Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:32 am BST

PDB ID	:	1L7V
Title	:	Bacterial ABC Transporter Involved in B12 Uptake
Authors	:	Locher, K.P.; Lee, A.T.; Rees, D.C.
Deposited on	:	2002-03-18
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 following versions of software and data (see references ⓘ) were used in the production of this report:

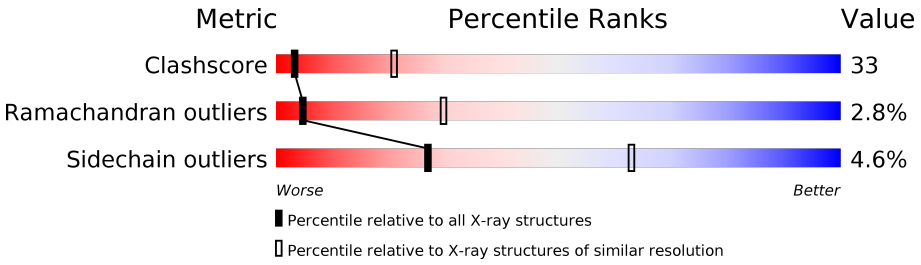
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	326	49% 47%
1	B	326	52% 45%
2	C	249	46% 43% 7%
2	D	249	45% 44% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	V4O	C	250	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	V4O	D	250	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8410 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 VITAMIN B12 TRANSPORT SYSTEM PERMEASE PROTEIN BTUC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	Se	163	0	0
			2441	1611	418	393	8	11			
1	B	324	Total	C	N	O	S	Se	183	0	0
			2441	1611	418	393	8	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	23	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	77	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	160	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	176	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	179	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	180	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	194	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	211	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	213	MSE	MET	MODIFIED RESIDUE	UNP P06609
A	242	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	1	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	23	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	77	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	160	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	176	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	179	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	180	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	194	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	211	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	213	MSE	MET	MODIFIED RESIDUE	UNP P06609
B	242	MSE	MET	MODIFIED RESIDUE	UNP P06609

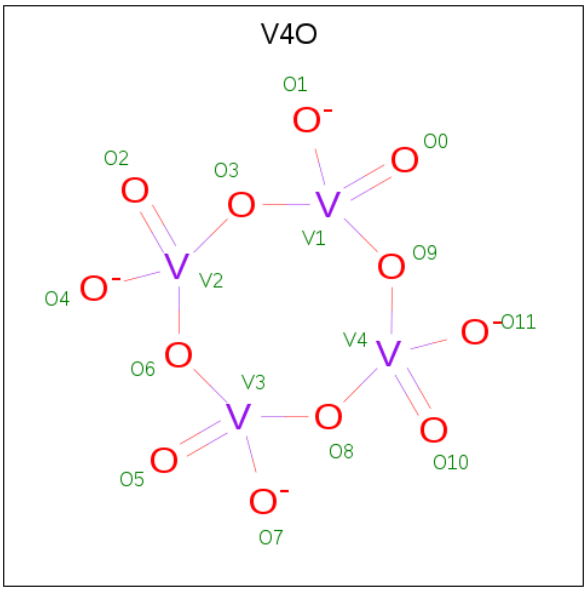
- Molecule 2 is a protein called Vitamin B12 transport ATP-binding protein btuD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	231	Total	C	N	O	S	Se	59	0	0
			1748	1094	322	324	1	7			
2	D	231	Total	C	N	O	S	Se	59	0	0
			1748	1094	322	324	1	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	5	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	46	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	49	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	161	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	188	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	211	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	232	MSE	MET	MODIFIED RESIDUE	UNP P06611
C	244	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	1	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	5	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	46	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	49	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	161	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	188	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	211	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	232	MSE	MET	MODIFIED RESIDUE	UNP P06611
D	244	MSE	MET	MODIFIED RESIDUE	UNP P06611

- Molecule 3 is CYCLO-TETRAMETAVANADATE (three-letter code: V4O) (formula: $O_{12}V_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O V 16 12 4	0	0
3	D	1	Total O V 16 12 4	0	0

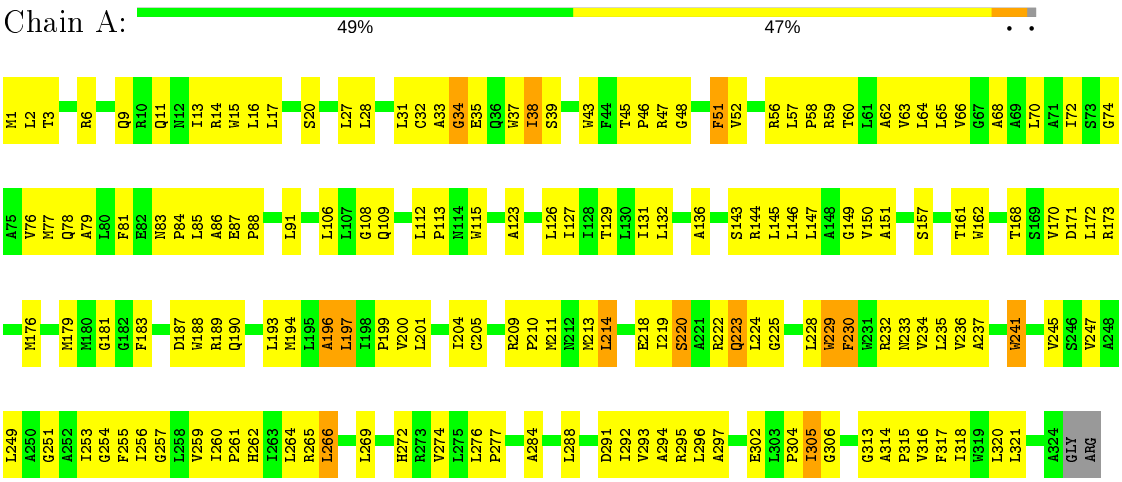
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

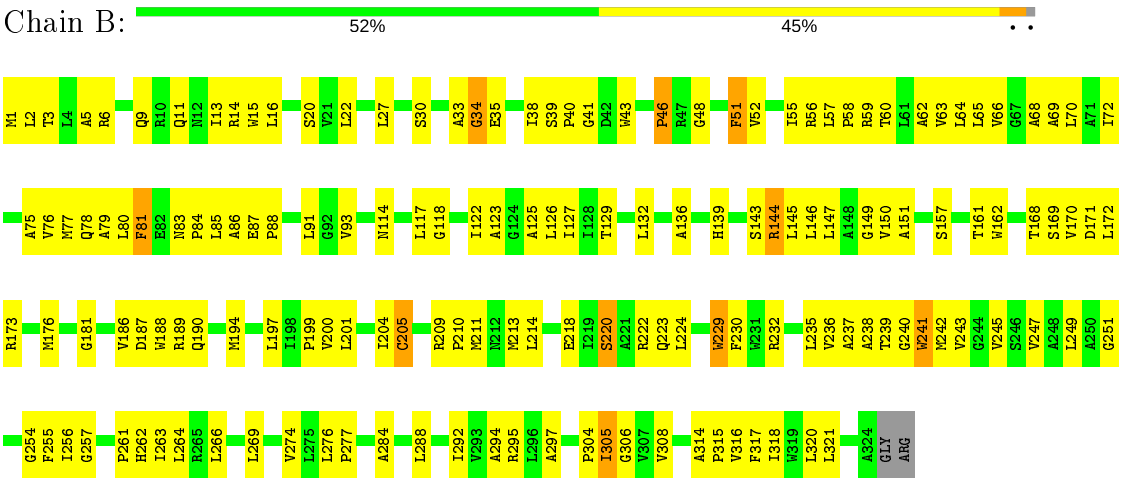
• Molecule 1: VITAMIN B12 TRANSPORT SYSTEM PERMEASE PROTEIN BTUC

Chain A:



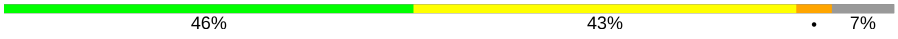
• Molecule 1: VITAMIN B12 TRANSPORT SYSTEM PERMEASE PROTEIN BTUC

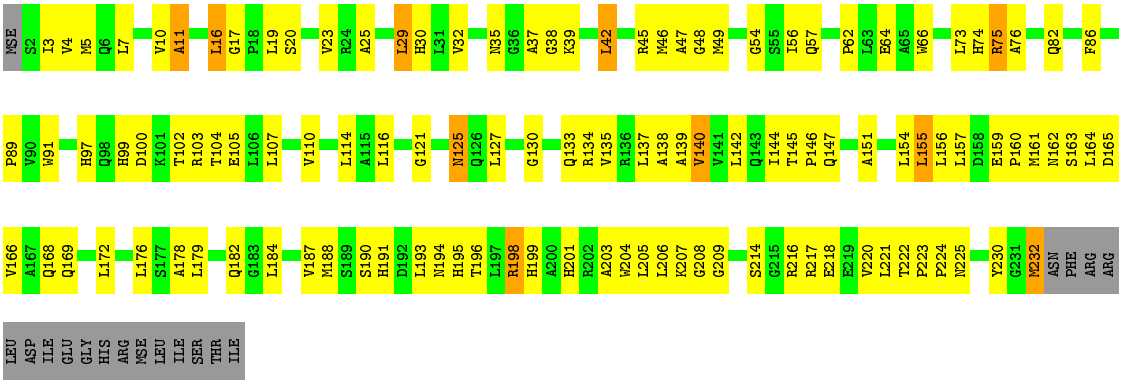
Chain B:



