Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 08:12 PM EDT

PDB ID	:	3VR3
Title	:	Crystal structure of AMP-PNP bound A3B3 complex from Enterococcus hirae V-ATPase [bA3B3]
Authors	:	Arai, S.; Saijo, S.; Suzuki, K.; Mizutani, K.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Ohsawa, N.; Terada, T.; Shirouzu, M.; Yokoyama, S.; Iwata, S.; Yamato, I.; Murata, T.
Deposited on	:	2012-04-03
Resolution	:	3.40 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 (i) 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 (i)) were used in the production of this report:

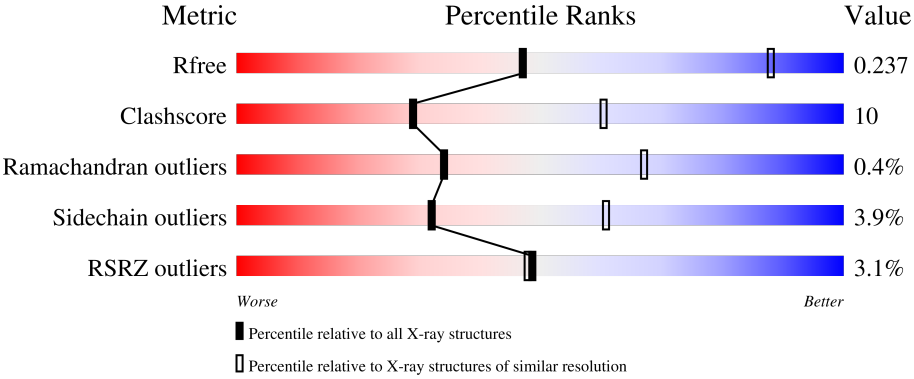
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	600	4% 74% 22% • •
1	B	600	6% 78% 18% • •
1	C	600	75% 20% • •
2	D	465	3% 76% 19% • •
2	E	465	3% 75% 22% •

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Mol	Chain	Length	Quality of chain
2	F	465	% 74% 22%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24266 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	586	4562	2866	766	904	3	23	0	0	0
1	B	586	4539	2851	763	899	3	23	0	0	0
1	C	584	4525	2844	758	897	3	23	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

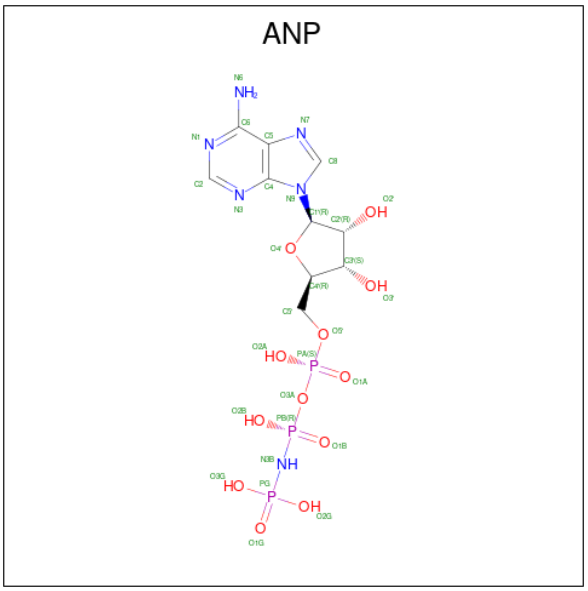
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	D	447	3449	2179	596	660	14	0	0	0
2	E	451	3533	2238	606	675	14	0	0	0
2	F	451	3523	2233	602	674	14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0
3	C	1	31	10	6	12	3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0
4	C	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	12	12	12	0	0
5	B	6	6	6	0	0
5	C	16	16	16	0	0
5	D	13	13	13	0	0
5	E	10	10	10	0	0

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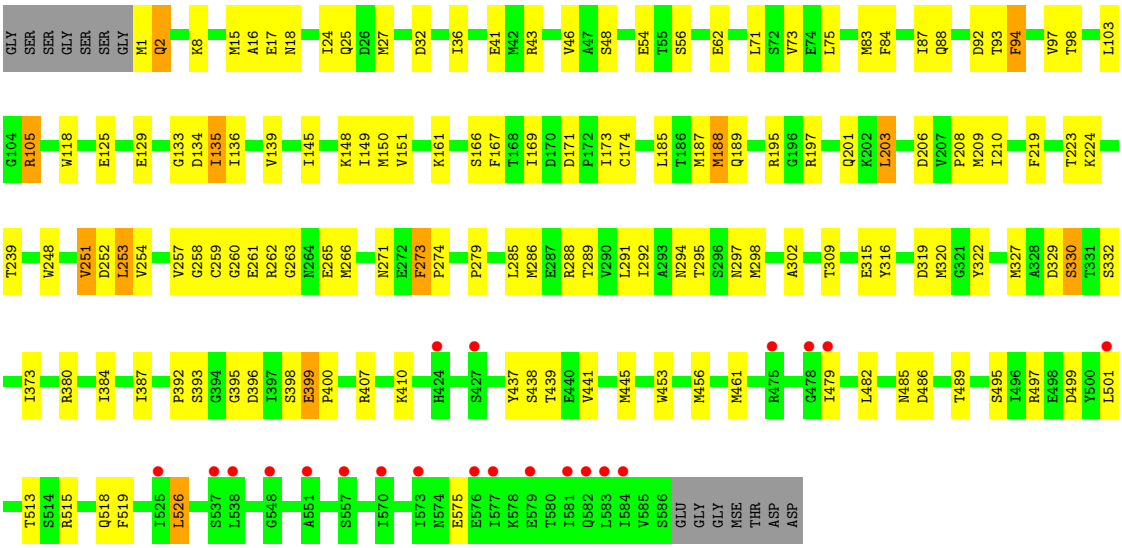
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	F	14	14	14	0	0

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.

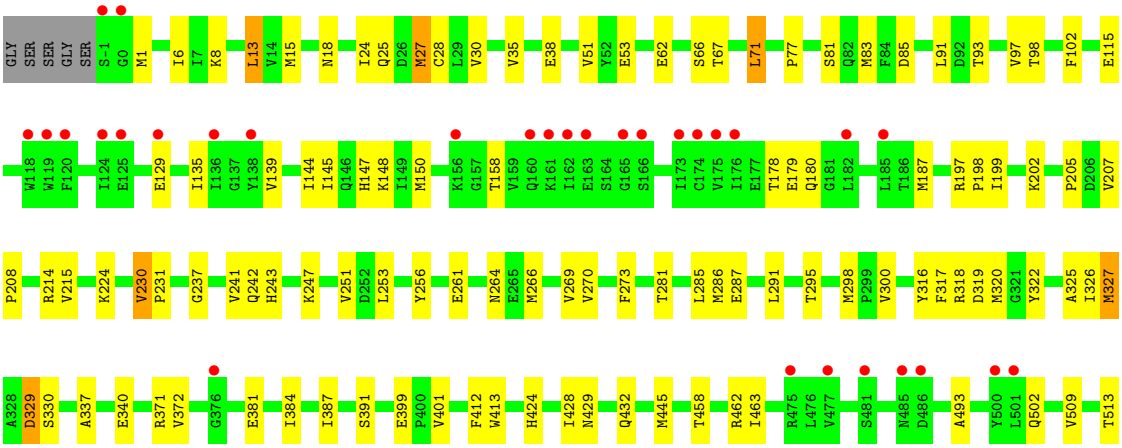
• Molecule 1: V-type sodium ATPase catalytic subunit A

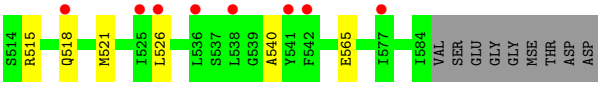
Chain A:



• Molecule 1: V-type sodium ATPase catalytic subunit A

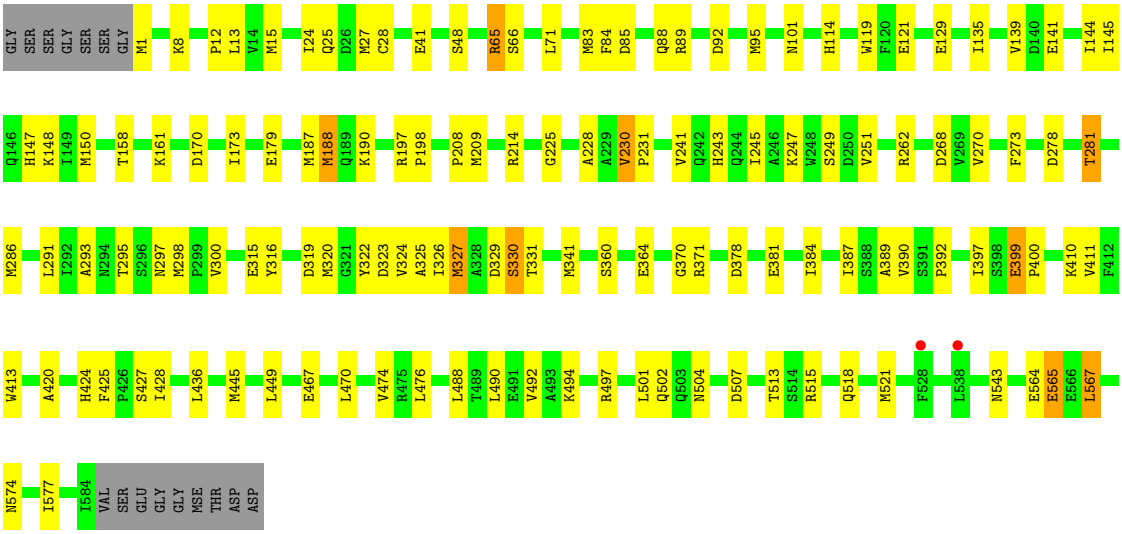
Chain B:





