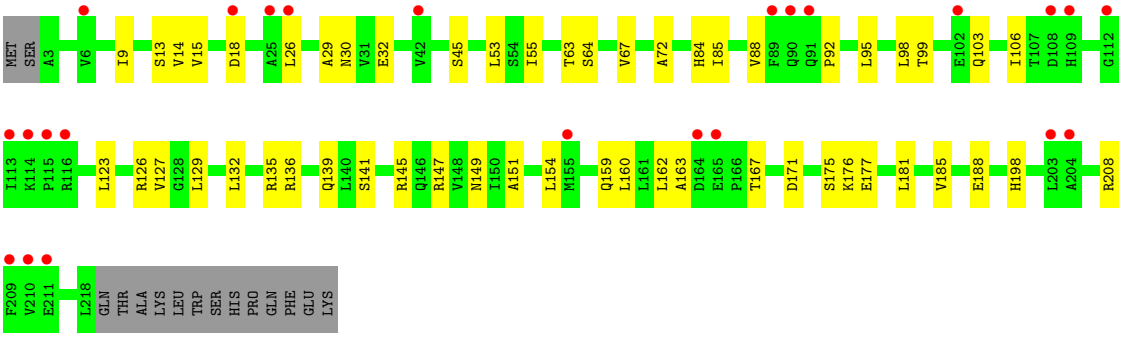
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 4 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

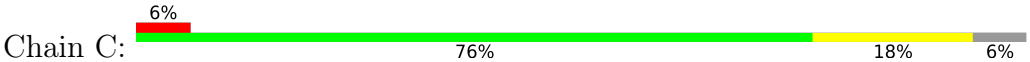
• Molecule 1: Putative ABC transport system, ATP-binding protein

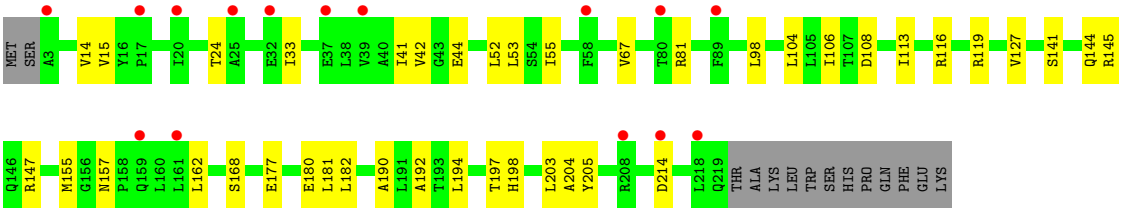
Chain A:



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

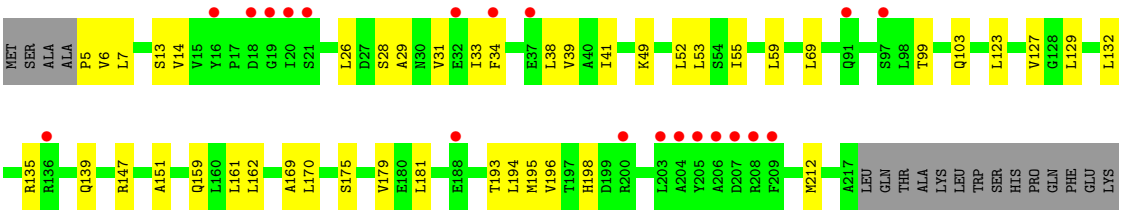
Chain C:



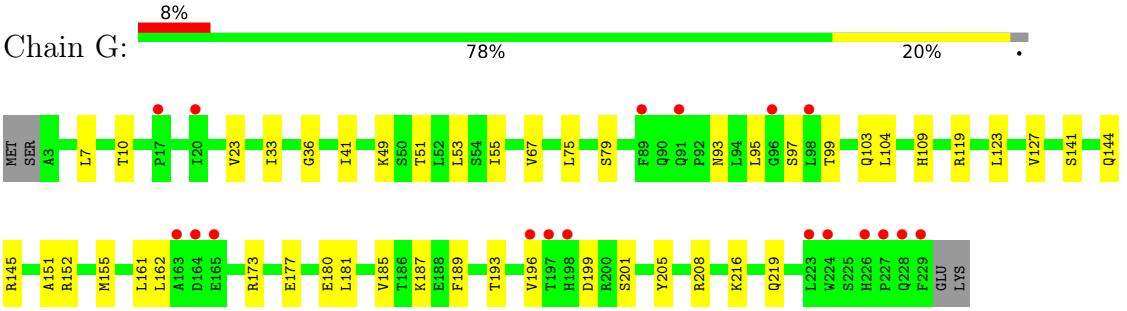


• Molecule 1: Putative ABC transport system, ATP-binding protein

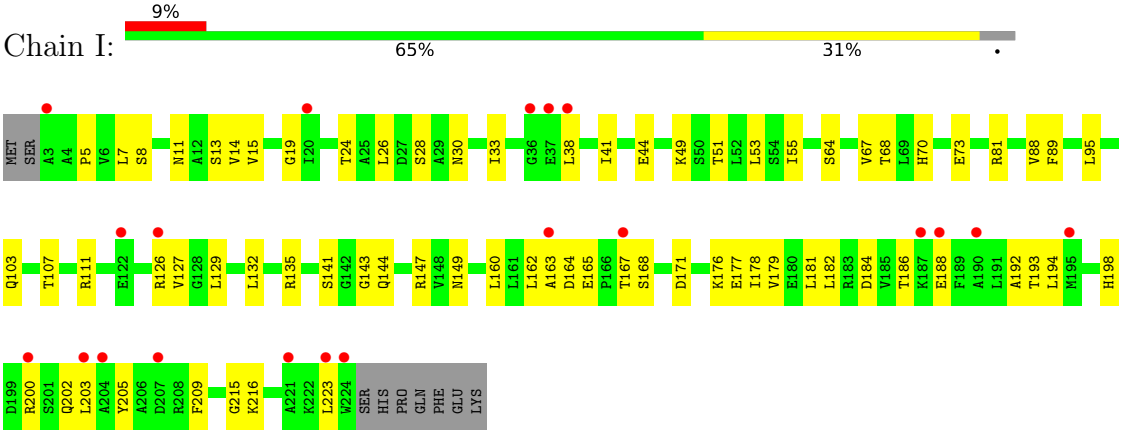
Chain E:



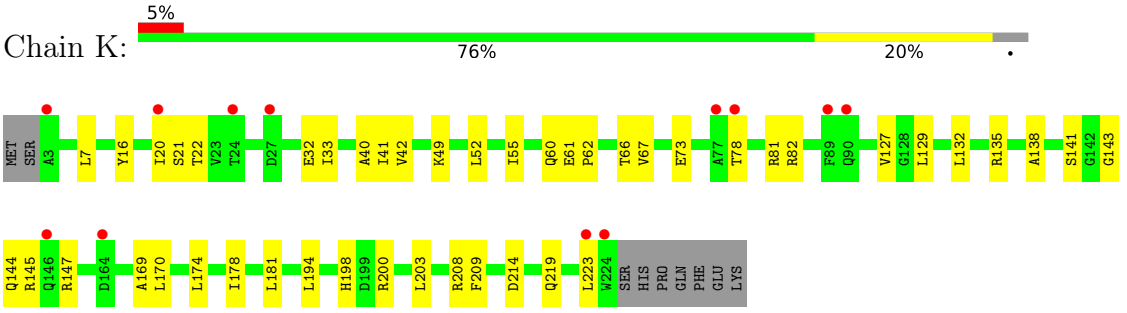
• Molecule 1: Putative ABC transport system, ATP-binding protein