• Molecule 2: Vitamin B12 transport ATP-binding protein btuD

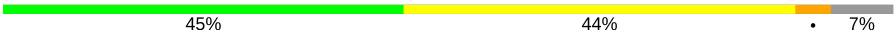
Chain C:

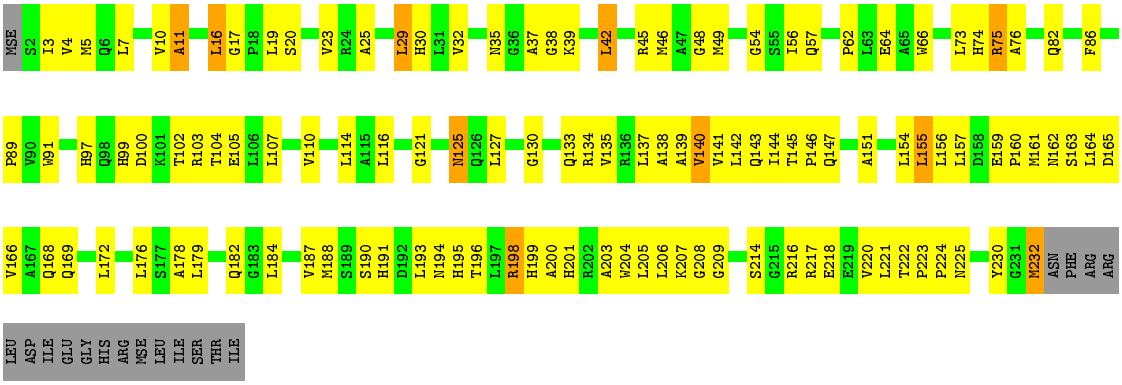




- Molecule 2: Vitamin B12 transport ATP-binding protein btuD

Chain D:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.99Å 106.29Å 95.54Å 90.00° 99.29° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.262 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8410	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V4O

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	0.32	0/2485	0.57	0/3378
1	B	0.34	0/2485	0.62	1/3378 (0.0%)
2	C	0.31	0/1773	0.59	0/2395
2	D	0.29	0/1773	0.58	0/2395
All	All	0.32	0/8516	0.59	1/11546 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	SER	N-CA-CB	-5.17	102.75	110.50

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	2441	0	2606	169	1
1	B	2441	0	2606	155	1
2	C	1748	0	1775	115	0
2	D	1748	0	1775	117	0
3	C	16	0	0	6	0
3	D	16	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8410	0	8762	533	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 33.