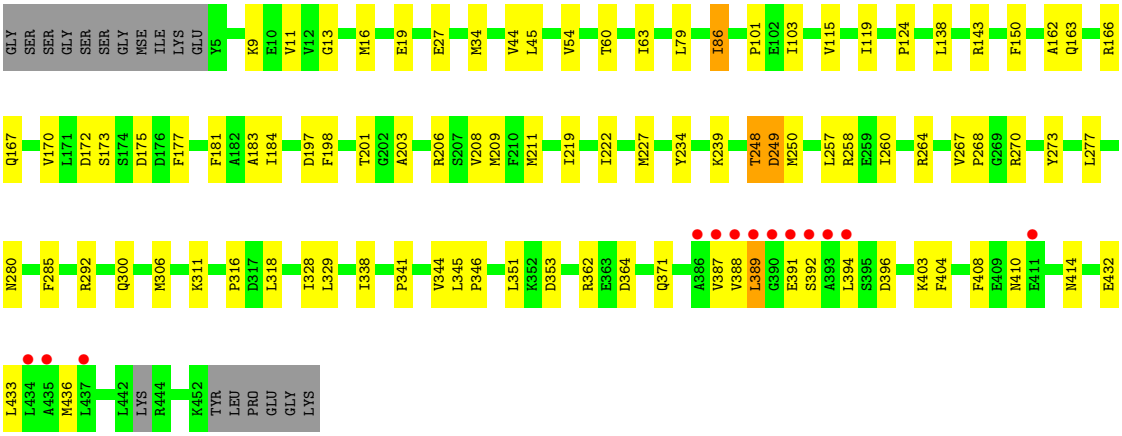
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C:



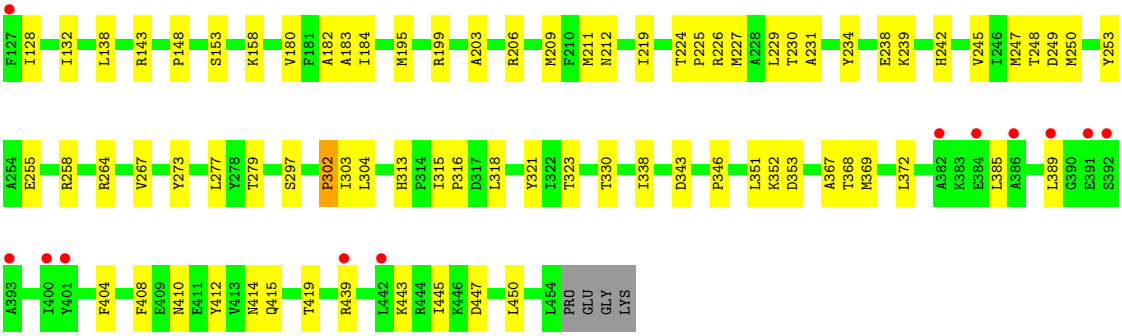
• Molecule 2: V-type sodium ATPase subunit B

Chain D:



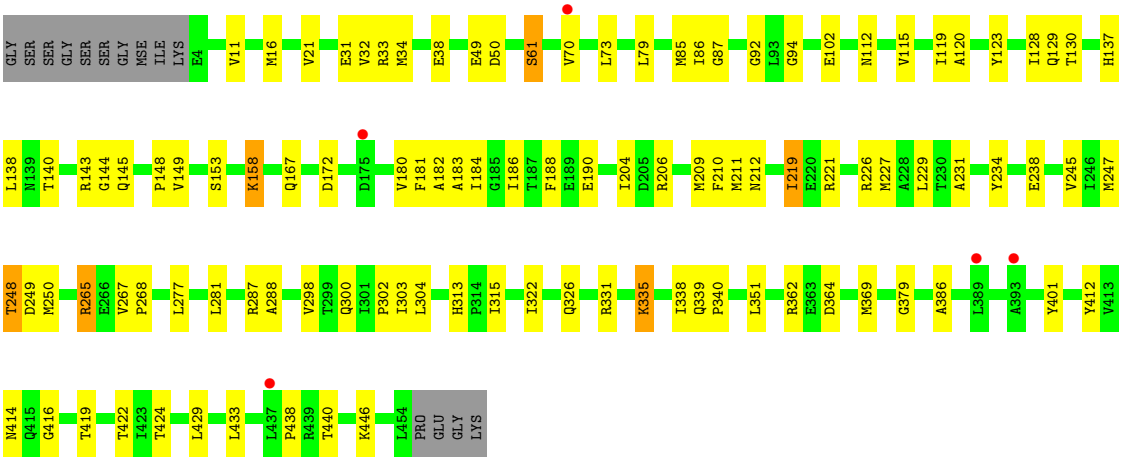
• Molecule 2: V-type sodium ATPase subunit B

Chain E:



- Molecule 2: V-type sodium ATPase subunit B

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.11Å 124.13Å 245.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.99 – 3.40 70.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.99-3.40) 99.6 (70.99-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.239 0.200 , 0.237	Depositor DCC
R_{free} test set	2653 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24266	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.36	0/4616	0.52	0/6209
1	B	0.36	0/4592	0.51	0/6176
1	C	0.36	0/4579	0.52	0/6162
2	D	0.37	0/3494	0.54	0/4699
2	E	0.35	0/3581	0.52	0/4818
2	F	0.35	0/3571	0.54	0/4806
All	All	0.36	0/24433	0.52	0/32870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4562	0	4528	94	0
1	B	4539	0	4483	87	0
1	C	4525	0	4468	90	0
2	D	3449	0	3425	65	0
2	E	3533	0	3543	74	0
2	F	3523	0	3526	71	0
3	B	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	0	13	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	12	0	0	0	0
5	B	6	0	0	0	0
5	C	16	0	0	0	0
5	D	13	0	0	1	0
5	E	10	0	0	0	0
5	F	14	0	0	0	0
All	All	24266	0	23999	461	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (461) 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)
1:C:27:MSE:HE3	1:C:71:LEU:HB2	1.23	1.15
2:E:77:LEU:HD23	2:E:111:ILE:CD1	1.76	1.14
2:E:77:LEU:HD23	2:E:111:ILE:HD11	1.10	1.09
1:B:242:GLN:OE1	1:B:329:ASP:HB2	1.58	1.04
1:A:320:MSE:HE2	1:A:322:TYR:HE2	1.28	0.98
1:B:261:GLU:HG3	1:B:329:ASP:OD2	1.67	0.95
2:E:77:LEU:CD2	2:E:111:ILE:HD11	1.98	0.92
1:A:148:LYS:H	1:A:320:MSE:HE3	1.35	0.91
2:E:234:TYR:O	2:E:238:GLU:HB2	1.73	0.89
2:D:391:GLU:O	2:D:391:GLU:HG2	1.71	0.88
1:B:320:MSE:HE3	1:B:322:TYR:HE2	1.38	0.87
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.55	0.86
2:F:412:TYR:HB2	2:F:433:LEU:HD11	1.58	0.84
2:F:219:ILE:HD12	2:F:219:ILE:H	1.41	0.84
1:C:129:GLU:HG2	1:C:158:THR:HG22	1.59	0.84
1:B:320:MSE:HE3	1:B:322:TYR:CE2	2.14	0.81
1:B:237:GLY:O	1:B:241:VAL:HG23	1.81	0.80
1:C:95:MSE:SE	2:F:120:ALA:HB2	2.31	0.80
1:C:513:THR:HG21	1:C:521:MSE:HE1	1.64	0.79
1:B:139:VAL:HG21	1:B:187:MSE:HE1	1.64	0.79
1:C:27:MSE:CE	1:C:71:LEU:HB2	2.09	0.79
1:C:273:PHE:HB2	1:C:286:MSE:HE2	1.63	0.79
1:B:139:VAL:HG21	1:B:187:MSE:CE	2.12	0.79
2:D:306:MSE:HE2	2:D:311:LYS:HA	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:MSE:CE	2:D:311:LYS:HA	2.13	0.79
2:D:13:GLY:O	2:D:60:THR:HG21	1.84	0.78
1:B:256:TYR:HE2	1:B:266:MSE:HE1	1.49	0.78
1:A:133:GLY:O	1:A:380:ARG:NH2	2.18	0.77
1:B:8:LYS:HB3	1:B:15:MSE:HG2	1.66	0.77
2:E:219:ILE:HD12	2:E:219:ILE:H	1.48	0.76
1:A:298:MSE:HE2	2:D:115:VAL:HG11	1.67	0.76
1:A:27:MSE:HE3	1:A:71:LEU:HB2	1.66	0.75
2:D:11:VAL:HG22	2:D:16:MSE:HG3	1.67	0.75
2:F:11:VAL:HG22	2:F:16:MSE:HG2	1.69	0.74
2:F:79:LEU:HD13	2:F:227:MSE:HE1	1.69	0.74
2:E:77:LEU:HB3	2:E:111:ILE:HG12	1.69	0.73
1:C:208:PRO:HG2	1:C:445:MSE:HE3	1.69	0.73
2:F:229:LEU:HG	2:F:247:MSE:HE1	1.71	0.73
1:A:297:ASN:ND2	2:D:115:VAL:HG13	2.05	0.72
1:A:392:PRO:HB2	1:A:396:ASP:H	1.54	0.72
2:E:184:ILE:CD1	2:E:250:MSE:HE1	2.19	0.71
1:A:392:PRO:HB3	1:A:399:GLU:HG2	1.71	0.71
1:A:169:ILE:HA	1:A:187:MSE:HB2	1.70	0.70
2:E:83:GLU:HB3	2:E:239:LYS:HE2	1.73	0.70
2:E:184:ILE:HD12	2:E:250:MSE:HE1	1.72	0.70
2:E:138:LEU:HA	2:E:369:MSE:HG3	1.73	0.70
2:D:391:GLU:O	2:D:391:GLU:CG	2.40	0.70
1:A:41:GLU:HG2	1:A:48:SER:HB2	1.74	0.69
1:C:141:GLU:OE2	1:C:147:HIS:HD2	1.75	0.69
1:B:25:GLN:HG3	2:F:61:SER:OG	1.92	0.69
1:C:27:MSE:HE3	1:C:71:LEU:CB	2.14	0.69
1:C:12:PRO:HG2	1:C:341:MSE:HE1	1.75	0.69
1:C:188:MSE:HE1	1:C:190:LYS:HG3	1.75	0.69
1:A:320:MSE:HE2	1:A:322:TYR:CE2	2.20	0.69
2:F:379:GLY:HA2	2:F:401:TYR:HB3	1.74	0.68
1:B:230:VAL:HG12	1:B:413:TRP:HB2	1.75	0.68
2:F:49:GLU:OE2	2:F:49:GLU:HA	1.94	0.68
2:D:270:ARG:NH1	5:D:509:HOH:O	2.24	0.67
2:D:181:PHE:HD2	2:D:211:MSE:HE1	1.59	0.67
2:E:229:LEU:HG	2:E:247:MSE:HE1	1.76	0.67
2:F:234:TYR:O	2:F:238:GLU:HB2	1.95	0.66
1:B:247:LYS:HB2	1:B:285:LEU:HD21	1.77	0.66
1:C:327:MSE:HG3	1:C:387:ILE:HB	1.78	0.66
1:B:27:MSE:HA	1:B:38:GLU:HA	1.78	0.66
1:B:24:ILE:HG22	1:B:25:GLN:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:MSE:HE1	1:C:190:LYS:CG	2.27	0.65
1:C:214:ARG:HD3	1:C:521:MSE:HE1	1.79	0.65
1:C:150:MSE:HE1	1:C:319:ASP:HB3	1.77	0.65
2:E:57:PHE:HA	2:E:219:ILE:HD13	1.79	0.64
2:D:181:PHE:CD2	2:D:211:MSE:HE1	2.32	0.64
1:B:264:ASN:ND2	2:E:121:ARG:HD3	2.13	0.64
1:C:445:MSE:HE1	1:C:515:ARG:CZ	2.28	0.64
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.32	0.64
1:C:320:MSE:CE	1:C:322:TYR:HE2	2.10	0.64
1:C:243:HIS:O	1:C:247:LYS:HG2	1.98	0.64
2:F:331:ARG:O	2:F:335:LYS:HB3	1.97	0.64
2:F:34:MSE:HE3	2:F:38:GLU:HB3	1.80	0.63
1:C:8:LYS:HB3	1:C:15:MSE:HG2	1.80	0.63
1:A:133:GLY:HA2	1:A:150:MSE:HE2	1.80	0.63
1:B:318:ARG:HD2	1:B:372:VAL:HG22	1.81	0.63
2:F:79:LEU:HD13	2:F:227:MSE:CE	2.28	0.63
1:A:188:MSE:HG2	1:A:189:GLN:N	2.14	0.62
1:A:189:GLN:HE22	1:A:197:ARG:HH22	1.47	0.62
1:B:129:GLU:HG2	1:B:158:THR:HG22	1.80	0.62
1:C:326:ILE:C	1:C:327:MSE:HE3	2.18	0.62
2:E:29:LEU:HD11	2:E:77:LEU:HD12	1.82	0.62
1:C:65:ARG:HB2	1:C:65:ARG:HH11	1.65	0.61
1:C:273:PHE:CB	1:C:286:MSE:HE2	2.31	0.61
2:D:345:LEU:HB2	2:D:346:PRO:HD3	1.83	0.61
2:E:250:MSE:HB2	2:E:304:LEU:HB3	1.83	0.61
1:A:94:PHE:O	1:A:98:THR:OG1	2.18	0.61
1:A:150:MSE:HE3	1:A:380:ARG:HH21	1.66	0.60
1:B:270:VAL:HA	1:B:286:MSE:CE	2.32	0.60
1:A:294:ASN:HD22	1:A:298:MSE:HG3	1.65	0.60
1:B:150:MSE:HE1	1:B:319:ASP:HB3	1.82	0.60
1:B:237:GLY:O	1:B:241:VAL:CG2	2.50	0.60
1:A:407:ARG:NH1	2:E:255:GLU:OE2	2.35	0.59
1:C:504:ASN:HD22	1:C:507:ASP:HB2	1.67	0.59
2:F:412:TYR:HD1	2:F:429:LEU:HD23	1.67	0.59
1:C:399:GLU:HG2	1:C:400:PRO:HD2	1.84	0.59
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.85	0.59
1:C:270:VAL:HA	1:C:286:MSE:HE3	1.82	0.59
2:E:89:VAL:HB	2:E:98:ASP:HB3	1.84	0.59
2:F:129:GLN:NE2	2:F:422:THR:HA	2.16	0.59
1:C:139:VAL:CG2	1:C:187:MSE:HE1	2.32	0.59
1:C:320:MSE:HE2	1:C:322:TYR:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ILE:HG22	1:C:25:GLN:HG2	1.84	0.59
2:E:90:PHE:HB3	2:E:94:GLY:HA2	1.85	0.59
1:C:12:PRO:CG	1:C:341:MSE:HE1	2.32	0.59
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.84	0.58
1:A:208:PRO:HG3	1:A:441:VAL:HG22	1.84	0.58
2:D:250:MSE:HE2	2:D:250:MSE:HA	1.84	0.58
1:A:330:SER:OG	1:A:332:SER:N	2.34	0.58
1:A:83:MSE:HE2	1:A:291:LEU:HD22	1.85	0.58
2:E:77:LEU:HD23	2:E:111:ILE:HD13	1.79	0.58
1:A:271:ASN:OD1	2:D:292:ARG:NH2	2.37	0.58
2:E:182:ALA:HB3	2:E:247:MSE:HG2	1.85	0.57
1:A:266:MSE:HE3	1:A:294:ASN:O	2.04	0.57
1:A:148:LYS:HB2	1:A:320:MSE:HG2	1.87	0.57
1:A:43:ARG:HG2	2:E:10:GLU:HG2	1.86	0.57
1:B:8:LYS:HG3	2:E:48:GLN:HB2	1.87	0.57
2:E:94:GLY:HA3	2:E:227:MSE:HE2	1.86	0.57
1:A:263:GLY:HA2	1:A:295:THR:HG22	1.86	0.57
2:D:249:ASP:C	2:D:249:ASP:OD1	2.43	0.57
2:F:229:LEU:HD13	2:F:287:ARG:HG3	1.87	0.57
1:A:298:MSE:CE	2:D:115:VAL:HG11	2.35	0.57
1:B:295:THR:OG1	1:B:298:MSE:HG3	2.05	0.56
1:B:230:VAL:HG13	1:B:413:TRP:HE3	1.70	0.56
1:B:329:ASP:OD2	1:B:329:ASP:C	2.42	0.56
2:E:408:PHE:O	2:E:412:TYR:HB3	2.05	0.56
1:A:274:PRO:HA	1:A:286:MSE:HG2	1.87	0.56
2:F:212:ASN:OD1	2:F:221:ARG:HG2	2.06	0.56
1:C:141:GLU:OE2	1:C:147:HIS:CD2	2.56	0.56
2:E:439:ARG:HE	2:E:450:LEU:HD13	1.70	0.56
2:E:79:LEU:HD13	2:E:227:MSE:CE	2.36	0.56
2:E:55:GLN:HE22	2:E:264:ARG:HE	1.52	0.55
1:B:424:HIS:CD2	1:B:502:GLN:HE21	2.24	0.55