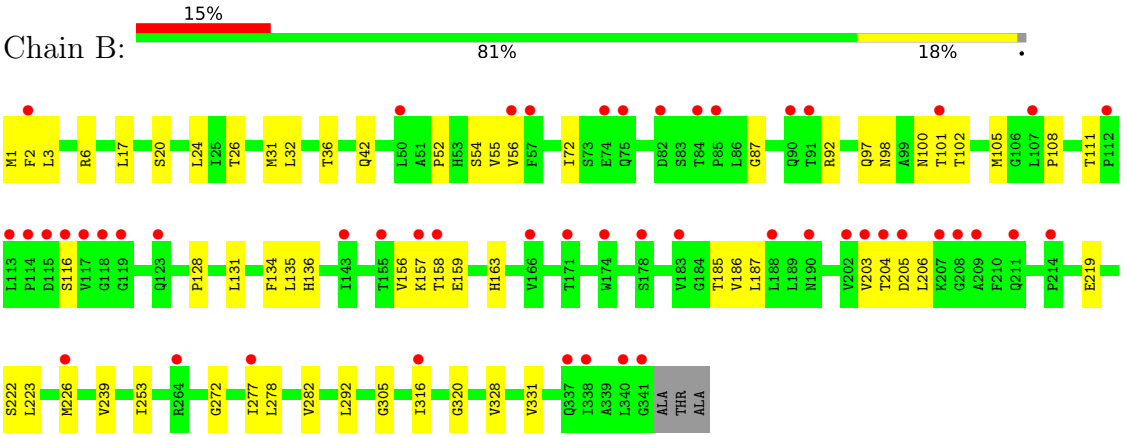
• Molecule 1: Putative ABC transport system, ATP-binding protein



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

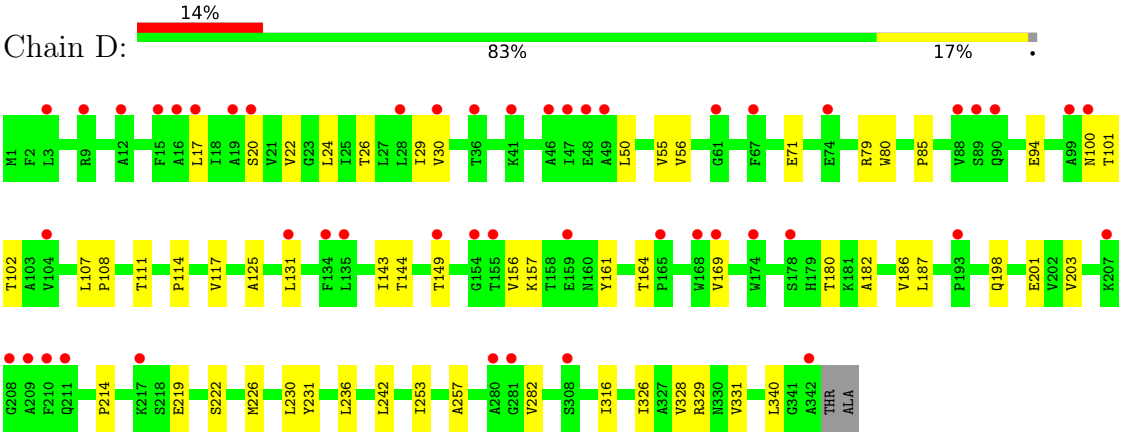


• Molecule 2: Putative ABC transport system integral membrane protein



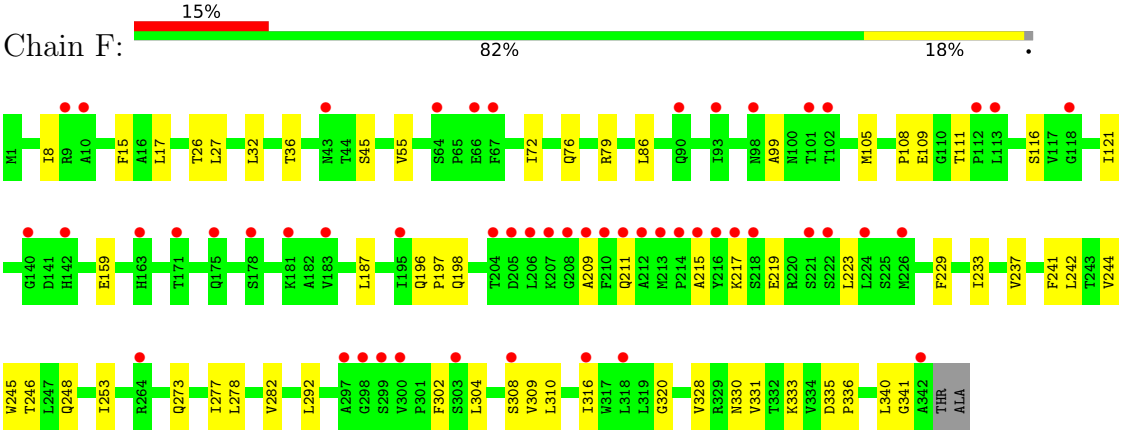
• Molecule 2: Putative ABC transport system integral membrane protein

Chain D:



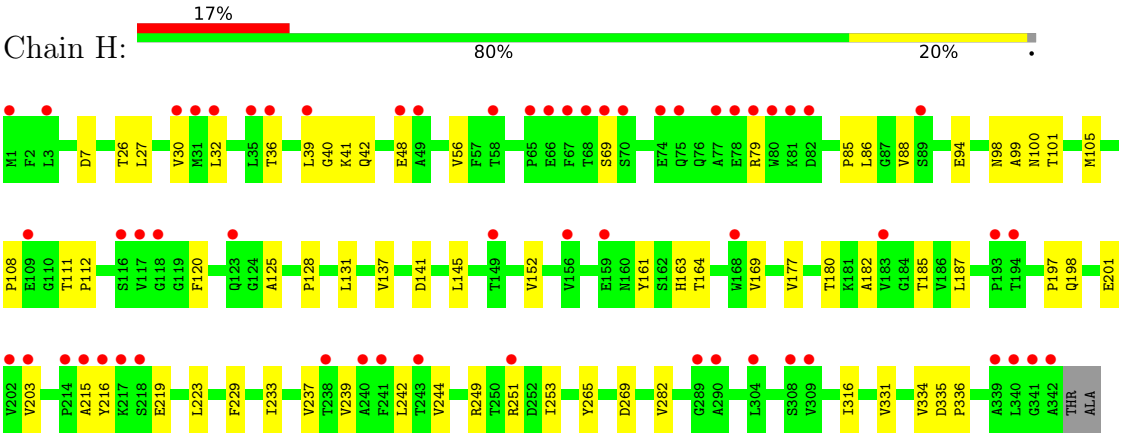
• Molecule 2: Putative ABC transport system integral membrane protein

Chain F:



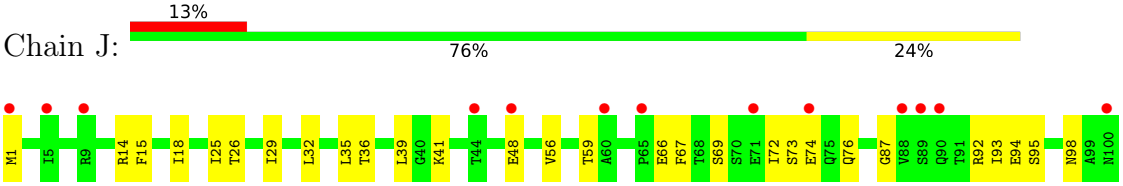
• Molecule 2: Putative ABC transport system integral membrane protein

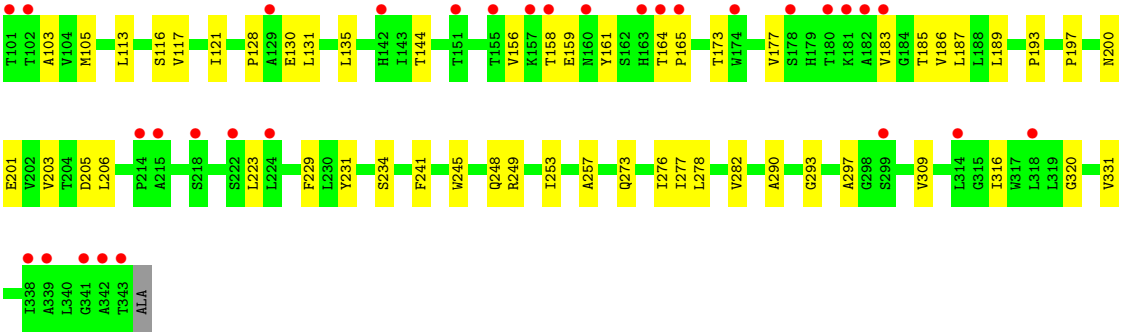
Chain H:



• Molecule 2: Putative ABC transport system integral membrane protein

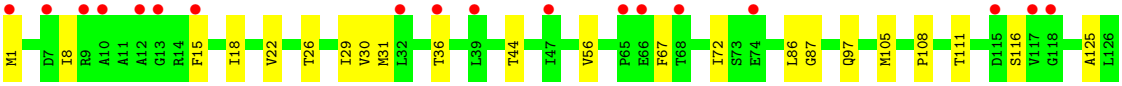
Chain J:

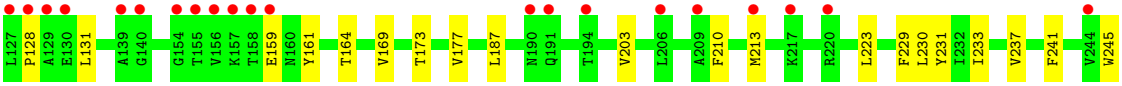


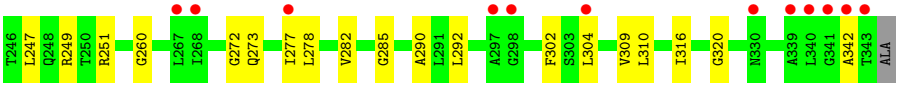


• Molecule 2: Putative ABC transport system integral membrane protein

Chain L:







4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	98274 reflections (3.12%)	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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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 (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%)	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%)	37	69
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/186 (92%)	172 (100%)	0	100	100
1	C	172/186 (92%)	171 (99%)	1 (1%)	84	92
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%)	89 94
All	All	2633/2706 (97%)	2631 (100%)	2 (0%)	92 98

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	$\#\|Z\| > 2$
3	AGA	B	501	-	24,24,29	0.48	0	28,29,35	0.72	1 (3%)
6	PEG	D	402	-	6,6,6	0.12	0	5,5,5	0.08	0
5	MNR	H	401	2	36,50,50	2.94	13 (36%)	34,82,82	2.31	12 (35%)
7	EDO	H	402	-	3,3,3	0.07	0	2,2,2	0.17	0
5	MNR	D	401	2	36,50,50	3.00	14 (38%)	34,82,82	2.63	14 (41%)
4	PGE	B	502	-	9,9,9	0.16	0	8,8,8	0.11	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
3	AGA	B	501	-	-	3/26/26/34	-
6	PEG	D	402	-	-	0/4/4/4	-
5	MNR	H	401	2	-	4/12/94/94	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	H	402	-	-	0/1/1/1	-
5	MNR	D	401	2	-	2/12/94/94	-
4	PGE	B	502	-	-	2/7/7/7	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	MNR	C3B-C2B	7.58	1.50	1.40
5	H	401	MNR	C3B-C2B	7.20	1.50	1.40
5	D	401	MNR	CHC-C1C	5.84	1.47	1.37
5	H	401	MNR	CHB-C4A	5.82	1.47	1.37
5	H	401	MNR	CHA-C1A	5.67	1.47	1.37
5	H	401	MNR	CHC-C1C	5.55	1.47	1.37
5	D	401	MNR	CHA-C1A	5.54	1.47	1.37
5	D	401	MNR	C3C-C2C	5.53	1.48	1.37
5	D	401	MNR	CHD-C4C	5.50	1.47	1.37
5	D	401	MNR	C2A-C3A	5.50	1.48	1.36
5	D	401	MNR	CHB-C4A	5.49	1.47	1.37
5	H	401	MNR	C2A-C3A	5.48	1.48	1.36
5	H	401	MNR	CHD-C4C	5.35	1.46	1.37
5	H	401	MNR	C3C-C2C	5.16	1.47	1.37
5	D	401	MNR	C3D-C2D	3.78	1.48	1.37
5	H	401	MNR	C3D-C2D	3.71	1.48	1.37
5	D	401	MNR	C3B-C4B	3.63	1.49	1.40
5	H	401	MNR	C3B-C4B	3.30	1.48	1.40
5	H	401	MNR	CHA-C4D	3.15	1.47	1.40
5	H	401	MNR	CHB-C1B	3.09	1.47	1.40
5	D	401	MNR	CHC-C4B	3.08	1.47	1.40
5	D	401	MNR	CHA-C4D	3.03	1.46	1.40
5	D	401	MNR	CHD-C1D	2.93	1.46	1.40
5	H	401	MNR	CHD-C1D	2.92	1.46	1.40
5	D	401	MNR	CHB-C1B	2.90	1.46	1.40
5	H	401	MNR	CHC-C4B	2.89	1.46	1.40
5	D	401	MNR	C4C-C3C	2.32	1.49	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	401	MNR	C4A-C3A-C2A	-7.26	102.57	108.61
5	H	401	MNR	C4A-C3A-C2A	-5.97	103.65	108.61
5	D	401	MNR	CHC-C1C-NC	5.50	125.70	120.84
5	H	401	MNR	CHB-C4A-NA	5.45	125.66	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	401	MNR	CHB-C4A-NA	4.78	125.06	120.84
5	D	401	MNR	CMB-C2B-C3B	4.38	132.87	124.68
5	D	401	MNR	CHD-C4C-NC	4.37	124.70	120.84
5	D	401	MNR	CHA-C1A-NA	4.24	124.59	120.84
5	H	401	MNR	CHC-C1C-NC	4.18	124.54	120.84
5	H	401	MNR	CHD-C4C-NC	4.13	124.49	120.84
5	H	401	MNR	CHA-C1A-NA	3.23	123.69	120.84
5	H	401	MNR	CMB-C2B-C3B	3.17	130.60	124.68
5	D	401	MNR	C4C-CHD-C1D	2.82	126.30	118.67
5	D	401	MNR	CMD-C2D-C3D	2.81	130.23	124.94
5	H	401	MNR	C1A-C2A-C3A	-2.63	103.39	113.64
5	D	401	MNR	C4A-CHB-C1B	2.60	125.70	118.67
5	D	401	MNR	C1A-C2A-C3A	-2.52	103.84	113.64
5	H	401	MNR	CMC-C2C-C1C	2.42	129.29	124.73
5	D	401	MNR	C1A-CHA-C4D	2.37	125.08	118.67
3	B	501	AGA	O3-P1-O4	2.36	119.90	110.68
5	D	401	MNR	CHD-C4C-C3C	-2.23	123.09	126.66
5	D	401	MNR	CAA-CBA-CGA	-2.15	108.97	113.60
5	H	401	MNR	C4C-CHD-C1D	2.15	124.48	118.67
5	H	401	MNR	C4A-CHB-C1B	2.09	124.33	118.67
5	H	401	MNR	C1A-CHA-C4D	2.07	124.27	118.67
5	H	401	MNR	CMD-C2D-C3D	2.07	128.84	124.94
5	D	401	MNR	C1C-CHC-C4B	2.05	124.21	118.67