All (533) 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:C:30:HIS:HE2	2:C:188:MSE:HE3	1.02	1.17
2:D:30:HIS:HE2	2:D:188:MSE:HE3	1.02	1.09
1:A:77:MSE:HE1	1:A:88:PRO:HG3	1.36	1.07
1:B:77:MSE:HE1	1:B:88:PRO:HG3	1.35	1.05
1:A:269:LEU:HD22	1:A:274:VAL:HG11	1.41	1.02
1:B:87:GLU:HG2	1:B:88:PRO:HD2	1.41	1.02
1:A:76:VAL:HA	1:A:211:MSE:HE1	1.40	1.01
1:A:87:GLU:HG2	1:A:88:PRO:HD2	1.39	0.99
2:D:30:HIS:NE2	2:D:188:MSE:HE3	1.78	0.98
2:C:30:HIS:NE2	2:C:188:MSE:HE3	1.78	0.97
1:B:76:VAL:HA	1:B:211:MSE:HE1	1.47	0.93
1:B:220:SER:HB2	2:D:82:GLN:HE22	1.35	0.90
2:D:57:GLN:HA	2:D:62:PRO:HA	1.56	0.88
1:A:58:PRO:HG3	1:A:188:TRP:CE2	2.10	0.87
2:C:57:GLN:HA	2:C:62:PRO:HA	1.56	0.85
1:B:58:PRO:HG3	1:B:188:TRP:CE2	2.12	0.85
1:B:209:ARG:HB2	1:B:210:PRO:HD3	1.59	0.84
1:B:65:LEU:HB3	1:B:197:LEU:HD23	1.60	0.83
1:B:232:ARG:O	1:B:236:VAL:HG23	1.79	0.83
1:A:87:GLU:HG2	1:A:88:PRO:CD	2.08	0.83
1:A:232:ARG:O	1:A:236:VAL:HG23	1.79	0.82
1:B:87:GLU:HG2	1:B:88:PRO:CD	2.10	0.81
1:A:209:ARG:HB2	1:A:210:PRO:HD3	1.62	0.81
1:A:81:PHE:HD2	1:A:145:LEU:HD13	1.45	0.81
1:A:316:VAL:O	1:A:320:LEU:HG	1.80	0.81
1:A:269:LEU:HD22	1:A:274:VAL:CG1	2.09	0.81
1:A:59:ARG:NH1	1:A:295:ARG:HH11	1.79	0.80
2:C:179:LEU:HD22	2:C:184:LEU:HD12	1.64	0.80
1:B:70:LEU:HB2	1:B:256:ILE:HD11	1.62	0.79
1:B:33:ALA:C	1:B:56:ARG:NH2	2.36	0.79
2:D:179:LEU:HD22	2:D:184:LEU:HD12	1.64	0.79
1:A:70:LEU:HB2	1:A:256:ILE:HD11	1.63	0.79
2:C:75:ARG:HD3	2:C:75:ARG:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ALA:HB2	1:B:145:LEU:HD21	1.66	0.78
2:D:75:ARG:O	2:D:75:ARG:HD3	1.83	0.78
1:A:62:ALA:HB2	1:A:194:MSE:HE2	1.65	0.77
1:B:211:MSE:HE3	1:B:235:LEU:HD13	1.66	0.77
1:B:187:ASP:HB3	1:B:189:ARG:HG2	1.66	0.77
1:B:269:LEU:HD22	1:B:274:VAL:HG11	1.63	0.77
1:A:129:THR:HG22	1:A:236:VAL:HG13	1.66	0.77
2:D:97:HIS:CD2	2:D:139:ALA:HB1	2.20	0.77
1:A:59:ARG:HH12	1:A:295:ARG:HH11	1.32	0.77
2:C:97:HIS:CD2	2:C:139:ALA:HB1	2.20	0.77
2:C:42:LEU:HD22	2:C:46:MSE:SE	2.35	0.77
1:A:33:ALA:C	1:A:56:ARG:HH21	1.88	0.76
1:A:65:LEU:HB3	1:A:197:LEU:HD23	1.66	0.76
1:B:254:GLY:O	1:B:255:PHE:HB2	1.86	0.76
2:D:42:LEU:HD22	2:D:46:MSE:SE	2.35	0.76
1:A:33:ALA:C	1:A:56:ARG:NH2	2.39	0.75
1:B:276:LEU:HB2	1:B:277:PRO:HD3	1.68	0.75
1:B:38:ILE:HG22	1:B:39:SER:H	1.52	0.74
2:C:157:LEU:HB3	2:C:160:PRO:HG3	1.71	0.73
2:D:157:LEU:HB3	2:D:160:PRO:HG3	1.71	0.73
1:A:276:LEU:HB2	1:A:277:PRO:HD3	1.69	0.73
1:B:59:ARG:HH12	1:B:295:ARG:NE	1.87	0.73
1:A:113:PRO:HB2	1:A:115:TRP:CD1	2.24	0.73
1:A:187:ASP:HB3	1:A:189:ARG:HG2	1.72	0.72
1:B:129:THR:HG22	1:B:236:VAL:HG13	1.72	0.71
1:B:79:ALA:CB	1:B:211:MSE:HE2	2.20	0.71
1:B:314:ALA:HB3	1:B:315:PRO:HD3	1.74	0.70
2:C:130:GLY:O	2:C:134:ARG:HG3	1.92	0.70
1:B:79:ALA:HB3	1:B:211:MSE:HE2	1.73	0.70
2:D:130:GLY:O	2:D:134:ARG:HG3	1.92	0.70
1:A:84:PRO:HB3	1:A:262:HIS:CE1	2.27	0.69
1:A:314:ALA:HB3	1:A:315:PRO:HD3	1.75	0.69
1:B:62:ALA:HB2	1:B:194:MSE:HE2	1.74	0.69
2:D:222:THR:HG22	2:D:225:ASN:ND2	2.08	0.69
1:B:81:PHE:HD2	1:B:145:LEU:HD13	1.58	0.69
1:B:80:LEU:HD21	1:B:235:LEU:HD12	1.74	0.69
1:A:220:SER:HB2	2:C:82:GLN:HE22	1.58	0.69
2:C:222:THR:HG22	2:C:225:ASN:ND2	2.08	0.68
1:A:76:VAL:HG21	1:A:204:ILE:HD11	1.75	0.68
1:B:38:ILE:HG22	1:B:39:SER:N	2.08	0.68
2:C:156:LEU:HD23	2:C:187:VAL:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:MSE:HE1	1:A:88:PRO:CG	2.20	0.68
1:B:143:SER:O	1:B:147:LEU:HG	1.94	0.67
2:D:196:THR:HG23	2:D:221:LEU:HD11	1.77	0.67
1:B:55:ILE:O	1:B:58:PRO:HD2	1.95	0.67
1:B:64:LEU:HD21	1:B:288:LEU:HD11	1.76	0.67
2:C:178:ALA:O	2:C:182:GLN:HG3	1.95	0.67
2:C:146:PRO:HB2	2:C:182:GLN:HE21	1.60	0.67
2:D:178:ALA:O	2:D:182:GLN:HG3	1.95	0.67
2:C:161:MSE:HG3	2:C:191:HIS:CE1	2.30	0.66
1:B:123:ALA:O	1:B:127:ILE:HG12	1.94	0.66
2:C:196:THR:HG23	2:C:221:LEU:HD11	1.77	0.66
2:D:146:PRO:HB2	2:D:182:GLN:HE21	1.60	0.66
2:D:156:LEU:HD23	2:D:187:VAL:HB	1.76	0.66
1:B:229:TRP:CE3	1:B:229:TRP:HA	2.31	0.66
1:A:33:ALA:O	1:A:56:ARG:NH2	2.28	0.66
2:D:161:MSE:HG3	2:D:191:HIS:CE1	2.29	0.66
2:D:207:LYS:C	2:D:209:GLY:H	1.99	0.65
1:A:146:LEU:O	1:A:150:VAL:HG23	1.97	0.65
2:D:64:GLU:H	2:D:64:GLU:CD	1.99	0.65
1:A:34:GLY:O	1:A:35:GLU:HB2	1.95	0.65
2:C:193:LEU:O	2:C:196:THR:HG22	1.96	0.65
2:C:64:GLU:H	2:C:64:GLU:CD	1.98	0.65
1:A:147:LEU:HD21	1:B:85:LEU:HD13	1.79	0.65
2:D:216:ARG:O	2:D:220:VAL:HG23	1.98	0.64
2:C:207:LYS:C	2:C:209:GLY:H	2.00	0.64
2:C:4:VAL:CG2	2:C:25:ALA:HB2	2.27	0.64
1:A:254:GLY:O	1:A:255:PHE:HB2	1.97	0.64
2:D:4:VAL:CG2	2:D:25:ALA:HB2	2.27	0.64
2:C:207:LYS:O	2:C:209:GLY:N	2.30	0.64
2:D:193:LEU:O	2:D:196:THR:HG22	1.97	0.64
2:C:216:ARG:O	2:C:220:VAL:HG23	1.98	0.64
2:D:207:LYS:O	2:D:209:GLY:N	2.30	0.63
1:B:269:LEU:HD22	1:B:274:VAL:CG1	2.27	0.63
1:A:129:THR:CG2	1:A:236:VAL:HG13	2.29	0.63
1:B:126:LEU:HD21	1:B:237:ALA:HA	1.81	0.63
1:A:168:THR:C	1:A:170:VAL:H	2.01	0.62
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.34	0.62
2:D:29:LEU:HD11	2:D:204:TRP:CE2	2.34	0.62
1:A:57:LEU:HB3	1:A:58:PRO:HD3	1.81	0.62
2:C:29:LEU:HD11	2:C:204:TRP:CE2	2.34	0.62
1:A:64:LEU:HD22	1:A:284:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:O	1:A:147:LEU:HG	2.00	0.62
1:A:274:VAL:O	1:A:277:PRO:HD2	2.00	0.61
1:A:81:PHE:CD2	1:A:145:LEU:HD13	2.31	0.61
1:A:210:PRO:O	1:A:214:LEU:HB2	2.00	0.61
1:A:2:LEU:HD23	1:A:3:THR:N	2.15	0.61
1:A:79:ALA:HB3	1:A:211:MSE:HE2	1.83	0.61
1:A:85:LEU:HD22	1:B:147:LEU:HD21	1.83	0.60
1:B:1:MSE:HE3	1:B:6:ARG:HB2	1.82	0.60
1:B:316:VAL:O	1:B:320:LEU:HG	2.01	0.60
2:C:30:HIS:HB3	2:C:190:SER:HB2	1.84	0.60
2:C:193:LEU:HA	2:C:196:THR:HG22	1.82	0.60
1:A:37:TRP:CH2	1:A:39:SER:HB3	2.36	0.60
2:D:193:LEU:HA	2:D:196:THR:HG22	1.83	0.60
2:D:30:HIS:HB3	2:D:190:SER:HB2	1.84	0.60
1:A:63:VAL:HG11	1:A:288:LEU:HA	1.83	0.60
1:A:317:PHE:HE2	1:B:147:LEU:HB3	1.67	0.60
2:C:10:VAL:O	2:C:11:ALA:HB2	2.02	0.60