2:D:433:LEU:HG	2:D:436:MSE:HE2	1.88	0.55
1:C:173:ILE:HD13	1:C:187:MSE:HG2	1.88	0.55
1:C:320:MSE:CE	1:C:322:TYR:CE2	2.90	0.55
2:F:137:HIS:HD2	2:F:412:TYR:OH	1.89	0.55
2:F:338:ILE:HG23	2:F:414:ASN:HB2	1.88	0.55
2:D:150:PHE:HB2	2:D:328:ILE:HD13	1.88	0.55
1:A:189:GLN:NE2	1:A:197:ARG:HH12	2.05	0.55
2:D:184:ILE:HD13	2:D:250:MSE:HE1	1.88	0.55
2:E:180:VAL:HB	2:E:245:VAL:HG22	1.89	0.54
1:B:327:MSE:HE2	1:B:387:ILE:HB	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:MSE:HB3	2:D:211:MSE:HE3	1.89	0.54
2:E:313:HIS:CE1	2:E:315:ILE:HG12	2.42	0.54
2:F:158:LYS:HE3	2:F:190:GLU:HG2	1.89	0.54
1:A:261:GLU:HG2	1:A:266:MSE:CE	2.38	0.54
1:B:6:ILE:HD12	1:B:62:GLU:HB2	1.89	0.54
1:C:249:SER:HB3	1:C:251:VAL:HG22	1.88	0.54
1:C:315:GLU:HA	1:C:384:ILE:HD11	1.88	0.54
2:D:285:PHE:HA	2:D:300:GLN:HE22	1.71	0.54
2:F:249:ASP:OD2	2:F:249:ASP:C	2.44	0.54
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.90	0.54
1:A:410:LYS:HD3	1:A:437:TYR:CZ	2.42	0.54
1:B:261:GLU:CG	1:B:329:ASP:OD2	2.48	0.54
2:D:143:ARG:HH21	2:D:170:VAL:HG11	1.72	0.54
1:A:513:THR:HG22	1:A:518:GLN:HG3	1.90	0.54
1:C:251:VAL:HB	1:C:323:ASP:O	2.08	0.54
2:E:209:MSE:HB3	2:E:211:MSE:HE3	1.89	0.54
1:B:77:PRO:HG2	1:B:187:MSE:HE2	1.90	0.54
2:D:163:GLN:HE21	2:D:167:GLN:HE22	1.55	0.54
1:A:219:PHE:HD1	1:A:461:MSE:HE2	1.73	0.53
2:E:111:ILE:HA	2:E:230:THR:OG1	2.08	0.53
1:A:259:CYS:SG	1:A:330:SER:O	2.65	0.53
1:A:201:GLN:HB3	1:A:373:ILE:HD12	1.90	0.53
2:D:173:SER:C	2:D:175:ASP:H	2.12	0.53
2:D:345:LEU:HB2	2:D:346:PRO:CD	2.38	0.53
1:A:456:MSE:HG2	1:A:526:LEU:HD13	1.90	0.53
2:D:184:ILE:N	2:D:248:THR:O	2.31	0.53
2:F:144:GLY:HA2	2:F:298:VAL:O	2.08	0.53
2:E:94:GLY:HA3	2:E:227:MSE:CE	2.38	0.53
1:B:230:VAL:CG1	1:B:413:TRP:HB2	2.39	0.53
2:E:367:ALA:HB1	2:E:445:ILE:HG12	1.90	0.53
1:B:214:ARG:CD	1:B:521:MSE:HE1	2.39	0.53
1:B:83:MSE:SE	1:B:91:LEU:HD12	2.59	0.52
1:C:270:VAL:HA	1:C:286:MSE:CE	2.38	0.52
2:E:224:THR:HB	2:E:225:PRO:HD3	1.92	0.52
2:D:362:ARG:HD2	2:D:364:ASP:OD1	2.09	0.52
2:F:209:MSE:HB3	2:F:211:MSE:HE3	1.91	0.52
2:E:258:ARG:HD2	2:E:273:TYR:CE1	2.45	0.52
2:D:119:ILE:O	2:D:292:ARG:NH1	2.42	0.52
1:A:456:MSE:HE1	1:A:519:PHE:HE1	1.74	0.52
1:C:225:GLY:O	1:C:370:GLY:HA2	2.10	0.52
2:E:410:ASN:O	2:E:414:ASN:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD22	1:A:298:MSE:HE1	1.92	0.52
1:C:425:PHE:HB3	3:C:601:ANP:C6	2.40	0.52
2:D:389:LEU:HD12	2:D:392:SER:HB2	1.92	0.52
2:E:203:ALA:HA	2:E:206:ARG:HH11	1.75	0.52
1:A:327:MSE:HA	1:A:387:ILE:O	2.10	0.51
1:B:318:ARG:HD3	1:B:384:ILE:HG13	1.92	0.51
1:C:135:ILE:HD12	1:C:148:LYS:HB3	1.92	0.51
2:F:412:TYR:HB2	2:F:433:LEU:CD1	2.37	0.51
1:B:371:ARG:NH1	1:B:381:GLU:OE2	2.43	0.51
2:E:85:MSE:HE1	2:E:231:ALA:CB	2.40	0.51
1:A:136:ILE:HD11	1:A:173:ILE:HD11	1.93	0.51
2:D:45:LEU:O	2:D:264:ARG:HD3	2.10	0.51
2:F:182:ALA:HB3	2:F:247:MSE:HG2	1.91	0.51
1:A:209:MSE:HE3	1:A:224:LYS:HG2	1.93	0.51
2:D:163:GLN:HE21	2:D:167:GLN:NE2	2.08	0.51
2:F:181:PHE:CD2	2:F:211:MSE:HE1	2.45	0.51
1:B:273:PHE:HB2	1:B:286:MSE:HE2	1.92	0.51
2:D:79:LEU:HD13	2:D:227:MSE:HE1	1.92	0.51
1:B:27:MSE:HE3	1:B:71:LEU:HA	1.92	0.51
1:A:134:ASP:O	1:A:151:VAL:HG23	2.11	0.51
1:C:8:LYS:HB3	1:C:15:MSE:CG	2.41	0.51
2:D:86:ILE:HA	2:D:208:VAL:HG22	1.93	0.51
2:E:79:LEU:HD13	2:E:227:MSE:HE1	1.92	0.50
2:F:138:LEU:HA	2:F:369:MSE:HG3	1.93	0.50
1:B:325:ALA:HB1	1:B:327:MSE:HE1	1.93	0.50
1:A:273:PHE:HB3	1:A:286:MSE:CE	2.42	0.50
2:E:415:GLN:O	2:E:419:THR:OG1	2.29	0.50
1:A:32:ASP:OD2	1:A:62:GLU:HG2	2.12	0.50
1:A:93:THR:O	1:A:97:VAL:HG23	2.12	0.50
2:E:248:THR:HA	2:E:303:ILE:HB	1.94	0.50
2:F:128:ILE:HG13	2:F:143:ARG:HG2	1.93	0.50
1:A:258:GLY:HA3	1:A:266:MSE:HE1	1.94	0.50
2:F:304:LEU:HD22	2:F:315:ILE:HG22	1.94	0.50
2:F:362:ARG:HD2	2:F:364:ASP:OD1	2.11	0.50
2:F:438:PRO:HB2	2:F:440:THR:HG22	1.93	0.50
2:F:265:ARG:HB2	2:F:265:ARG:HH11	1.77	0.50
2:E:29:LEU:HD11	2:E:77:LEU:CD1	2.42	0.50
1:A:197:ARG:NE	1:A:319:ASP:OD2	2.42	0.50
1:C:399:GLU:HG2	1:C:400:PRO:CD	2.41	0.50
1:A:174:CYS:HB3	1:A:185:LEU:HB2	1.93	0.49
2:E:195:MSE:HE3	2:E:199:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:ILE:HD12	2:F:250:MSE:HE1	1.92	0.49
1:B:85:ASP:HB3	1:B:91:LEU:HD21	1.94	0.49
2:E:277:LEU:HD23	2:E:318:LEU:HD12	1.95	0.49
1:C:83:MSE:HE2	1:C:291:LEU:HD23	1.94	0.49
2:F:181:PHE:HD2	2:F:211:MSE:HE1	1.77	0.49
2:F:339:GLN:HE21	2:F:416:GLY:HA2	1.78	0.49
2:F:112:ASN:ND2	2:F:226:ARG:HD3	2.27	0.49
1:A:254:VAL:O	1:A:289:THR:HA	2.13	0.49
2:F:219:ILE:H	2:F:219:ILE:CD1	2.13	0.49
1:A:87:ILE:HG23	1:A:302:ALA:HA	1.95	0.49
1:A:257:VAL:HA	1:A:292:ILE:HB	1.94	0.49
1:C:114:HIS:HB3	1:C:170:ASP:OD2	2.12	0.49
2:E:89:VAL:HG22	2:E:209:MSE:HB2	1.95	0.49
1:B:147:HIS:HE1	1:B:316:TYR:OH	1.96	0.49
1:B:513:THR:HG21	1:B:521:MSE:HE1	1.95	0.49
1:C:494:LYS:HA	1:C:497:ARG:NH1	2.28	0.49
2:E:247:MSE:HB3	2:E:250:MSE:CE	2.43	0.49
1:B:463:ILE:HG22	1:B:493:ALA:HB2	1.95	0.48
2:D:166:ARG:HD3	2:D:197:ASP:OD2	2.13	0.48
1:A:203:LEU:HD11	1:A:373:ILE:HG13	1.96	0.48
1:C:424:HIS:CD2	1:C:502:GLN:HE21	2.32	0.48
2:E:85:MSE:HE1	2:E:231:ALA:HB1	1.94	0.48
2:E:148:PRO:HA	2:E:302:PRO:HD2	1.94	0.48
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.96	0.48
2:E:447:ASP:HA	2:E:450:LEU:HD12	1.95	0.48
2:F:94:GLY:CA	2:F:227:MSE:HE2	2.43	0.48
1:B:144:ILE:HG13	1:B:145:ILE:HG12	1.95	0.48
2:E:29:LEU:CD1	2:E:77:LEU:HD12	2.43	0.48
1:B:329:ASP:HA	1:B:330:SER:HA	1.67	0.48
1:C:513:THR:HG21	1:C:521:MSE:CE	2.40	0.48
1:B:202:LYS:HB2	2:F:188:PHE:CE1	2.49	0.48
1:B:214:ARG:HD3	1:B:521:MSE:HE1	1.95	0.48
1:C:209:MSE:HE2	1:C:251:VAL:CG1	2.44	0.48
1:A:261:GLU:CG	1:A:266:MSE:HE2	2.44	0.47
1:A:445:MSE:HG2	1:A:453:TRP:CE3	2.48	0.47
1:C:324:VAL:HG12	1:C:325:ALA:N	2.29	0.47
2:D:9:LYS:HD2	2:D:19:GLU:CD	2.34	0.47
2:D:34:MSE:SE	2:D:63:ILE:HG12	2.64	0.47
2:D:285:PHE:HA	2:D:300:GLN:NE2	2.28	0.47
2:E:143:ARG:HD3	2:E:242:HIS:CD2	2.49	0.47
1:A:105:ARG:HB2	1:A:105:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASP:HA	1:C:293:ALA:O	2.14	0.47
1:C:413:TRP:HB3	1:C:428:ILE:HD12	1.95	0.47
1:B:413:TRP:HB3	1:B:428:ILE:HD12	1.96	0.47
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.95	0.47
1:C:231:PRO:HA	1:C:390:VAL:O	2.15	0.47
2:F:248:THR:HA	2:F:249:ASP:HA	1.60	0.47
1:A:173:ILE:HG21	1:A:187:MSE:HG2	1.96	0.47
1:C:320:MSE:HE2	1:C:322:TYR:CD2	2.50	0.47
2:D:306:MSE:HG2	2:D:316:PRO:HG3	1.97	0.47
2:F:149:VAL:HB	2:F:303:ILE:HG12	1.97	0.47
2:E:184:ILE:HD12	2:E:250:MSE:CE	2.42	0.47
1:C:467:GLU:HG3	1:C:490:LEU:HD23	1.96	0.47
2:E:338:ILE:HG23	2:E:414:ASN:HB2	1.96	0.47
1:A:482:LEU:HB3	1:A:486:ASP:HB2	1.97	0.47
2:D:222:ILE:HD12	2:D:260:ILE:HD13	1.96	0.47
1:B:518:GLN:HA	1:B:521:MSE:HE2	1.97	0.46
1:C:262:ARG:NE	2:F:322:ILE:O	2.46	0.46
1:B:28:CYS:HB2	1:B:66:SER:HA	1.98	0.46
1:A:208:PRO:HA	1:A:223:THR:HA	1.98	0.46
1:C:13:LEU:HD23	1:C:15:MSE:HE1	1.96	0.46
2:E:132:ILE:HA	2:E:415:GLN:HE22	1.81	0.46
1:A:210:ILE:HD11	1:A:515:ARG:HE	1.80	0.46
1:C:144:ILE:HG13	1:C:145:ILE:HG12	1.96	0.46
2:E:112:ASN:ND2	2:E:226:ARG:HD3	2.31	0.46
1:A:258:GLY:O	1:A:294:ASN:HB2	2.16	0.46
1:A:149:ILE:HD11	1:A:187:MSE:HE2	1.97	0.46
1:C:209:MSE:HE2	1:C:251:VAL:HG13	1.98	0.46
2:D:389:LEU:CD1	2:D:392:SER:HB2	2.45	0.46
2:D:222:ILE:CD1	2:D:260:ILE:HD13	2.45	0.46
2:D:249:ASP:OD1	2:D:250:MSE:N	2.48	0.45
2:F:210:PHE:O	2:F:211:MSE:HE2	2.17	0.45
1:A:497:ARG:HA	1:A:501:LEU:HD12	1.98	0.45