There are no chirality outliers.

All (11) 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	C2D-C3D-CAD-CBD
5	D	401	MNR	C4D-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

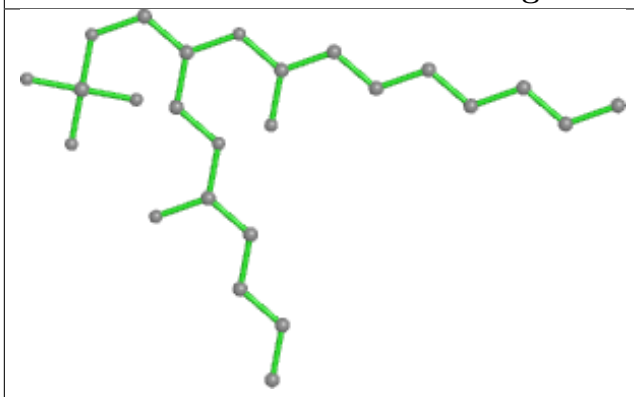
There are no ring outliers.

3 monomers are involved in 17 short contacts:

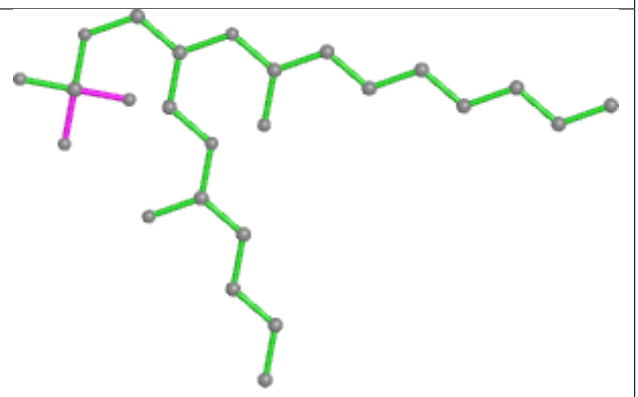
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	401	MNR	10	0
5	D	401	MNR	6	0
4	B	502	PGE	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