2:D:102:THR:O	2:D:104:THR:N	2.34	0.60
1:B:63:VAL:HG11	1:B:288:LEU:HD23	1.84	0.60
1:B:66:VAL:HG23	1:B:249:LEU:HD23	1.83	0.59
2:D:42:LEU:HD12	2:D:206:LEU:HD11	1.84	0.59
2:C:190:SER:OG	2:C:196:THR:HB	2.03	0.59
2:C:222:THR:HG22	2:C:225:ASN:HD22	1.67	0.59
2:D:190:SER:OG	2:D:196:THR:HB	2.03	0.59
1:A:126:LEU:HD21	1:A:237:ALA:HA	1.84	0.59
1:A:123:ALA:O	1:A:127:ILE:HG12	2.02	0.59
2:C:102:THR:O	2:C:104:THR:N	2.34	0.59
2:D:10:VAL:O	2:D:11:ALA:HB2	2.02	0.59
1:B:84:PRO:HB3	1:B:262:HIS:CE1	2.37	0.59
2:C:75:ARG:HD3	2:C:75:ARG:C	2.24	0.59
2:D:222:THR:HG22	2:D:225:ASN:HD22	1.67	0.59
1:B:33:ALA:C	1:B:56:ARG:HH21	2.01	0.59
2:D:145:THR:HG22	2:D:147:GLN:H	1.68	0.59
3:D:250:V4O:O0	3:D:250:V4O:V1	1.58	0.59
3:D:250:V4O:O7	3:D:250:V4O:V3	1.58	0.59
1:A:295:ARG:HA	1:A:302:GLU:HG3	1.83	0.58
1:A:321:LEU:HD21	1:B:147:LEU:HD13	1.85	0.58
2:C:56:ILE:N	2:C:56:ILE:HD12	2.18	0.58
2:D:11:ALA:HB1	2:D:16:LEU:O	2.03	0.58
2:D:56:ILE:HD12	2:D:56:ILE:N	2.18	0.58
1:A:260:ILE:HB	1:A:261:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:MSE:HE2	1:B:239:THR:HG23	1.85	0.58
2:C:10:VAL:HG13	2:C:45:ARG:NH1	2.18	0.58
2:C:42:LEU:HD12	2:C:206:LEU:HD11	1.84	0.58
1:B:66:VAL:CG2	1:B:249:LEU:HD23	2.33	0.58
3:C:250:V4O:V1	3:C:250:V4O:O0	1.58	0.58
2:C:11:ALA:HB1	2:C:16:LEU:O	2.03	0.58
2:D:5:MSE:HB3	2:D:23:VAL:HB	1.84	0.58
1:A:147:LEU:HD13	1:B:321:LEU:HD21	1.86	0.58
3:C:250:V4O:V3	3:C:250:V4O:O7	1.58	0.58
1:A:27:LEU:HD13	1:A:64:LEU:HD11	1.86	0.57
2:C:5:MSE:HB3	2:C:23:VAL:HB	1.84	0.57
2:D:91:TRP:HD1	2:D:121:GLY:HA2	1.69	0.57
1:A:147:LEU:HD21	1:B:85:LEU:HD22	1.85	0.57
1:B:2:LEU:HD23	1:B:3:THR:N	2.19	0.57
1:B:81:PHE:CD2	1:B:145:LEU:HD13	2.40	0.57
1:B:51:PHE:HA	1:B:55:ILE:HD12	1.86	0.57
1:A:222:ARG:HB2	2:C:49:MSE:HE1	1.86	0.57
2:D:75:ARG:C	2:D:75:ARG:HD3	2.25	0.57
1:B:224:LEU:HD23	2:D:143:GLN:NE2	2.20	0.57
2:D:161:MSE:HE1	2:D:172:LEU:HD22	1.87	0.57
1:A:85:LEU:HD13	1:B:147:LEU:HD21	1.86	0.57
2:C:145:THR:HG22	2:C:147:GLN:H	1.68	0.57
1:B:63:VAL:CG1	1:B:288:LEU:HD23	2.35	0.56
2:C:161:MSE:HE1	2:C:172:LEU:HD22	1.87	0.56
2:D:134:ARG:HD3	2:D:168:GLN:HE21	1.70	0.56
2:D:10:VAL:HG13	2:D:45:ARG:NH1	2.18	0.56
1:A:70:LEU:CB	1:A:256:ILE:HD11	2.35	0.56
1:A:79:ALA:CB	1:A:211:MSE:HE2	2.34	0.56
1:B:229:TRP:HE3	1:B:229:TRP:HA	1.68	0.56
2:C:91:TRP:HD1	2:C:121:GLY:HA2	1.69	0.56
1:A:147:LEU:HD22	1:B:317:PHE:CZ	2.40	0.56
1:B:186:VAL:HA	1:B:190:GLN:OE1	2.05	0.56
1:B:201:LEU:O	1:B:205:CYS:HB2	2.05	0.56
1:A:72:ILE:O	1:A:76:VAL:HG23	2.05	0.56
1:B:129:THR:CG2	1:B:236:VAL:HG13	2.36	0.56
1:B:243:VAL:O	1:B:247:VAL:HG23	2.05	0.56
1:B:43:TRP:O	1:B:48:GLY:HA3	2.06	0.56
2:C:164:LEU:HD22	2:C:168:GLN:HE21	1.71	0.56
2:C:29:LEU:HD23	2:C:30:HIS:N	2.21	0.56
2:D:146:PRO:HB2	2:D:182:GLN:NE2	2.21	0.56
2:C:127:LEU:HD13	2:C:135:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:HA	1:B:292:ILE:HD11	1.88	0.55
2:D:127:LEU:HD13	2:D:135:VAL:HG21	1.88	0.55
1:A:143:SER:HB3	1:B:85:LEU:HD11	1.87	0.55
1:A:197:LEU:HD13	1:A:245:VAL:HG11	1.89	0.55
1:B:200:VAL:HG13	1:B:201:LEU:N	2.21	0.55
2:C:137:LEU:HD13	2:C:172:LEU:HD12	1.88	0.55
2:D:29:LEU:HD23	2:D:30:HIS:N	2.21	0.55
2:D:7:LEU:HD23	2:D:56:ILE:HG23	1.89	0.55
2:C:134:ARG:HD3	2:C:168:GLN:HE21	1.71	0.55
1:B:59:ARG:HH12	1:B:295:ARG:CZ	2.18	0.55
1:A:264:LEU:HD22	1:A:269:LEU:HD12	1.87	0.55
1:B:136:ALA:CB	1:B:145:LEU:HD21	2.37	0.55
1:B:229:TRP:CZ3	1:B:232:ARG:HD2	2.41	0.55
1:B:41:GLY:C	1:B:43:TRP:H	2.10	0.55
1:A:16:LEU:O	1:A:20:SER:HB2	2.07	0.55
1:B:27:LEU:HD12	1:B:60:THR:CG2	2.37	0.55
1:B:40:PRO:O	1:B:43:TRP:HB2	2.07	0.55
2:C:100:ASP:OD2	2:C:102:THR:HB	2.07	0.55
1:A:259:VAL:HG11	1:A:316:VAL:HG21	1.88	0.55
2:D:35:ASN:HB3	3:D:250:V4O:O4	2.07	0.54
2:D:164:LEU:HD22	2:D:168:GLN:HE21	1.71	0.54
2:D:137:LEU:HD13	2:D:172:LEU:HD12	1.88	0.54
2:D:11:ALA:HB2	2:D:17:GLY:O	2.08	0.54
1:B:118:GLY:O	1:B:122:ILE:HG13	2.07	0.54
1:A:274:VAL:C	1:A:277:PRO:HD2	2.28	0.54
1:B:200:VAL:HG13	1:B:201:LEU:H	1.73	0.54
2:C:7:LEU:HD23	2:C:56:ILE:HG23	1.88	0.54
1:A:11:GLN:O	1:A:15:TRP:HD1	1.90	0.54
1:A:78:GLN:HA	1:A:86:ALA:HB3	1.89	0.54
1:B:27:LEU:HD12	1:B:60:THR:HG21	1.90	0.54
2:D:100:ASP:OD2	2:D:102:THR:HB	2.07	0.54
2:D:107:LEU:HD23	2:D:107:LEU:C	2.28	0.54
1:A:229:TRP:HE3	1:A:229:TRP:HA	1.72	0.54
1:A:66:VAL:CG2	1:A:249:LEU:HD23	2.38	0.54
1:A:1:MSE:HE3	1:A:6:ARG:HB2	1.90	0.54
2:C:11:ALA:HB2	2:C:17:GLY:O	2.08	0.54
2:C:146:PRO:HB2	2:C:182:GLN:NE2	2.21	0.54
2:C:64:GLU:N	2:C:64:GLU:OE2	2.39	0.54
1:A:87:GLU:HG3	1:A:257:GLY:C	2.29	0.53
2:C:107:LEU:HA	2:C:142:LEU:HD11	1.91	0.53
1:A:33:ALA:HB1	1:A:296:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:CB	1:B:256:ILE:HD11	2.36	0.53
2:D:134:ARG:HD3	2:D:168:GLN:NE2	2.24	0.53
1:A:147:LEU:HB3	1:B:317:PHE:CE2	2.44	0.53
2:D:107:LEU:HA	2:D:142:LEU:HD11	1.91	0.53
1:A:147:LEU:HD11	1:B:85:LEU:HD21	1.90	0.53
2:C:107:LEU:HD23	2:C:107:LEU:C	2.28	0.53
2:C:137:LEU:HD13	2:C:172:LEU:CD1	2.39	0.53
1:A:108:GLY:HA3	1:A:112:LEU:HD11	1.91	0.53
1:B:63:VAL:HG11	1:B:288:LEU:HA	1.91	0.53
1:A:211:MSE:HE3	1:A:235:LEU:HD13	1.89	0.53
2:D:137:LEU:HD13	2:D:172:LEU:CD1	2.39	0.53
2:D:39:LYS:HE3	3:D:250:V4O:O0	2.09	0.53
1:A:147:LEU:HB3	1:B:317:PHE:HE2	1.73	0.52
1:A:257:GLY:O	1:A:261:PRO:HG2	2.09	0.52
2:D:64:GLU:N	2:D:64:GLU:OE2	2.39	0.52
1:A:213:MSE:HE2	1:A:213:MSE:HA	1.91	0.52
1:A:59:ARG:NH1	1:A:295:ARG:NH1	2.54	0.52
1:A:265:ARG:HA	1:A:269:LEU:O	2.09	0.52
1:B:77:MSE:HE1	1:B:88:PRO:CG	2.25	0.52
2:C:134:ARG:HD3	2:C:168:GLN:NE2	2.24	0.52
2:D:172:LEU:HD21	2:D:176:LEU:HD11	1.91	0.52
1:B:210:PRO:O	1:B:214:LEU:HB2	2.10	0.52
2:C:172:LEU:HD21	2:C:176:LEU:HD11	1.91	0.52
1:A:200:VAL:HB	1:A:241:TRP:CZ3	2.44	0.52
1:B:34:GLY:HA2	1:B:295:ARG:HD2	1.92	0.52
2:D:19:LEU:HD23	2:D:20:SER:N	2.25	0.52
2:C:161:MSE:HE2	2:C:161:MSE:HA	1.92	0.52
1:A:157:SER:O	1:A:161:THR:HG23	2.10	0.52