1:B:147:HIS:CE1	1:B:316:TYR:OH	2.70	0.45
1:B:256:TYR:CE2	1:B:266:MSE:HE1	2.39	0.45
1:B:327:MSE:CE	1:B:387:ILE:HB	2.47	0.45
1:C:92:ASP:HA	2:F:119:ILE:HG21	1.97	0.45
2:D:248:THR:HA	2:D:249:ASP:HA	1.77	0.45
2:F:362:ARG:HH21	2:F:424:THR:HG23	1.82	0.45
2:F:31:GLU:HG3	2:F:73:LEU:HD11	1.98	0.45
2:E:44:VAL:HA	2:E:54:VAL:HG12	1.98	0.45
1:C:119:TRP:HE1	1:C:121:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LYS:HB3	1:C:436:LEU:HB2	1.98	0.45
2:D:183:ALA:HA	2:D:248:THR:O	2.17	0.45
1:A:261:GLU:HG2	1:A:266:MSE:HE2	1.97	0.45
1:C:449:LEU:HD21	1:C:515:ARG:HG2	1.98	0.45
1:C:497:ARG:HA	1:C:501:LEU:HD12	1.99	0.45
1:B:28:CYS:HA	1:B:67:THR:HG23	1.98	0.45
1:B:51:VAL:HG12	1:B:53:GLU:H	1.82	0.45
1:B:317:PHE:O	1:B:322:TYR:HB2	2.17	0.45
1:C:420:ALA:HB2	1:C:427:SER:OG	2.17	0.45
2:E:55:GLN:NE2	2:E:264:ARG:HE	2.13	0.45
1:B:135:ILE:HD12	1:B:148:LYS:HB3	1.99	0.45
1:B:300:VAL:HG22	2:E:279:THR:HG21	1.98	0.45
1:B:429:ASN:OD1	1:B:432:GLN:HG2	2.17	0.45
2:F:277:LEU:O	2:F:281:LEU:HG	2.17	0.45
1:B:83:MSE:HG3	1:B:291:LEU:HB3	1.99	0.45
2:F:137:HIS:CD2	2:F:412:TYR:OH	2.70	0.45
1:A:129:GLU:CD	1:A:129:GLU:H	2.20	0.44
1:A:56:SER:HB2	2:D:27:GLU:OE2	2.18	0.44
1:A:399:GLU:HA	1:A:400:PRO:HD3	1.91	0.44
2:E:128:ILE:HG13	2:E:143:ARG:HG2	1.99	0.44
2:F:34:MSE:CE	2:F:38:GLU:HB3	2.45	0.44
2:F:184:ILE:CD1	2:F:250:MSE:HE1	2.47	0.44
2:D:408:PHE:HA	2:D:433:LEU:HD21	2.00	0.44
1:A:248:TRP:CZ3	1:A:279:PRO:HB3	2.52	0.44
2:D:138:LEU:HD12	2:D:344:VAL:HG11	1.99	0.44
2:E:183:ALA:HB3	2:E:211:MSE:HA	2.00	0.44
1:A:252:ASP:O	1:A:288:ARG:HD2	2.18	0.44
1:A:261:GLU:HB2	1:A:266:MSE:HE2	1.99	0.44
1:A:329:ASP:HA	1:A:330:SER:HA	1.63	0.44
1:B:458:THR:HG22	1:B:462:ARG:HH12	1.82	0.44
2:D:277:LEU:HD23	2:D:318:LEU:HD12	2.00	0.44
2:F:94:GLY:HA3	2:F:227:MSE:CE	2.48	0.44
1:A:139:VAL:CG2	1:A:187:MSE:HE1	2.47	0.44
1:C:101:ASN:HD22	2:F:120:ALA:HB1	1.82	0.44
2:D:177:PHE:O	2:D:206:ARG:HG2	2.17	0.44
2:D:338:ILE:HG23	2:D:414:ASN:HB2	2.00	0.44
2:D:410:ASN:O	2:D:414:ASN:HB3	2.18	0.44
1:C:329:ASP:HA	1:C:330:SER:HA	1.76	0.44
1:A:1:MSE:HG2	1:A:2:GLN:N	2.33	0.44
1:A:16:ALA:O	1:A:46:VAL:HA	2.18	0.44
1:A:206:ASP:O	1:A:208:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:MSE:HB3	2:E:250:MSE:HE3	2.00	0.44
1:C:188:MSE:HE1	1:C:190:LYS:HG2	1.98	0.43
1:C:241:VAL:O	1:C:245:ILE:HG12	2.18	0.43
2:D:391:GLU:HG3	2:D:394:LEU:HB2	1.99	0.43
1:B:81:SER:OG	1:B:287:GLU:HA	2.18	0.43
1:B:243:HIS:O	1:B:247:LYS:HG2	2.18	0.43
1:B:445:MSE:HE1	1:B:515:ARG:CZ	2.48	0.43
1:B:205:PRO:HB3	1:B:224:LYS:O	2.19	0.43
2:E:250:MSE:O	2:E:253:TYR:HB3	2.19	0.43
1:A:73:VAL:HG11	1:A:309:THR:HG23	2.00	0.43
1:B:269:VAL:O	1:B:273:PHE:HB2	2.19	0.43
1:B:318:ARG:HD2	1:B:372:VAL:CG2	2.48	0.43
1:B:326:ILE:C	1:B:327:MSE:HE3	2.39	0.43
1:C:268:ASP:HB2	2:F:123:TYR:CE1	2.53	0.43
1:C:390:VAL:O	1:C:392:PRO:HD3	2.19	0.43
2:F:21:VAL:HG22	2:F:50:ASP:O	2.19	0.43
1:B:30:VAL:HB	1:B:35:VAL:HG23	2.01	0.43
1:C:147:HIS:HE1	1:C:316:TYR:OH	2.00	0.43
2:E:315:ILE:HB	2:E:316:PRO:CD	2.49	0.43
1:A:17:GLU:O	1:A:18:ASN:HB2	2.18	0.43
1:A:286:MSE:HA	1:A:289:THR:HB	2.00	0.43
1:A:315:GLU:HA	1:A:384:ILE:HD11	2.01	0.42
1:C:488:LEU:O	1:C:492:VAL:HG23	2.19	0.42
2:E:385:LEU:HD11	2:E:389:LEU:HD12	2.01	0.42
1:A:210:ILE:HD11	1:A:515:ARG:NE	2.33	0.42
1:B:197:ARG:HA	1:B:198:PRO:HD3	1.91	0.42
1:B:27:MSE:HG3	1:B:71:LEU:HD12	2.00	0.42
2:D:150:PHE:HB3	2:D:306:MSE:SE	2.69	0.42
1:C:228:ALA:HA	1:C:411:VAL:HB	2.01	0.42
2:E:113:GLY:O	2:E:114:GLU:HG3	2.19	0.42
2:E:352:LYS:HD2	2:E:369:MSE:SE	2.69	0.42
2:F:130:THR:O	2:F:167:GLN:HB2	2.19	0.42
2:D:329:LEU:HA	2:D:341:PRO:O	2.19	0.42
2:E:183:ALA:O	2:E:212:ASN:HB3	2.19	0.42
2:F:183:ALA:HB1	2:F:186:ILE:CD1	2.49	0.42
1:B:317:PHE:CD1	1:B:320:MSE:HE2	2.55	0.42
1:B:391:SER:HB3	2:E:321:TYR:CE2	2.55	0.42
1:B:399:GLU:OE1	1:B:401:VAL:HB	2.20	0.42
1:C:371:ARG:NH1	1:C:381:GLU:OE2	2.48	0.42
1:A:8:LYS:HB3	1:A:15:MSE:HG3	2.01	0.42
1:A:262:ARG:HB2	1:A:265:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:CYS:HB3	1:C:66:SER:HA	2.01	0.42
2:E:227:MSE:HE3	2:E:227:MSE:HB3	1.98	0.42
1:B:247:LYS:HB2	1:B:285:LEU:CD2	2.49	0.42
2:D:404:PHE:CD1	2:D:436:MSE:HE3	2.54	0.42
1:B:230:VAL:CG1	1:B:413:TRP:HE3	2.33	0.41
1:B:270:VAL:HA	1:B:286:MSE:HE1	2.02	0.41
1:C:331:THR:HG22	1:C:389:ALA:O	2.20	0.41
1:C:565:GLU:CD	1:C:565:GLU:H	2.23	0.41
2:F:148:PRO:HA	2:F:302:PRO:O	2.20	0.41
2:F:446:LYS:HA	2:F:446:LYS:HD3	1.87	0.41
1:C:197:ARG:HA	1:C:198:PRO:HD3	1.87	0.41
1:C:360:SER:O	1:C:364:GLU:HG3	2.20	0.41
2:D:44:VAL:HA	2:D:54:VAL:HG12	2.01	0.41
2:D:162:ALA:O	2:D:166:ARG:HG3	2.20	0.41
2:D:388:VAL:O	2:D:389:LEU:HB3	2.20	0.41
1:B:199:ILE:HG21	1:B:372:VAL:HG21	2.03	0.41
2:D:198:PHE:HA	2:D:203:ALA:HB3	2.02	0.41
1:B:13:LEU:HD23	1:B:15:MSE:HE1	2.02	0.41
1:B:327:MSE:HE2	1:B:387:ILE:CG1	2.51	0.41
1:C:399:GLU:HG2	1:C:400:PRO:N	2.35	0.41
1:C:513:THR:HG22	1:C:518:GLN:HG3	2.03	0.41
2:F:32:VAL:HG22	2:F:70:VAL:HG22	2.02	0.41
2:F:339:GLN:HA	2:F:340:PRO:HA	1.95	0.41
1:C:297:ASN:ND2	2:F:115:VAL:HG22	2.35	0.41
2:F:145:GLN:HG3	2:F:351:LEU:HD12	2.02	0.41
2:F:245:VAL:HG11	2:F:247:MSE:HE3	2.03	0.41
1:B:178:THR:C	1:B:180:GLN:H	2.24	0.41
1:B:337:ALA:O	1:B:340:GLU:HB3	2.21	0.41
2:E:343:ASP:O	2:E:346:PRO:HD2	2.21	0.41
2:E:372:LEU:HD23	2:E:404:PHE:HZ	1.85	0.41
1:A:118:TRP:O	1:A:166:SER:HA	2.21	0.41
1:B:93:THR:O	1:B:97:VAL:HG23	2.20	0.41
1:C:278:ASP:O	1:C:281:THR:HG23	2.21	0.41
1:C:397:ILE:C	1:C:399:GLU:H	2.24	0.41
1:C:564:GLU:O	1:C:567:LEU:HG	2.20	0.41
2:D:166:ARG:HD2	2:D:201:THR:HG21	2.03	0.41
2:D:258:ARG:HD2	2:D:273:TYR:CE1	2.56	0.41
2:D:267:VAL:HA	2:D:268:PRO:HD3	1.94	0.41
2:F:288:ALA:HB2	2:F:300:GLN:HE21	1.84	0.41
1:A:135:ILE:H	1:A:135:ILE:HG13	1.78	0.41
1:A:209:MSE:HE2	1:A:251:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PHE:HB3	2:E:114:GLU:HB3	2.03	0.41
1:B:270:VAL:HA	1:B:286:MSE:HE3	2.03	0.41
1:B:513:THR:HG22	1:B:518:GLN:HG3	2.03	0.41
1:C:295:THR:H	1:C:298:MSE:SE	2.54	0.41
1:C:574:ASN:HA	1:C:577:ILE:HD12	2.03	0.41
1:C:230:VAL:HG13	1:C:413:TRP:HB2	2.02	0.40
2:F:85:MSE:HE1	2:F:231:ALA:HB1	2.03	0.40
2:F:87:GLY:HA2	2:F:204:ILE:O	2.21	0.40
1:A:495:SER:O	1:A:499:ASP:HB2	2.21	0.40
1:C:470:LEU:O	1:C:474:VAL:HG23	2.21	0.40
2:D:234:TYR:CZ	2:D:239:LYS:HE3	2.55	0.40
2:E:148:PRO:HG3	2:E:323:THR:HG21	2.03	0.40
2:F:180:VAL:O	2:F:245:VAL:HA	2.21	0.40
1:B:207:VAL:HA	1:B:208:PRO:HD3	1.89	0.40
2:D:173:SER:C	2:D:175:ASP:N	2.74	0.40
2:E:242:HIS:HA	2:E:297:SER:H	1.87	0.40
1:A:1:MSE:CG	1:A:2:GLN:N	2.85	0.40
1:A:145:ILE:HG21	1:A:253:LEU:HD11	2.03	0.40
2:F:148:PRO:HD2	2:F:326:GLN:HA	2.04	0.40
1:A:54:GLU:HB2	1:A:105:ARG:HE	1.87	0.40
1:A:75:LEU:HD13	1:A:316:TYR:HB2	2.02	0.40
1:A:188:MSE:HE2	1:A:188:MSE:HB3	1.90	0.40
1:A:210:ILE:HD11	1:A:515:ARG:HG3	2.04	0.40
1:B:231:PRO:HG2	1:B:412:PHE:HE1	1.86	0.40
1:B:513:THR:HG21	1:B:521:MSE:CE	2.51	0.40
2:F:92:GLY:O	2:F:227:MSE:HG3	2.22	0.40
2:F:267:VAL:HA	2:F:268:PRO:HD3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/600 (97%)	542 (93%)	38 (6%)	4 (1%)	22	55
1	B	584/600 (97%)	548 (94%)	35 (6%)	1 (0%)	47	78
1	C	582/600 (97%)	549 (94%)	33 (6%)	0	100	100
2	D	443/465 (95%)	403 (91%)	38 (9%)	2 (0%)	29	61
2	E	449/465 (97%)	420 (94%)	26 (6%)	3 (1%)	22	55
2	F	449/465 (97%)	422 (94%)	25 (6%)	2 (0%)	34	67
All	All	3091/3195 (97%)	2884 (93%)	195 (6%)	12 (0%)	34	67