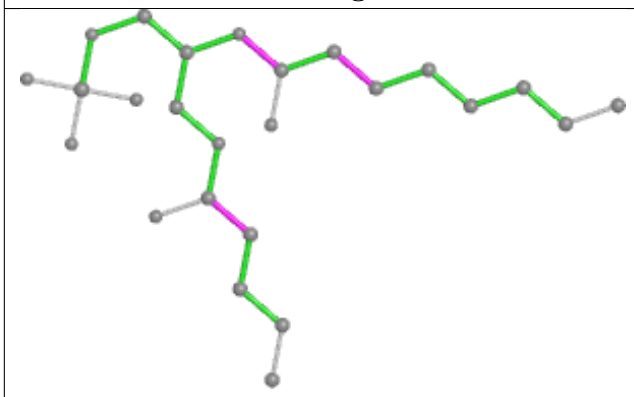
Ligand AGA B 501



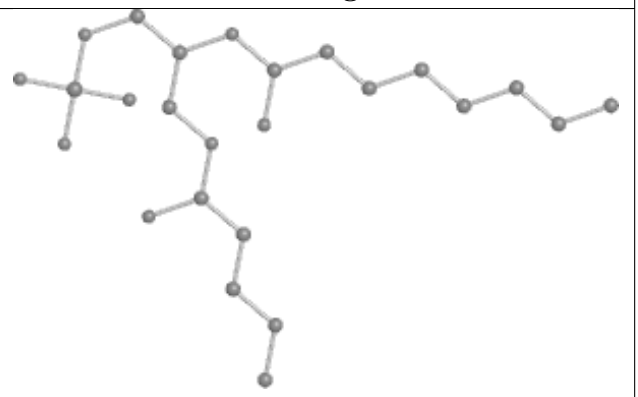
Bond lengths



Bond angles

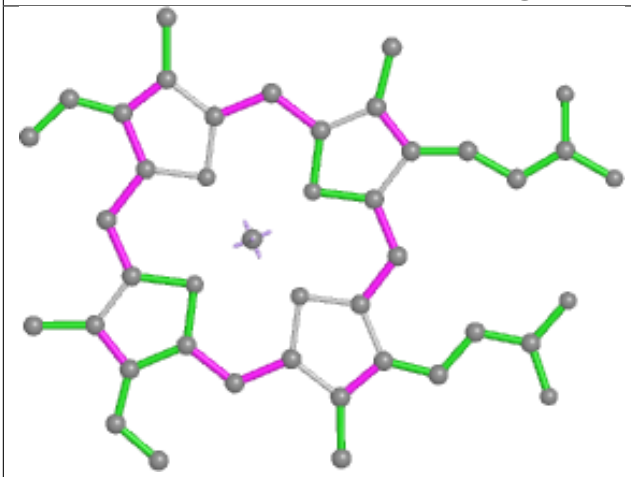


Torsions

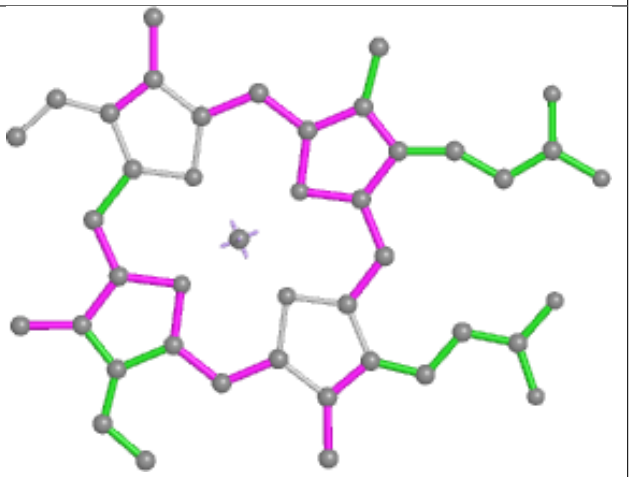


Rings

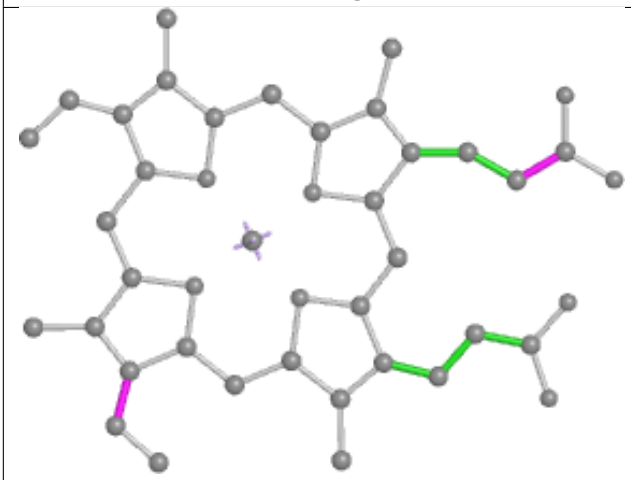
Ligand MNR H 401



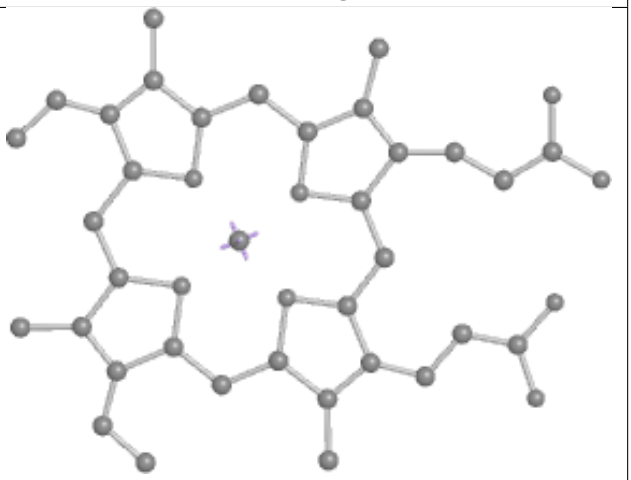
Bond lengths



Bond angles

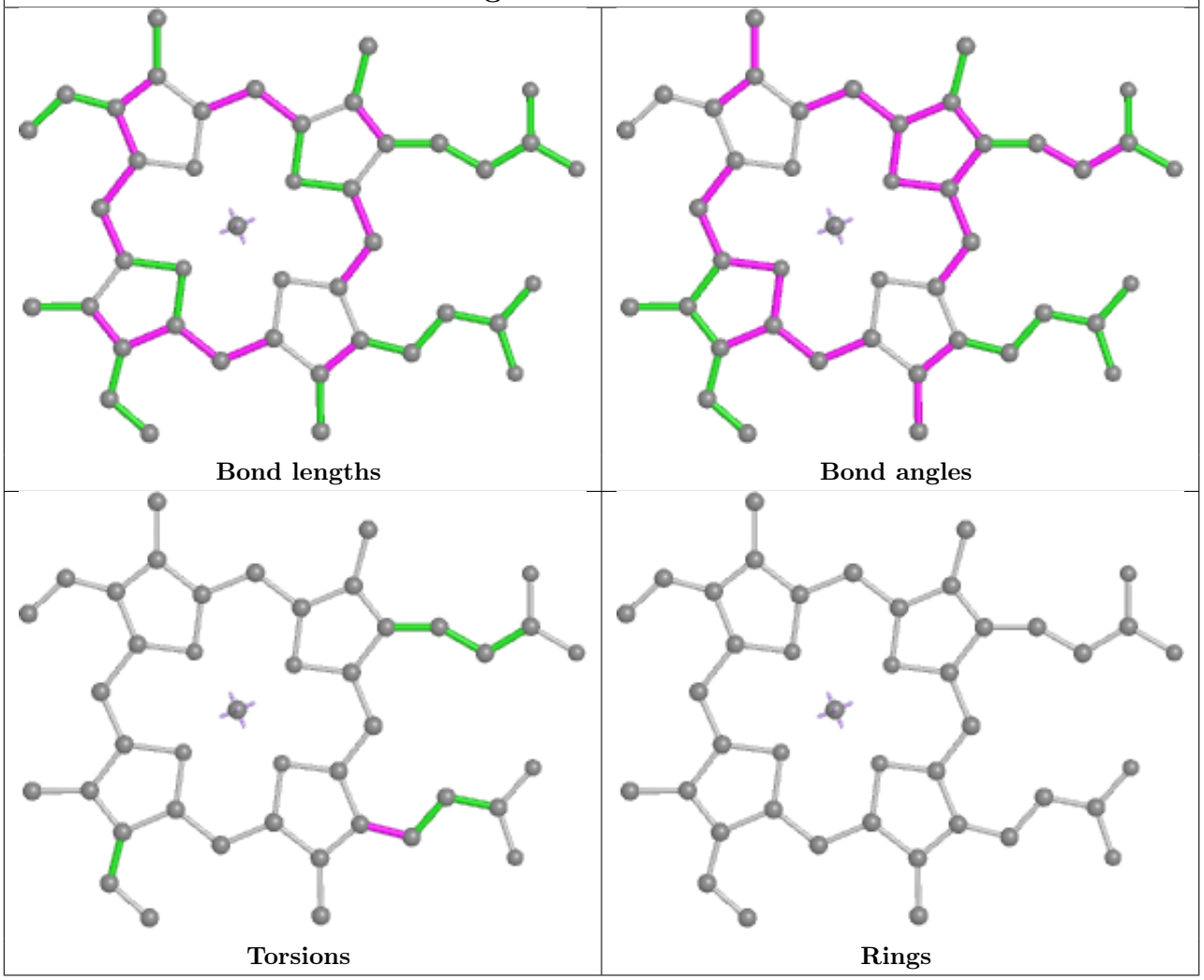


Torsions



Rings

Ligand MNR D 401



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, 95^{th} 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%)	0.72	24 (11%) 12 8	89, 109, 128, 145	0
1	C	217/231 (93%)	0.47	15 (6%) 24 17	74, 99, 118, 127	0
1	E	213/231 (92%)	0.55	20 (9%) 15 11	101, 136, 163, 220	0
1	G	227/231 (98%)	0.38	18 (7%) 20 14	81, 106, 144, 166	0
1	I	222/231 (96%)	0.45	20 (9%) 17 11	77, 98, 115, 133	0
1	K	222/231 (96%)	0.31	12 (5%) 32 22	70, 91, 122, 172	0
2	B	341/344 (99%)	0.84	50 (14%) 7 5	96, 116, 167, 210	0
2	D	342/344 (99%)	0.86	48 (14%) 7 5	88, 162, 220, 249	0
2	F	342/344 (99%)	0.92	52 (15%) 6 5	109, 129, 168, 202	0
2	H	342/344 (99%)	0.85	59 (17%) 5 4	109, 169, 214, 254	0
2	J	343/344 (99%)	0.84	44 (12%) 9 7	91, 149, 185, 213	0
2	L	343/344 (99%)	0.89	51 (14%) 7 5	82, 142, 185, 211	0
All	All	3370/3450 (97%)	0.71	413 (12%) 9 7	70, 124, 194, 254	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	158	THR	10.6
2	F	211	GLN	9.5
2	L	155	THR	9.3
1	E	208	ARG	8.1
2	B	207	LYS	7.8
2	F	298	GLY	7.5
1	E	204	ALA	7.3
2	J	163	HIS	7.3
2	F	210	PHE	7.3
2	B	118	GLY	7.2
2	L	156	VAL	7.1