2:C:19:LEU:HD23	2:C:20:SER:N	2.25	0.52
2:C:196:THR:CG2	2:C:221:LEU:HD11	2.39	0.52
2:C:223:PRO:HB2	2:C:224:PRO:HD3	1.92	0.52
2:D:223:PRO:HB2	2:D:224:PRO:HD3	1.92	0.52
1:A:14:ARG:O	1:A:17:LEU:HB3	2.10	0.51
1:A:64:LEU:HD21	1:A:288:LEU:HD11	1.92	0.51
1:B:204:ILE:HD12	1:B:238:ALA:HB1	1.92	0.51
1:A:136:ALA:HB2	1:A:145:LEU:HD21	1.91	0.51
2:D:161:MSE:HA	2:D:161:MSE:HE2	1.92	0.51
1:A:317:PHE:CE2	1:B:147:LEU:HB3	2.44	0.51
1:B:200:VAL:HB	1:B:241:TRP:CE3	2.46	0.51
2:D:196:THR:CG2	2:D:221:LEU:HD11	2.39	0.51
1:A:305:ILE:HG22	1:A:306:GLY:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:VAL:HG23	2:D:25:ALA:HB2	1.92	0.51
2:C:4:VAL:HG23	2:C:25:ALA:HB2	1.92	0.51
2:D:127:LEU:CD1	2:D:135:VAL:HG21	2.41	0.51
1:B:81:PHE:HB3	1:B:145:LEU:HD13	1.92	0.51
1:B:1:MSE:HE3	1:B:6:ARG:CB	2.40	0.51
1:B:213:MSE:HA	1:B:213:MSE:HE2	1.92	0.51
1:B:69:ALA:HA	1:B:242:MSE:HE2	1.92	0.51
2:C:127:LEU:CD1	2:C:135:VAL:HG21	2.41	0.51
1:B:57:LEU:HB3	1:B:58:PRO:HD3	1.93	0.51
2:C:66:TRP:HZ3	2:C:74:HIS:CD2	2.29	0.51
1:A:45:THR:HG23	1:A:46:PRO:HD2	1.91	0.51
1:B:229:TRP:HZ3	1:B:232:ARG:HD2	1.76	0.51
2:D:206:LEU:HD23	2:D:206:LEU:N	2.26	0.51
1:A:27:LEU:HD12	1:A:60:THR:HG21	1.93	0.50
2:D:66:TRP:HZ3	2:D:74:HIS:CD2	2.29	0.50
1:B:274:VAL:O	1:B:277:PRO:HD2	2.11	0.50
2:C:11:ALA:HB2	2:C:17:GLY:C	2.32	0.50
2:D:216:ARG:HG2	2:D:218:GLU:H	1.76	0.50
2:C:206:LEU:HD23	2:C:206:LEU:N	2.26	0.50
1:A:58:PRO:HG3	1:A:188:TRP:CZ2	2.46	0.50
2:D:125:ASN:O	2:D:125:ASN:ND2	2.45	0.50
2:D:207:LYS:C	2:D:209:GLY:N	2.65	0.50
1:A:70:LEU:HD12	1:A:256:ILE:HD11	1.92	0.50
1:B:257:GLY:O	1:B:261:PRO:HG2	2.11	0.50
2:C:162:ASN:O	2:C:163:SER:HB2	2.12	0.50
1:B:11:GLN:O	1:B:15:TRP:HD1	1.94	0.50
1:B:209:ARG:HB2	1:B:210:PRO:CD	2.38	0.50
2:D:162:ASN:O	2:D:163:SER:HB2	2.12	0.50
1:A:318:ILE:HD11	1:B:151:ALA:HB3	1.94	0.49
1:A:219:ILE:HG23	2:C:49:MSE:HE2	1.94	0.49
1:B:16:LEU:O	1:B:20:SER:HB2	2.12	0.49
1:B:34:GLY:HA2	1:B:295:ARG:CD	2.42	0.49
2:C:125:ASN:O	2:C:125:ASN:ND2	2.45	0.49
1:B:238:ALA:O	1:B:242:MSE:HG3	2.13	0.49
2:C:216:ARG:HG2	2:C:218:GLU:H	1.76	0.49
1:A:200:VAL:HB	1:A:241:TRP:CE3	2.47	0.49
1:A:59:ARG:NH1	1:A:291:ASP:OD2	2.46	0.49
1:B:2:LEU:O	1:B:5:ALA:HB3	2.13	0.49
2:C:196:THR:HG23	2:C:221:LEU:CD1	2.43	0.49
1:B:64:LEU:CD2	1:B:288:LEU:HD11	2.40	0.49
1:B:78:GLN:HG2	1:B:84:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TRP:O	1:A:233:ASN:ND2	2.46	0.49
1:A:85:LEU:HD21	1:B:147:LEU:HD11	1.94	0.49
1:A:188:TRP:C	1:A:190:GLN:H	2.16	0.49
1:B:76:VAL:CA	1:B:211:MSE:HE1	2.33	0.49
1:A:247:VAL:O	1:A:251:GLY:N	2.42	0.48
1:B:239:THR:O	1:B:243:VAL:HG23	2.13	0.48
1:B:78:GLN:HA	1:B:86:ALA:HB3	1.93	0.48
2:D:196:THR:HG23	2:D:221:LEU:CD1	2.43	0.48
1:B:222:ARG:HB2	2:D:49:MSE:HE1	1.95	0.48
2:C:10:VAL:HA	2:C:54:GLY:HA3	1.95	0.48
2:D:10:VAL:HA	2:D:54:GLY:HA3	1.95	0.48
2:D:11:ALA:HB2	2:D:17:GLY:C	2.33	0.48
2:D:76:ALA:HB1	2:D:140:VAL:HG22	1.94	0.48
1:A:183:PHE:CE1	1:A:253:ILE:HD11	2.49	0.48
1:A:318:ILE:O	1:A:321:LEU:HB2	2.13	0.48
1:B:229:TRP:HZ3	1:B:232:ARG:HH11	1.61	0.48
2:D:10:VAL:HG13	2:D:45:ARG:HH12	1.79	0.48
1:B:229:TRP:CA	1:B:229:TRP:CE3	2.97	0.47
1:B:200:VAL:HB	1:B:241:TRP:CZ3	2.49	0.47
2:C:75:ARG:HA	2:C:144:ILE:CD1	2.44	0.47
1:A:291:ASP:O	1:A:294:ALA:HB3	2.14	0.47
2:C:76:ALA:HB1	2:C:140:VAL:HG22	1.94	0.47
2:C:10:VAL:HG13	2:C:45:ARG:HH12	1.79	0.47
1:A:34:GLY:HA2	1:A:296:LEU:HD21	1.96	0.47
1:A:48:GLY:O	1:A:52:VAL:HB	2.14	0.47
1:B:294:ALA:HB2	1:B:308:VAL:HG21	1.96	0.47
2:C:75:ARG:HA	2:C:154:LEU:O	2.15	0.47
2:D:161:MSE:CE	2:D:172:LEU:HD22	2.44	0.47
1:A:32:CYS:HA	1:A:38:ILE:CD1	2.45	0.47
1:B:269:LEU:HB3	1:B:274:VAL:HG12	1.96	0.47
2:D:75:ARG:HA	2:D:154:LEU:O	2.14	0.47
1:B:146:LEU:O	1:B:150:VAL:HG23	2.14	0.47
1:A:9:GLN:O	1:A:13:ILE:HG12	2.15	0.47
1:B:87:GLU:HG3	1:B:257:GLY:C	2.35	0.47
2:C:161:MSE:CE	2:C:172:LEU:HD22	2.44	0.47
1:A:106:LEU:C	1:A:108:GLY:H	2.17	0.47
1:A:33:ALA:N	1:A:56:ARG:NH2	2.63	0.47
2:D:114:LEU:O	2:D:116:LEU:HG	2.14	0.47
1:B:38:ILE:CG2	1:B:39:SER:N	2.78	0.46
1:B:81:PHE:CD1	1:B:81:PHE:N	2.82	0.46
2:C:157:LEU:O	2:C:188:MSE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:ARG:HA	2:D:144:ILE:CD1	2.45	0.46
1:A:136:ALA:CA	1:A:145:LEU:HD21	2.45	0.46
1:A:230:PHE:CZ	1:A:234:VAL:HG21	2.50	0.46
1:B:55:ILE:C	1:B:58:PRO:HD2	2.36	0.46
2:C:110:VAL:HG11	2:C:142:LEU:HD22	1.98	0.46
2:C:114:LEU:O	2:C:116:LEU:HG	2.14	0.46
1:A:91:LEU:HA	1:A:149:GLY:HA3	1.97	0.46
1:A:171:ASP:O	1:A:173:ARG:N	2.49	0.46
2:C:201:HIS:O	2:C:217:ARG:HG3	2.16	0.46
1:A:109:GLN:H	1:A:112:LEU:HD11	1.81	0.46
2:D:157:LEU:O	2:D:188:MSE:HA	2.15	0.46
1:B:9:GLN:O	1:B:13:ILE:HG12	2.16	0.46
2:D:194:ASN:OD1	2:D:195:HIS:N	2.48	0.46
2:D:201:HIS:O	2:D:217:ARG:HG3	2.16	0.46
1:B:139:HIS:HB3	1:B:144:ARG:HD2	1.98	0.46
2:C:207:LYS:C	2:C:209:GLY:N	2.65	0.46
2:C:39:LYS:HB2	3:C:250:V4O:O0	2.16	0.46
2:D:74:HIS:CE1	2:D:151:ALA:HB1	2.51	0.46
2:D:39:LYS:HB2	3:D:250:V4O:O0	2.15	0.46
1:A:32:CYS:O	1:A:37:TRP:CD1	2.68	0.46
1:A:57:LEU:HD23	1:A:188:TRP:HZ2	1.80	0.46
1:A:223:GLN:HE21	1:A:224:LEU:HG	1.81	0.45
2:C:222:THR:OG1	2:C:224:PRO:HD2	2.16	0.45
1:A:76:VAL:CA	1:A:211:MSE:HE1	2.30	0.45
1:A:57:LEU:HD23	1:A:188:TRP:CZ2	2.51	0.45
1:B:114:ASN:O	1:B:117:LEU:HB2	2.16	0.45
2:C:176:LEU:O	2:C:179:LEU:HB2	2.16	0.45
1:A:229:TRP:CZ3	1:A:232:ARG:HD2	2.51	0.45
1:A:56:ARG:NH1	1:A:56:ARG:HG3	2.31	0.45
1:A:68:ALA:O	1:A:72:ILE:HG13	2.16	0.45
2:D:110:VAL:HG11	2:D:142:LEU:HD22	1.98	0.45
2:D:214:SER:O	2:D:220:VAL:HG22	2.17	0.45
1:A:64:LEU:CD2	1:A:284:ALA:HB1	2.45	0.45
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.85	0.45
1:B:91:LEU:HB3	1:B:132:LEU:HD11	1.98	0.45
1:B:304:PRO:O	1:B:305:ILE:C	2.54	0.45
1:A:37:TRP:CZ3	1:A:39:SER:HB3	2.51	0.45
1:B:197:LEU:HD13	1:B:245:VAL:HG11	1.98	0.45
2:C:194:ASN:OD1	2:C:195:HIS:N	2.50	0.45