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	SER
2	F	172	ASP
2	E	126	GLU
2	F	386	ALA
2	E	249	ASP
1	A	395	GLY
1	A	479	ILE
1	B	540	ALA
2	E	96	PRO
1	A	260	GLY
2	D	101	PRO
2	D	103	ILE

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	502/487 (103%)	477 (95%)	25 (5%)	24	54
1	B	495/487 (102%)	477 (96%)	18 (4%)	35	63
1	C	494/487 (101%)	477 (97%)	17 (3%)	37	65
2	D	360/372 (97%)	346 (96%)	14 (4%)	32	61
2	E	374/372 (100%)	361 (96%)	13 (4%)	36	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	372/372 (100%)	359 (96%)	13 (4%)	36	65
All	All	2597/2577 (101%)	2497 (96%)	100 (4%)	32	61

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	36	ILE
1	A	92	ASP
1	A	94	PHE
1	A	105	ARG
1	A	125	GLU
1	A	135	ILE
1	A	161	LYS
1	A	188	MSE
1	A	195	ARG
1	A	203	LEU
1	A	239	THR
1	A	251	VAL
1	A	253	LEU
1	A	273	PHE
1	A	285	LEU
1	A	330	SER
1	A	398	SER
1	A	399	GLU
1	A	438	SER
1	A	439	THR
1	A	485	ASN
1	A	489	THR
1	A	526	LEU
1	A	575	GLU
1	B	1	MSE
1	B	13	LEU
1	B	18	ASN
1	B	27	MSE
1	B	71	LEU
1	B	98	THR
1	B	115	GLU
1	B	179	GLU
1	B	215	VAL
1	B	230	VAL
1	B	251	VAL