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Mol	Chain	Res	Type	RSRZ
2	J	101	THR	6.9
1	E	19	GLY	6.8
2	L	154	GLY	6.8
1	E	203	LEU	6.7
1	G	164	ASP	6.7
1	E	206	ALA	6.6
2	D	48	GLU	6.6
2	L	157	LYS	6.5
2	J	90	GLN	6.4
1	A	114	LYS	6.1
2	L	12	ALA	6.0
1	K	224	TRP	6.0
2	F	299	SER	6.0
2	B	115	ASP	6.0
1	A	164	ASP	5.9
1	G	229	PHE	5.9
2	B	190	ASN	5.8
2	J	215	ALA	5.7
2	D	209	ALA	5.7
2	L	191	GLN	5.6
2	L	297	ALA	5.6
2	F	215	ALA	5.6
2	F	10	ALA	5.5
2	H	341	GLY	5.5
2	F	163	HIS	5.5
2	H	241	PHE	5.5
2	H	215	ALA	5.4
1	A	210	VAL	5.4
1	A	209	PHE	5.3
1	I	204	ALA	5.2
2	F	209	ALA	5.2
2	B	205	ASP	5.1
2	B	112	PRO	5.1
2	H	217	LYS	5.0
2	B	117	VAL	5.0
2	J	342	ALA	5.0
1	A	211	GLU	5.0
2	H	214	PRO	4.9
2	L	118	GLY	4.9
1	A	18	ASP	4.9
2	H	77	ALA	4.8
2	D	90	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	342	ALA	4.8
1	I	188	GLU	4.7
2	L	117	VAL	4.7
1	A	90	GLN	4.7
2	F	342	ALA	4.7
1	I	224	TRP	4.7
1	E	37	GLU	4.6
2	L	342	ALA	4.6
2	F	207	LYS	4.6
2	F	9	ARG	4.5
2	F	297	ALA	4.5
1	C	20	ILE	4.5
1	G	165	GLU	4.5
2	F	206	LEU	4.5
2	F	216	TYR	4.5
1	E	34	PHE	4.4
1	I	223	LEU	4.4
2	B	188	LEU	4.3
1	A	115	PRO	4.3
2	B	113	LEU	4.3
2	F	204	THR	4.2
1	I	190	ALA	4.2
2	F	205	ASP	4.2
2	D	16	ALA	4.2
2	J	5	ILE	4.1
2	H	80	TRP	4.1
1	A	112	GLY	4.1
2	J	9	ARG	4.1
1	K	89	PHE	4.1
2	B	183	VAL	4.1
2	H	74	GLU	4.0
2	B	340	LEU	4.0
1	G	228	GLN	4.0
2	B	341	GLY	4.0
2	B	174	TRP	4.0
2	B	116	SER	4.0
2	H	48	GLU	4.0
2	H	339	ALA	4.0
2	J	339	ALA	4.0
2	F	93	ILE	3.9
2	J	100	ASN	3.9
2	L	129	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	91	GLN	3.9
2	J	341	GLY	3.9
2	D	174	TRP	3.9
2	H	218	SER	3.9
1	E	32	GLU	3.8
2	B	157	LYS	3.8
2	L	127	LEU	3.8
2	H	68	THR	3.8
2	L	267	LEU	3.8
2	F	217	LYS	3.8
2	H	78	GLU	3.8
2	F	208	GLY	3.8
2	J	48	GLU	3.7
2	J	60	ALA	3.7
1	E	97	SER	3.7
2	F	175	GLN	3.7
2	J	165	PRO	3.7
2	F	183	VAL	3.7
1	E	91	GLN	3.7
2	H	123	GLN	3.7
2	J	314	LEU	3.6
2	L	10	ALA	3.6
2	D	47	ILE	3.6
1	K	27	ASP	3.6
1	E	207	ASP	3.6
2	D	88	VAL	3.6
2	B	85	PRO	3.6
2	H	82	ASP	3.5
1	E	21	SER	3.5
2	J	71	GLU	3.4
2	H	69	SER	3.4
2	H	1	MET	3.4
2	L	343	THR	3.4
1	G	89	PHE	3.4
1	E	136	ARG	3.4
2	B	204	THR	3.4
2	F	195	ILE	3.4
1	K	164	ASP	3.4
2	F	181	LYS	3.4
1	G	227	PRO	3.4
2	F	112	PRO	3.4
2	H	109	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	20	ILE	3.4
2	L	194	THR	3.4
2	L	268	ILE	3.4
2	F	222	SER	3.4
2	B	166	VAL	3.3
2	B	84	THR	3.3
2	H	116	SER	3.3
2	D	342	ALA	3.3
2	D	207	LYS	3.3
1	I	36	GLY	3.3
2	B	74	GLU	3.3
2	F	113	LEU	3.3
1	A	116	ARG	3.3
2	H	39	LEU	3.3
2	D	28	LEU	3.2
2	B	211	GLN	3.1
2	D	134	PHE	3.1
2	L	47	ILE	3.1
2	H	36	THR	3.1
2	J	158	THR	3.1
2	H	340	LEU	3.1
1	G	198	HIS	3.1
2	D	19	ALA	3.1
2	D	67	PHE	3.1
1	C	3	ALA	3.1
2	L	115	ASP	3.1
2	J	164	THR	3.1
2	L	13	GLY	3.1
2	B	50	LEU	3.1
1	A	165	GLU	3.0
1	A	25	ALA	3.0
2	L	209	ALA	3.0
1	E	188	GLU	3.0
2	F	213	MET	3.0
2	L	206	LEU	3.0
1	E	16	TYR	3.0
1	G	224	TRP	3.0
2	J	222	SER	3.0
2	F	300	VAL	3.0
1	A	203	LEU	3.0
2	D	280	ALA	3.0
2	D	41	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	281	GLY	3.0
2	L	341	GLY	3.0
2	B	91	THR	3.0
2	F	90	GLN	2.9
2	H	183	VAL	2.9
2	D	89	SER	2.9
2	H	159	GLU	2.9
2	B	316	ILE	2.9
1	E	18	ASP	2.9
2	D	308	SER	2.9
2	L	190	ASN	2.9
1	I	187	LYS	2.9
2	F	316	ILE	2.9
2	B	208	GLY	2.9
2	D	208	GLY	2.9
2	F	214	PRO	2.9
2	J	214	PRO	2.9
2	J	174	TRP	2.9
2	F	221	SER	2.9
2	H	308	SER	2.9
2	L	304	LEU	2.9
2	H	30	VAL	2.9
2	L	130	GLU	2.8
2	D	3	LEU	2.8
2	L	66	GLU	2.8
2	B	155	THR	2.8
1	G	163	ALA	2.8
2	B	214	PRO	2.8
2	B	56	VAL	2.8
2	H	65	PRO	2.7
2	L	139	ALA	2.7
1	I	200	ARG	2.7
2	J	183	VAL	2.7