2:C:214:SER:O	2:C:220:VAL:HG22	2.16	0.45
2:C:74:HIS:CE1	2:C:151:ALA:HB1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:GLY:HA2	3:D:250:V4O:O11	2.16	0.45
1:A:136:ALA:HA	1:A:145:LEU:HD21	1.98	0.45
1:B:91:LEU:HA	1:B:149:GLY:HA3	1.98	0.45
1:A:63:VAL:HG11	1:A:288:LEU:HD23	1.98	0.45
2:C:156:LEU:CD2	2:C:187:VAL:HB	2.47	0.45
1:A:45:THR:CG2	1:A:46:PRO:HD2	2.47	0.45
2:C:159:GLU:N	2:C:160:PRO:HD3	2.32	0.45
2:D:76:ALA:HB3	2:D:155:LEU:HD23	1.99	0.45
2:D:176:LEU:O	2:D:179:LEU:HB2	2.16	0.44
2:D:230:TYR:HB2	2:D:232:MSE:HE2	1.99	0.44
2:D:32:VAL:O	2:D:205:LEU:HD12	2.17	0.44
1:A:168:THR:C	1:A:170:VAL:N	2.70	0.44
1:A:32:CYS:HA	1:A:38:ILE:HD12	1.99	0.44
1:B:168:THR:C	1:B:170:VAL:H	2.20	0.44
1:B:222:ARG:O	1:B:224:LEU:N	2.50	0.44
2:C:203:ALA:O	2:C:220:VAL:HG11	2.18	0.44
2:C:222:THR:CG2	2:C:225:ASN:ND2	2.80	0.44
1:A:31:LEU:HD21	1:A:57:LEU:HA	2.00	0.44
1:A:193:LEU:O	1:A:196:ALA:HB3	2.16	0.44
1:B:33:ALA:O	1:B:295:ARG:NH1	2.50	0.44
1:B:70:LEU:HD12	1:B:256:ILE:HD11	1.99	0.44
1:B:83:ASN:HA	1:B:84:PRO:HD3	1.74	0.44
2:C:179:LEU:O	2:C:184:LEU:HB2	2.18	0.44
2:C:35:ASN:HB3	3:C:250:V4O:O4	2.17	0.44
2:D:222:THR:CG2	2:D:225:ASN:ND2	2.80	0.44
1:A:272:HIS:C	1:A:274:VAL:N	2.71	0.44
1:B:157:SER:O	1:B:161:THR:HG23	2.17	0.44
1:B:264:LEU:HD22	1:B:269:LEU:HD12	2.00	0.44
1:B:91:LEU:HB3	1:B:132:LEU:CD1	2.48	0.44
1:A:136:ALA:CB	1:A:145:LEU:HD21	2.48	0.44
1:A:229:TRP:CE3	1:A:229:TRP:CA	3.00	0.44
1:A:51:PHE:C	1:A:56:ARG:HG2	2.38	0.44
2:C:133:GLN:HG2	2:C:162:ASN:O	2.18	0.44
2:C:73:LEU:HD23	2:C:99:HIS:CE1	2.53	0.44
2:D:159:GLU:N	2:D:160:PRO:HD3	2.32	0.44
2:D:222:THR:OG1	2:D:224:PRO:HD2	2.16	0.44
2:D:45:ARG:O	2:D:48:GLY:N	2.51	0.44
2:C:76:ALA:HB3	2:C:155:LEU:HD23	1.99	0.44
2:C:45:ARG:O	2:C:48:GLY:N	2.51	0.44
2:C:5:MSE:HE1	2:C:46:MSE:O	2.18	0.44
2:D:42:LEU:CD2	2:D:46:MSE:SE	3.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:O	1:A:224:LEU:N	2.51	0.43
2:C:198:ARG:HD2	2:C:199:HIS:CD2	2.53	0.43
2:C:230:TYR:HB2	2:C:232:MSE:HE2	1.99	0.43
2:D:203:ALA:O	2:D:220:VAL:HG11	2.18	0.43
1:A:200:VAL:HG13	1:A:201:LEU:N	2.34	0.43
2:C:91:TRP:CD1	2:C:121:GLY:HA2	2.52	0.43
2:D:133:GLN:HG2	2:D:162:ASN:O	2.18	0.43
2:D:73:LEU:HD23	2:D:99:HIS:CE1	2.53	0.43
1:A:91:LEU:HB3	1:A:132:LEU:HD11	2.00	0.43
1:A:56:ARG:HG3	1:A:56:ARG:HH11	1.84	0.43
1:A:70:LEU:CD1	1:A:256:ILE:HD11	2.48	0.43
1:B:247:VAL:HA	1:B:251:GLY:O	2.18	0.43
2:C:138:ALA:O	2:C:142:LEU:HD23	2.19	0.43
2:D:179:LEU:O	2:D:184:LEU:HB2	2.18	0.43
2:D:138:ALA:O	2:D:142:LEU:HD23	2.19	0.43
1:A:84:PRO:HB3	1:A:262:HIS:HE1	1.81	0.43
1:B:68:ALA:O	1:B:72:ILE:HG13	2.19	0.43
2:C:165:ASP:O	2:C:166:VAL:C	2.57	0.43
1:A:70:LEU:HB2	1:A:256:ILE:CD1	2.43	0.43
1:A:83:ASN:HA	1:A:84:PRO:HD3	1.87	0.43
1:A:147:LEU:HD22	1:B:317:PHE:HZ	1.81	0.43
2:C:32:VAL:O	2:C:205:LEU:HD12	2.17	0.43
2:C:42:LEU:CD2	2:C:46:MSE:SE	3.12	0.43
2:D:5:MSE:HE1	2:D:46:MSE:O	2.18	0.43
1:B:197:LEU:O	1:B:201:LEU:HB2	2.19	0.43
2:D:86:PHE:HA	2:D:125:ASN:HB2	2.01	0.43
2:D:165:ASP:O	2:D:166:VAL:C	2.56	0.43
1:B:222:ARG:NH2	2:D:49:MSE:HA	2.34	0.43
1:A:127:ILE:O	1:A:131:ILE:HG13	2.19	0.43
2:C:104:THR:HG23	2:C:105:GLU:N	2.34	0.43
1:A:45:THR:O	1:A:47:ARG:N	2.52	0.42
2:C:86:PHE:HA	2:C:125:ASN:HB2	2.01	0.42
2:C:222:THR:HG23	2:C:224:PRO:HD2	2.00	0.42
2:C:74:HIS:HA	2:C:151:ALA:O	2.19	0.42
2:C:39:LYS:HE3	3:C:250:V4O:O0	2.20	0.42
2:D:104:THR:HG23	2:D:105:GLU:N	2.34	0.42
1:A:81:PHE:CD1	1:A:81:PHE:N	2.87	0.42
1:B:22:LEU:HD12	1:B:22:LEU:O	2.19	0.42
1:A:293:VAL:O	1:A:297:ALA:HB2	2.18	0.42
1:A:321:LEU:O	1:B:144:ARG:NH1	2.53	0.42
1:A:76:VAL:HG21	1:A:204:ILE:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ALA:HB1	1:B:240:GLY:HA2	2.01	0.42
2:C:89:PRO:HB2	2:C:91:TRP:CD1	2.55	0.42
1:B:38:ILE:CG2	1:B:39:SER:H	2.24	0.42
1:B:11:GLN:O	1:B:14:ARG:HB3	2.19	0.42
1:B:59:ARG:HH12	1:B:295:ARG:HE	1.64	0.42
2:D:198:ARG:HD2	2:D:199:HIS:CD2	2.53	0.42
2:D:74:HIS:HA	2:D:151:ALA:O	2.19	0.42
1:A:209:ARG:HB2	1:A:210:PRO:CD	2.42	0.42
2:D:91:TRP:CD1	2:D:121:GLY:HA2	2.52	0.42
1:A:1:MSE:HE3	1:A:6:ARG:CB	2.49	0.42
1:A:317:PHE:CZ	1:B:147:LEU:HD22	2.55	0.42
1:A:43:TRP:O	1:A:48:GLY:HA3	2.19	0.42
1:B:201:LEU:HG	1:B:242:MSE:HE3	2.00	0.42
1:B:72:ILE:O	1:B:75:ALA:HB3	2.19	0.42
2:C:38:GLY:HA2	3:C:250:V4O:O11	2.20	0.42
2:D:10:VAL:O	2:D:11:ALA:CB	2.67	0.42
2:D:222:THR:HG23	2:D:224:PRO:HD2	2.00	0.42
1:A:222:ARG:O	1:A:225:GLY:N	2.39	0.41
1:A:304:PRO:O	1:A:305:ILE:C	2.58	0.41
1:B:64:LEU:HD22	1:B:284:ALA:HB1	2.02	0.41
1:A:292:ILE:O	1:A:295:ARG:HG2	2.19	0.41
2:C:161:MSE:SE	2:C:169:GLN:HG2	2.71	0.41
2:D:89:PRO:HB2	2:D:91:TRP:CD1	2.55	0.41
1:A:63:VAL:HA	1:A:183:PHE:CE2	2.56	0.41
2:D:196:THR:O	2:D:200:ALA:HB3	2.21	0.41
1:B:305:ILE:HG22	1:B:306:GLY:N	2.35	0.41
1:B:305:ILE:CG2	1:B:306:GLY:N	2.83	0.41
2:D:161:MSE:SE	2:D:169:GLN:HG2	2.71	0.41
1:A:266:LEU:HD13	1:A:266:LEU:HA	1.86	0.41
1:B:274:VAL:C	1:B:277:PRO:HD2	2.41	0.41
1:A:187:ASP:OD1	1:A:188:TRP:N	2.52	0.41
1:A:313:GLY:O	1:A:316:VAL:HG22	2.21	0.41
2:D:140:VAL:CG1	2:D:141:VAL:N	2.84	0.41
1:A:151:ALA:HB3	1:B:318:ILE:HD11	2.02	0.40
1:B:72:ILE:HD12	1:B:201:LEU:HD23	2.03	0.40
2:C:3:ILE:HG13	2:C:3:ILE:O	2.21	0.40
1:A:220:SER:CB	2:C:82:GLN:HE22	2.31	0.40
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.90	0.40
1:B:197:LEU:HD13	1:B:245:VAL:CG1	2.51	0.40
1:A:109:GLN:H	1:A:112:LEU:CD1	2.34	0.40
1:B:171:ASP:O	1:B:173:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ALA:CB	2:D:17:GLY:C	2.90	0.40
2:D:3:ILE:HG13	2:D:3:ILE:O	2.21	0.40
1:A:74:GLY:HA3	1:A:257:GLY:O	2.21	0.40
2:C:45:ARG:O	2:C:47:ALA:N	2.55	0.40
1:B:263:ILE:O	1:B:266:LEU:HB2	2.21	0.40
1:B:93:VAL:HG12	1:B:243:VAL:HG11	2.04	0.40
2:C:11:ALA:CB	2:C:17:GLY:C	2.89	0.40
2:D:162:ASN:O	2:D:163:SER:CB	2.70	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:47:ARG:NH1	1:B:35:GLU:OE2[2_657]	1.49	0.71