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Mol	Chain	Res	Type
1	B	253	LEU
1	B	281	THR
1	B	327	MSE
1	B	329	ASP
1	B	509	VAL
1	B	526	LEU
1	B	565	GLU
1	C	1	MSE
1	C	65	ARG
1	C	89	ARG
1	C	161	LYS
1	C	179	GLU
1	C	188	MSE
1	C	230	VAL
1	C	281	THR
1	C	300	VAL
1	C	327	MSE
1	C	330	SER
1	C	378	ASP
1	C	399	GLU
1	C	476	LEU
1	C	543	ASN
1	C	565	GLU
1	C	567	LEU
2	D	86	ILE
2	D	172	ASP
2	D	219	ILE
2	D	248	THR
2	D	249	ASP
2	D	257	LEU
2	D	280	ASN
2	D	353	ASP
2	D	371	GLN
2	D	387	VAL
2	D	389	LEU
2	D	396	ASP
2	D	403	LYS
2	D	432	GLU
2	E	7	THR
2	E	33	ARG
2	E	61	SER
2	E	102	GLU

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Mol	Chain	Res	Type
2	E	153	SER
2	E	158	LYS
2	E	267	VAL
2	E	302	PRO
2	E	330	THR
2	E	351	LEU
2	E	353	ASP
2	E	368	THR
2	E	443	LYS
2	F	33	ARG
2	F	61	SER
2	F	86	ILE
2	F	102	GLU
2	F	140	THR
2	F	153	SER
2	F	158	LYS
2	F	206	ARG
2	F	219	ILE
2	F	248	THR
2	F	265	ARG
2	F	335	LYS
2	F	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	189	GLN
1	A	294	ASN
1	A	404	ASN
1	A	485	ASN
1	A	520	ASN
1	B	2	GLN
1	B	50	GLN
1	B	101	ASN
1	B	147	HIS
1	B	264	ASN
1	B	294	ASN
1	B	424	HIS
1	B	450	GLN
1	B	518	GLN
1	B	520	ASN

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Mol	Chain	Res	Type
1	C	2	GLN
1	C	50	GLN
1	C	101	ASN
1	C	147	HIS
1	C	264	ASN
1	C	450	GLN
1	C	502	GLN
2	D	99	ASN
2	D	167	GLN
2	D	252	ASN
2	D	300	GLN
2	D	339	GLN
2	D	365	HIS
2	E	55	GLN
2	E	112	ASN
2	E	167	GLN
2	E	365	HIS
2	E	370	ASN
2	F	55	GLN
2	F	67	ASN
2	F	112	ASN
2	F	137	HIS
2	F	157	HIS
2	F	242	HIS
2	F	300	GLN
2	F	339	GLN
2	F	370	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	B	601	4	29,33,33	1.96	7 (24%)	31,52,52	1.82	8 (25%)
3	ANP	C	601	4	29,33,33	1.80	6 (20%)	31,52,52	1.87	8 (25%)

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	ANP	B	601	4	-	4/14/38/38	0/3/3/3
3	ANP	C	601	4	-	5/14/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	ANP	PG-N3B	4.91	1.76	1.63
3	B	601	ANP	PB-N3B	4.63	1.75	1.63
3	C	601	ANP	PG-N3B	4.25	1.74	1.63
3	C	601	ANP	PB-N3B	4.07	1.74	1.63
3	B	601	ANP	PG-O1G	3.58	1.51	1.46
3	B	601	ANP	PB-O1B	3.46	1.51	1.46
3	C	601	ANP	PB-O1B	3.09	1.51	1.46
3	C	601	ANP	PG-O1G	3.05	1.51	1.46
3	C	601	ANP	C5-C4	2.85	1.48	1.40
3	B	601	ANP	PB-O3A	2.77	1.62	1.59
3	B	601	ANP	C5-C4	2.73	1.48	1.40
3	B	601	ANP	C2-N3	2.02	1.35	1.32
3	C	601	ANP	PB-O3A	2.01	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	ANP	O1G-PG-N3B	-4.52	105.11	111.77
3	C	601	ANP	O2B-PB-O1B	4.49	119.33	109.92
3	C	601	ANP	O1G-PG-N3B	-4.20	105.58	111.77
3	C	601	ANP	O1B-PB-N3B	-4.06	105.79	111.77
3	B	601	ANP	O2B-PB-O1B	3.79	117.88	109.92
3	B	601	ANP	N3-C2-N1	-3.43	123.31	128.68
3	C	601	ANP	N3-C2-N1	-3.26	123.59	128.68
3	C	601	ANP	PB-O3A-PA	-3.18	121.42	132.62
3	B	601	ANP	O1B-PB-N3B	-3.06	107.26	111.77
3	C	601	ANP	O2G-PG-O3G	2.83	115.17	107.64
3	B	601	ANP	C3'-C2'-C1'	2.70	105.05	100.98
3	B	601	ANP	PB-O3A-PA	-2.46	123.97	132.62
3	B	601	ANP	O2G-PG-O3G	2.45	114.15	107.64
3	C	601	ANP	C4-C5-N7	-2.43	106.87	109.40
3	B	601	ANP	C4-C5-N7	-2.35	106.95	109.40
3	C	601	ANP	C2-N1-C6	2.08	122.32	118.75

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	ANP	PB-N3B-PG-O1G
3	B	601	ANP	PG-N3B-PB-O1B
3	B	601	ANP	PG-N3B-PB-O3A
3	C	601	ANP	PB-N3B-PG-O1G
3	C	601	ANP	PG-N3B-PB-O1B
3	C	601	ANP	PG-N3B-PB-O3A
3	C	601	ANP	O4'-C4'-C5'-O5'
3	C	601	ANP	C3'-C4'-C5'-O5'
3	B	601	ANP	O4'-C4'-C5'-O5'

There are no ring outliers.

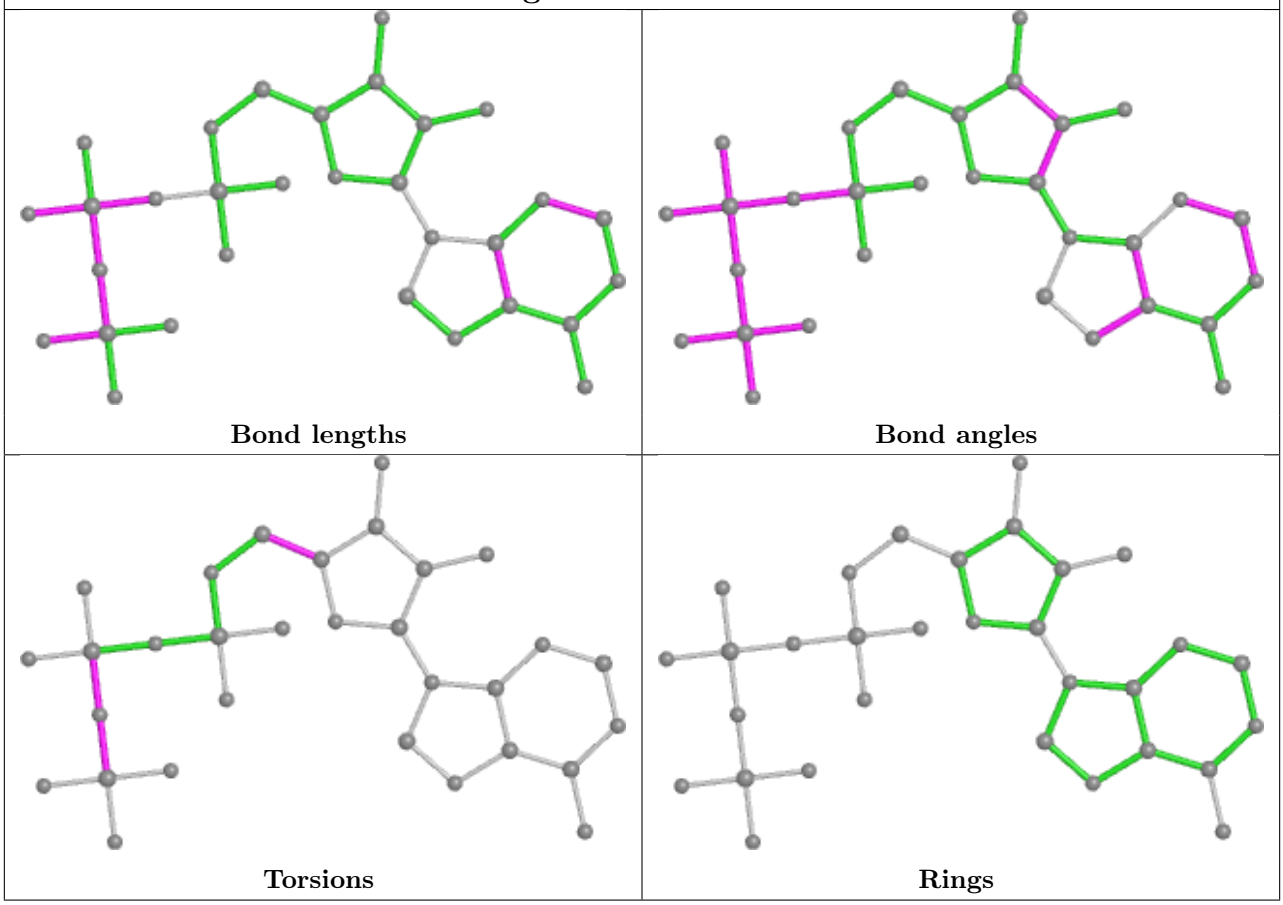
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	ANP	1	0