2	D	154	GLY	2.7
2	B	107	LEU	2.7
1	E	205	TYR	2.7
1	A	89	PHE	2.7
1	I	167	THR	2.7
2	H	194	THR	2.7
2	L	68	THR	2.7
1	I	207	ASP	2.7
2	D	159	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	15	PHE	2.7
2	H	243	THR	2.7
1	A	109	HIS	2.7
2	L	32	LEU	2.7
2	L	339	ALA	2.7
1	C	39	VAL	2.7
2	B	178	SER	2.6
2	F	98	ASN	2.6
1	K	78	THR	2.6
2	F	101	THR	2.6
2	H	240	ALA	2.6
2	J	44	THR	2.6
2	B	203	VAL	2.6
2	H	203	VAL	2.6
2	L	220	ARG	2.6
1	E	20	ILE	2.6
1	K	20	ILE	2.6
1	C	58	PHE	2.6
2	L	298	GLY	2.6
2	L	340	LEU	2.6
1	K	3	ALA	2.6
2	J	182	ALA	2.6
2	L	128	PRO	2.6
2	J	151	THR	2.6
2	B	264	ARG	2.6
2	D	135	LEU	2.6
2	L	159	GLU	2.6
2	B	114	PRO	2.6
2	D	165	PRO	2.6
2	F	218	SER	2.6
2	J	1	MET	2.6
1	I	122	GLU	2.6
2	D	9	ARG	2.6
1	C	214	ASP	2.6
2	B	82	ASP	2.6
2	L	7	ASP	2.6
1	I	20	ILE	2.5
2	B	123	GLN	2.5
2	D	12	ALA	2.5
2	D	99	ALA	2.5
2	D	193	PRO	2.5
2	H	193	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	17	LEU	2.5
2	D	131	LEU	2.5
2	H	35	LEU	2.5
1	C	25	ALA	2.5
2	J	155	THR	2.5
1	I	163	ALA	2.5
2	B	338	ILE	2.5
1	A	26	LEU	2.5
2	H	70	SER	2.5
1	K	146	GLN	2.5
2	B	75	GLN	2.5
2	B	119	GLY	2.5
1	C	89	PHE	2.5
1	E	209	PHE	2.5
2	H	118	GLY	2.5
2	J	218	SER	2.5
2	D	100	ASN	2.5
2	J	160	ASN	2.5
1	A	155	MET	2.5
2	F	264	ARG	2.4
2	J	102	THR	2.4
2	L	36	THR	2.4
2	D	46	ALA	2.4
2	H	49	ALA	2.4
2	J	65	PRO	2.4
1	C	32	GLU	2.4
2	L	15	PHE	2.4
2	J	157	LYS	2.4
1	I	195	MET	2.4
2	D	49	ALA	2.4
2	H	31	MET	2.4
2	J	129	ALA	2.4
2	F	212	ALA	2.4
1	A	42	VAL	2.4
2	H	75	GLN	2.4
2	H	156	VAL	2.4
2	J	299	SER	2.4
2	J	142	HIS	2.4
2	D	155	THR	2.4
1	A	113	ILE	2.4
2	F	118	GLY	2.4
1	A	204	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	196	VAL	2.4
2	B	337	GLN	2.4
2	H	79	ARG	2.4
1	C	80	THR	2.3
1	I	203	LEU	2.3
2	H	67	PHE	2.3
2	F	303	SER	2.3
2	H	309	VAL	2.3
2	B	158	THR	2.3
2	L	277	ILE	2.3
2	F	318	LEU	2.3
2	D	36	THR	2.3
1	A	6	VAL	2.3
1	K	77	ALA	2.3
2	F	178	SER	2.3
2	F	140	GLY	2.3
2	J	181	LYS	2.3
1	C	218	LEU	2.3
2	F	142	HIS	2.3
2	F	224	LEU	2.3
2	D	168	TRP	2.3
1	K	24	THR	2.3
1	A	91	GLN	2.3
2	B	90	GLN	2.3
2	D	30	VAL	2.3
2	L	140	GLY	2.3
1	C	17	PRO	2.2
2	J	318	LEU	2.2
2	J	74	GLU	2.2
2	J	178	SER	2.2
1	A	108	ASP	2.2
2	B	171	THR	2.2
2	H	58	THR	2.2
2	J	343	THR	2.2
1	E	200	ARG	2.2
2	H	81	LYS	2.2
2	L	213	MET	2.2
2	L	217	LYS	2.2
2	L	244	VAL	2.2
2	B	277	ILE	2.2
2	F	66	GLU	2.2
2	F	64	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	89	SER	2.2
2	L	65	PRO	2.2
1	C	159	GLN	2.2
2	B	226	MET	2.2
1	I	221	ALA	2.2
1	G	226	HIS	2.2
2	B	2	PHE	2.2
2	F	226	MET	2.2
2	J	180	THR	2.2
1	I	38	LEU	2.2
1	K	90	GLN	2.2
2	B	143	ILE	2.2
2	L	9	ARG	2.2
2	L	74	GLU	2.2
2	H	168	TRP	2.2
1	K	223	LEU	2.2
2	B	101	THR	2.2
2	H	238	THR	2.2
2	D	61	GLY	2.1
1	C	208	ARG	2.1
1	G	17	PRO	2.1
1	G	98	LEU	2.1
2	F	308	SER	2.1
2	F	67	PHE	2.1
1	A	102	GLU	2.1
2	H	304	LEU	2.1
2	L	1	MET	2.1
2	F	102	THR	2.1
2	H	216	TYR	2.1
1	I	37	GLU	2.1
2	D	74	GLU	2.1
2	H	66	GLU	2.1
2	J	224	LEU	2.1
2	H	117	VAL	2.1
1	I	3	ALA	2.1
1	G	197	THR	2.1
2	D	178	SER	2.1
2	F	171	THR	2.1
2	H	289	GLY	2.1
1	C	161	LEU	2.1
2	L	39	LEU	2.1
2	B	202	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	104	VAL	2.1
2	B	209	ALA	2.1
2	D	217	LYS	2.1
2	D	149	THR	2.1
2	D	20	SER	2.1
2	H	89	SER	2.1
2	F	43	ASN	2.1
2	B	57	PHE	2.1
2	H	3	LEU	2.1
2	H	32	LEU	2.1
2	D	169	VAL	2.1
2	J	88	VAL	2.1
2	H	290	ALA	2.0
2	J	338	ILE	2.0
2	D	210	PHE	2.0
2	L	330	ASN	2.0
1	G	223	LEU	2.0
2	H	202	VAL	2.0
1	C	37	GLU	2.0
2	H	251	ARG	2.0
1	G	96	GLY	2.0
2	H	149	THR	2.0
2	D	211	GLN	2.0
1	I	126	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