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	322/326 (99%)	258 (80%)	53 (16%)	11 (3%)	3	24
1	B	322/326 (99%)	255 (79%)	55 (17%)	12 (4%)	3	22
2	C	229/249 (92%)	194 (85%)	31 (14%)	4 (2%)	9	42
2	D	229/249 (92%)	195 (85%)	30 (13%)	4 (2%)	9	42
All	All	1102/1150 (96%)	902 (82%)	169 (15%)	31 (3%)	5	29

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	PHE
1	B	181	GLY

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Mol	Chain	Res	Type
2	C	103	ARG
2	D	103	ARG
1	A	172	LEU
1	A	181	GLY
1	A	218	GLU
1	B	52	VAL
1	B	218	GLU
2	C	37	ALA
2	C	208	GLY
2	D	37	ALA
2	D	208	GLY
1	A	196	ALA
1	A	223	GLN
1	B	172	LEU
1	B	223	GLN
1	B	230	PHE
2	C	11	ALA
2	D	11	ALA
1	A	51	PHE
1	B	241	TRP
1	A	199	PRO
1	A	230	PHE
1	B	297	ALA
1	A	34	GLY
1	A	228	LEU
1	A	241	TRP
1	B	34	GLY
1	B	46	PRO
1	B	199	PRO

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	249/239 (104%)	236 (95%)	13 (5%)	23 59
1	B	249/239 (104%)	240 (96%)	9 (4%)	35 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	184/192 (96%)	175 (95%)	9 (5%)	25 61
2	D	184/192 (96%)	175 (95%)	9 (5%)	25 61
All	All	866/862 (100%)	826 (95%)	40 (5%)	27 63

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	38	ILE
1	A	144	ARG
1	A	162	TRP
1	A	176	MSE
1	A	179	MSE
1	A	197	LEU
1	A	205	CYS
1	A	214	LEU
1	A	220	SER
1	A	229	TRP
1	A	266	LEU
1	A	305	ILE
1	B	46	PRO
1	B	81	PHE
1	B	144	ARG
1	B	162	TRP
1	B	176	MSE
1	B	205	CYS
1	B	220	SER
1	B	229	TRP
1	B	305	ILE
2	C	16	LEU
2	C	29	LEU
2	C	42	LEU
2	C	75	ARG
2	C	125	ASN
2	C	140	VAL
2	C	155	LEU
2	C	198	ARG
2	C	232	MSE
2	D	16	LEU
2	D	29	LEU
2	D	42	LEU

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Mol	Chain	Res	Type
2	D	75	ARG
2	D	125	ASN
2	D	140	VAL
2	D	155	LEU
2	D	198	ARG
2	D	232	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	114	ASN
1	B	95	ASN
2	C	35	ASN
2	C	81	GLN
2	C	82	GLN
2	C	97	HIS
2	C	125	ASN
2	C	168	GLN
2	C	182	GLN
2	C	195	HIS
2	C	199	HIS
2	C	225	ASN
2	C	228	GLN
2	D	35	ASN
2	D	81	GLN
2	D	82	GLN
2	D	97	HIS
2	D	125	ASN
2	D	168	GLN
2	D	182	GLN
2	D	195	HIS
2	D	199	HIS
2	D	225	ASN
2	D	228	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	V4O	D	250	-	12,16,16	1.31	2 (16%)	-		
3	V4O	C	250	-	12,16,16	1.31	2 (16%)	-		

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	V4O	D	250	-	-	-	0/1/1/1
3	V4O	C	250	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	250	V4O	O8-V4	-2.41	1.71	1.77
3	D	250	V4O	O8-V4	-2.37	1.71	1.77
3	C	250	V4O	O3-V2	-2.31	1.71	1.77
3	D	250	V4O	O3-V2	-2.29	1.72	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

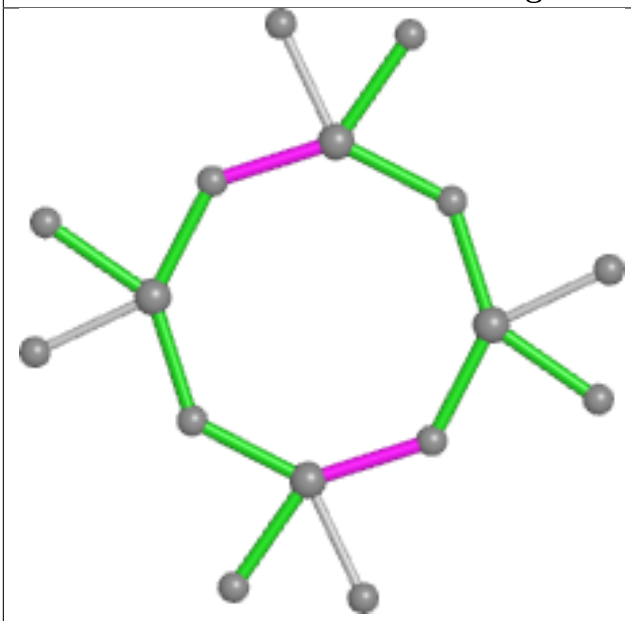
There are no ring outliers.

2 monomers are involved in 12 short contacts:

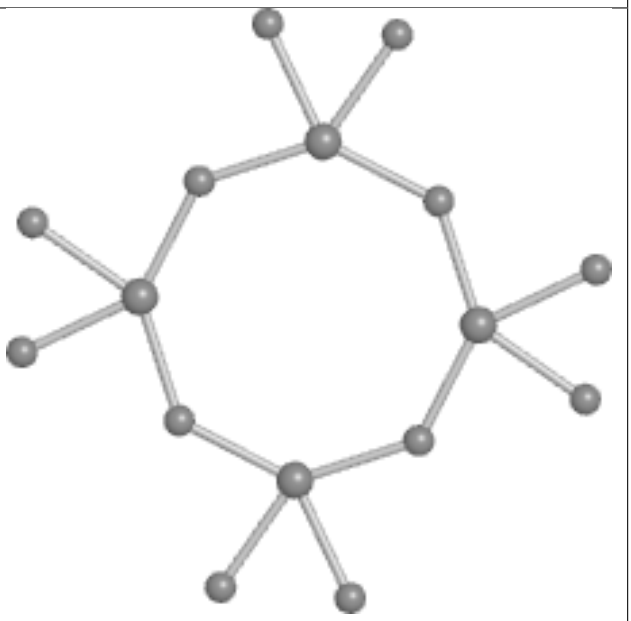
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	250	V4O	6	0
3	C	250	V4O	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

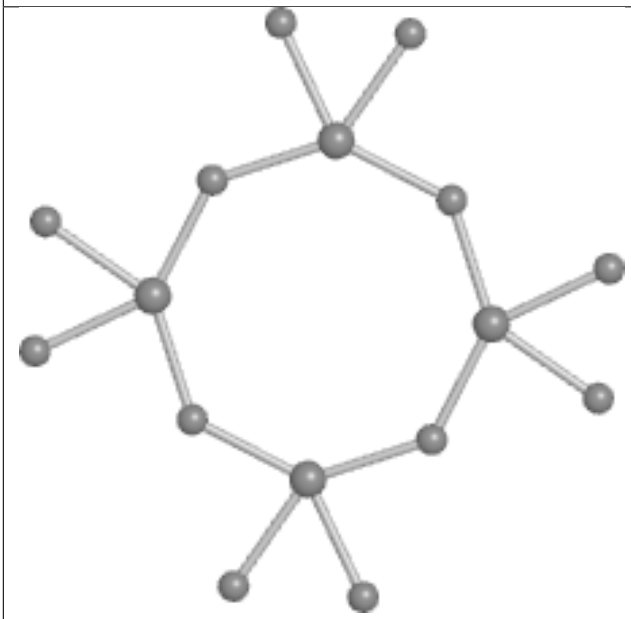
Ligand V4O D 250



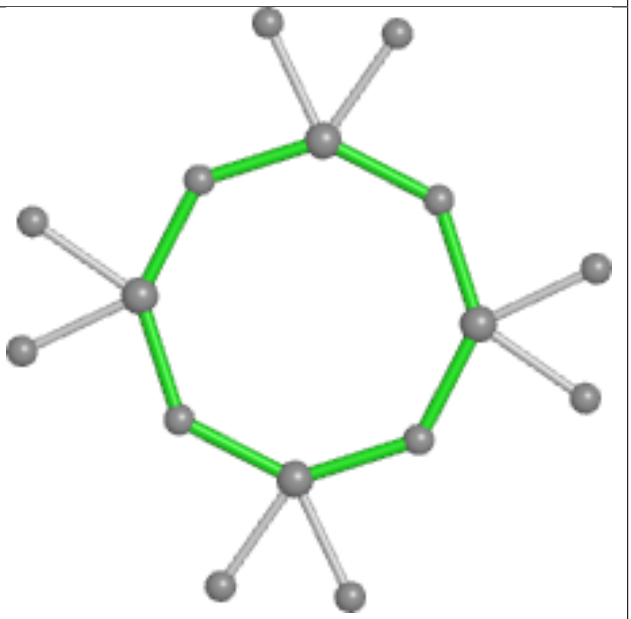
Bond lengths



Bond angles

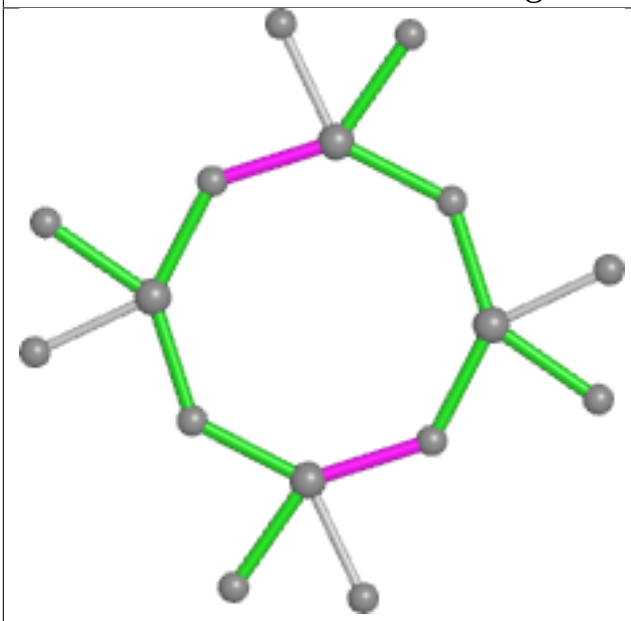


Torsions

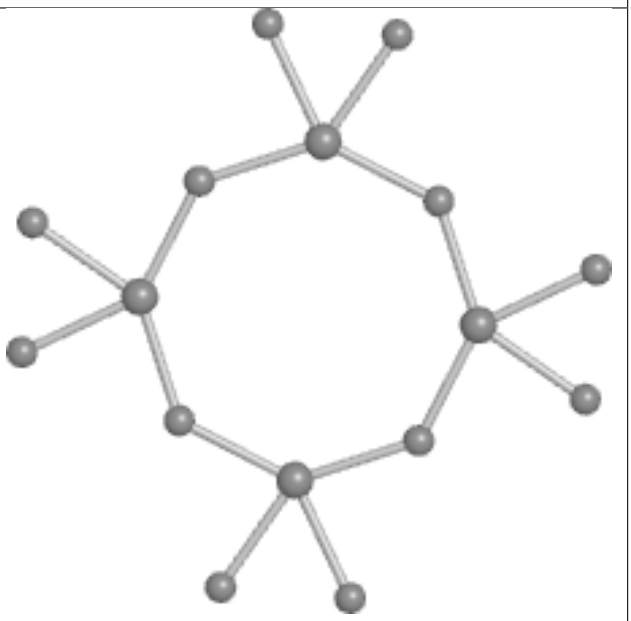


Rings

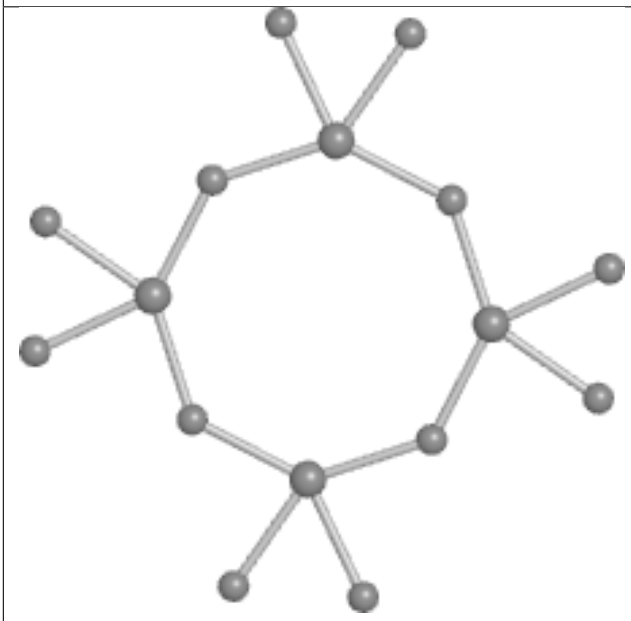
Ligand V4O C 250



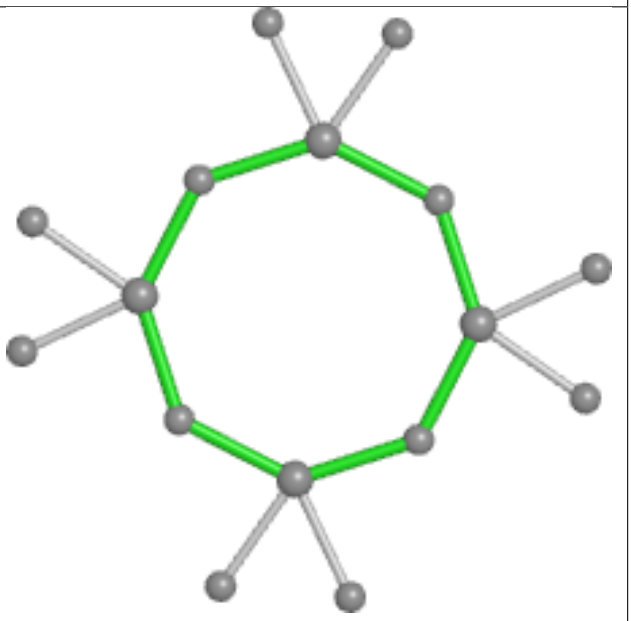
Bond lengths



Bond angles



Torsions



Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.