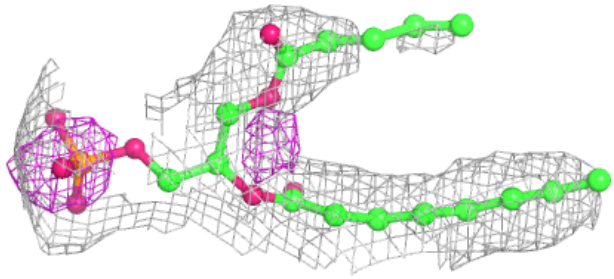
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

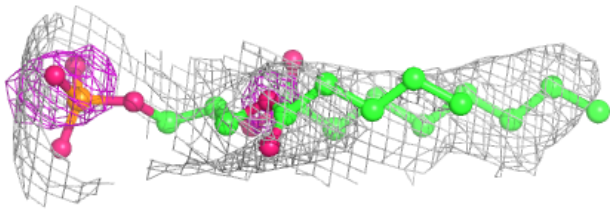
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	H	402	4/4	0.28	0.37	142,142,142,142	0
4	PGE	B	502	10/10	0.59	0.14	102,102,102,102	0
6	PEG	D	402	7/7	0.60	0.24	142,142,142,142	0
3	AGA	B	501	25/30	0.78	0.23	107,107,107,107	0
5	MNR	H	401	43/43	0.86	0.29	477,482,484,485	0
5	MNR	D	401	43/43	0.93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

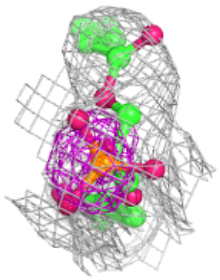
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

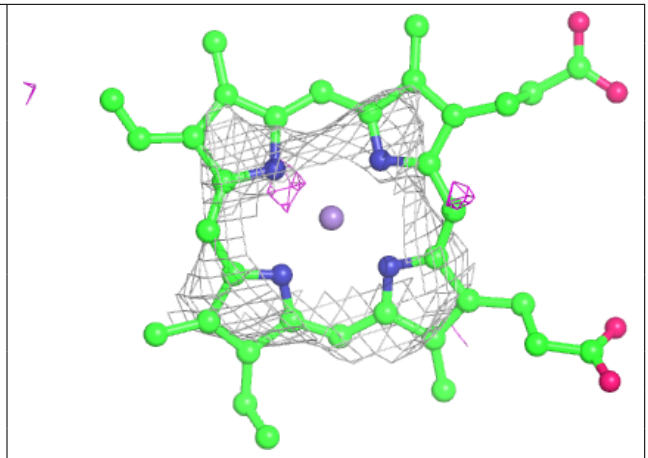


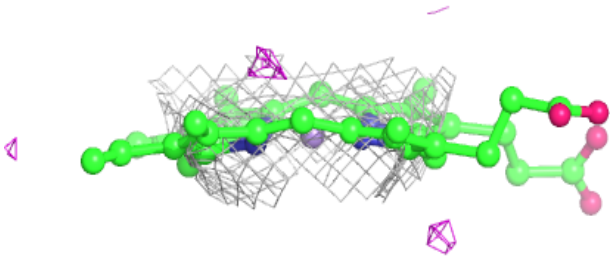


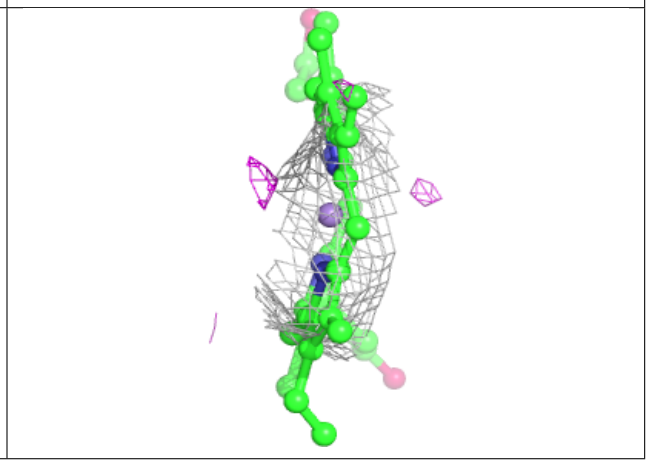


Electron density around MNR H 401:

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

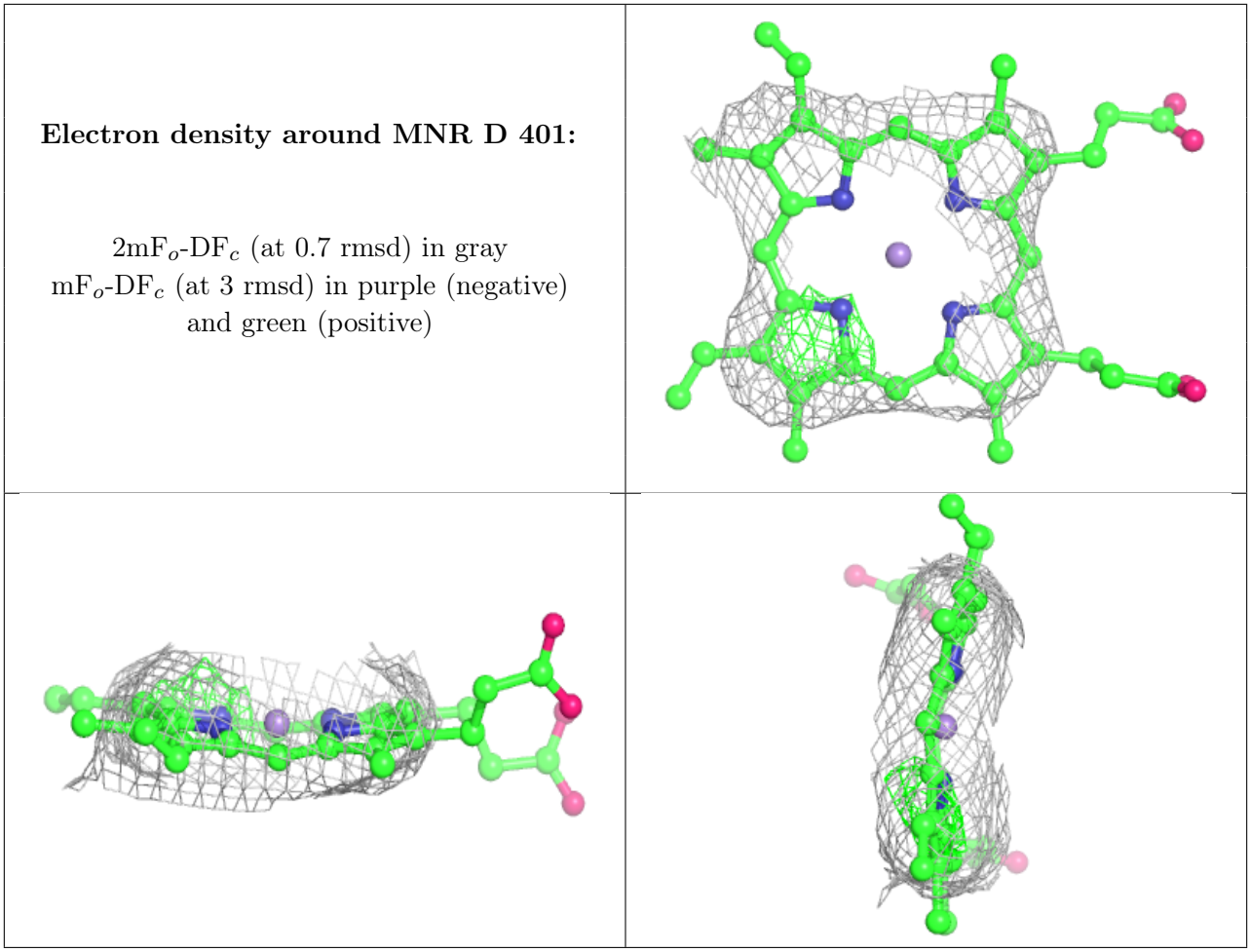






Electron density around MNR D 401:

$2mF_o$-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

There are no such residues in this entry.