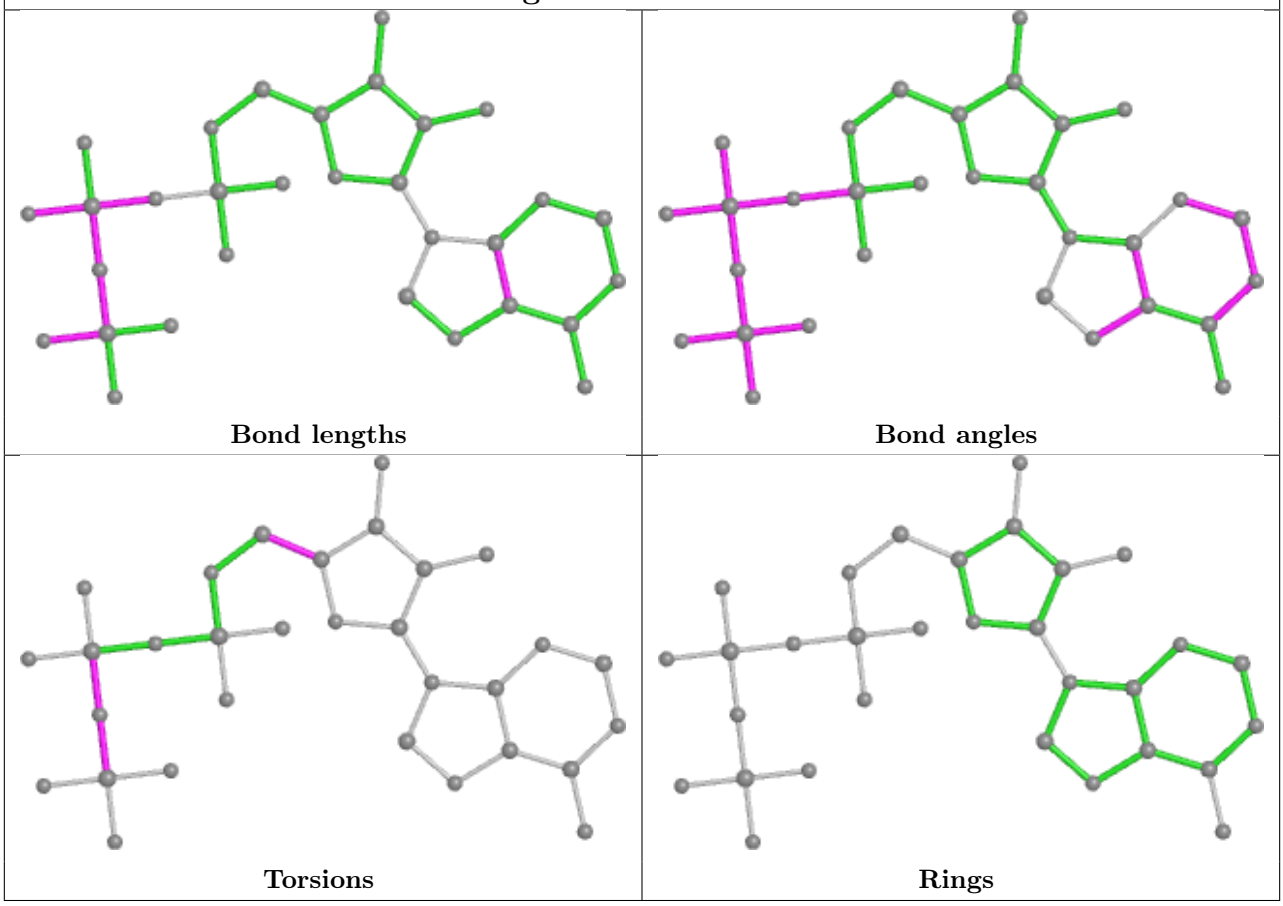
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ANP B 601



Ligand ANP C 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	563/600 (93%)	0.28	21 (3%)	41	40	51, 82, 151, 165	0
1	B	563/600 (93%)	0.42	39 (6%)	16	18	61, 105, 153, 204	0
1	C	561/600 (93%)	-0.02	2 (0%)	92	92	39, 71, 123, 153	0
2	D	433/465 (93%)	0.18	13 (3%)	50	49	47, 77, 156, 193	0
2	E	437/465 (93%)	0.25	13 (2%)	50	49	58, 102, 168, 193	0
2	F	437/465 (93%)	0.14	5 (1%)	80	79	47, 84, 141, 173	0
All	All	2994/3195 (93%)	0.21	93 (3%)	49	48	39, 87, 150, 204	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	LEU	6.0
2	D	392	SER	5.9
2	F	389	LEU	5.0
2	D	388	VAL	4.7
1	A	577	ILE	4.3
2	D	390	GLY	4.2
1	B	136	ILE	4.2
2	D	393	ALA	4.1
1	A	538	LEU	3.9
1	B	162	ILE	3.9
1	B	174	CYS	3.6
2	E	386	ALA	3.6
1	B	477	VAL	3.5
2	E	393	ALA	3.3
1	B	175	VAL	3.3
1	A	570	ILE	3.3
1	B	173	ILE	3.2
1	B	542	PHE	3.2
2	E	392	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	478	GLY	3.2
1	B	536	LEU	3.1
1	B	525	ILE	3.0
2	D	387	VAL	3.0
1	B	541	TYR	3.0
2	E	389	LEU	3.0
1	B	185	LEU	2.9
2	F	437	LEU	2.9
1	A	579	GLU	2.9
1	B	166	SER	2.9
2	D	434	LEU	2.9
1	B	125	GLU	2.9
2	E	442	LEU	2.8
2	E	400	ILE	2.7
1	B	577	ILE	2.7
2	E	401	TYR	2.7
1	A	583	LEU	2.7
1	B	0	GLY	2.7
1	A	479	ILE	2.7
1	A	576	GLU	2.7
1	B	119	TRP	2.7
1	A	581	ILE	2.7
2	F	175	ASP	2.6
1	B	129	GLU	2.6
1	A	427	SER	2.6
1	B	156	LYS	2.6
1	A	475	ARG	2.6
1	B	538	LEU	2.6
1	B	161	LYS	2.6
2	E	391	GLU	2.6
1	B	526	LEU	2.5
1	B	500	TYR	2.5
1	A	584	ILE	2.5
1	A	501	LEU	2.5
2	F	393	ALA	2.5
1	B	138	TYR	2.5
2	D	394	LEU	2.5
1	B	124	ILE	2.5
2	E	384	GLU	2.5
1	A	525	ILE	2.5
1	A	537	SER	2.4
2	D	391	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	182	LEU	2.4
1	B	485	ASN	2.4
2	E	42	GLY	2.3
1	A	573	ILE	2.3
1	C	538	LEU	2.3
1	B	163	GLU	2.3
1	B	120	PHE	2.3
1	B	481	SER	2.3
2	E	382	ALA	2.3
2	D	435	ALA	2.2
1	B	176	ILE	2.2
1	B	165	GLY	2.2
1	B	118	TRP	2.2
1	B	160	GLN	2.2
1	A	557	SER	2.2
1	A	548	GLY	2.2
1	B	-1	SER	2.1
2	E	439	ARG	2.1
1	B	518	GLN	2.1
1	B	501	LEU	2.1
1	B	376	GLY	2.1
2	D	411	GLU	2.1
1	B	475	ARG	2.1
2	F	70	VAL	2.1
2	D	437	LEU	2.1
1	A	424	HIS	2.1
1	C	528	PHE	2.0
2	E	127	PHE	2.0
1	A	582	GLN	2.0
1	B	486	ASP	2.0
2	D	386	ALA	2.0
1	A	551	ALA	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)

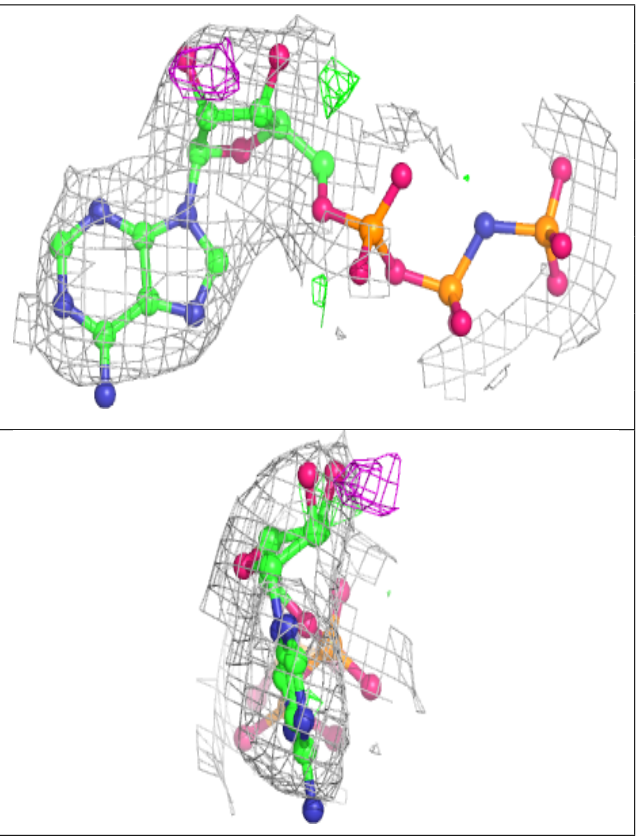
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	602	1/1	0.91	0.23	62,62,62,62	0
3	ANP	B	601	31/31	0.94	0.18	64,67,72,73	0
3	ANP	C	601	31/31	0.96	0.20	53,54,57,58	0
4	MG	C	602	1/1	0.97	0.30	46,46,46,46	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.

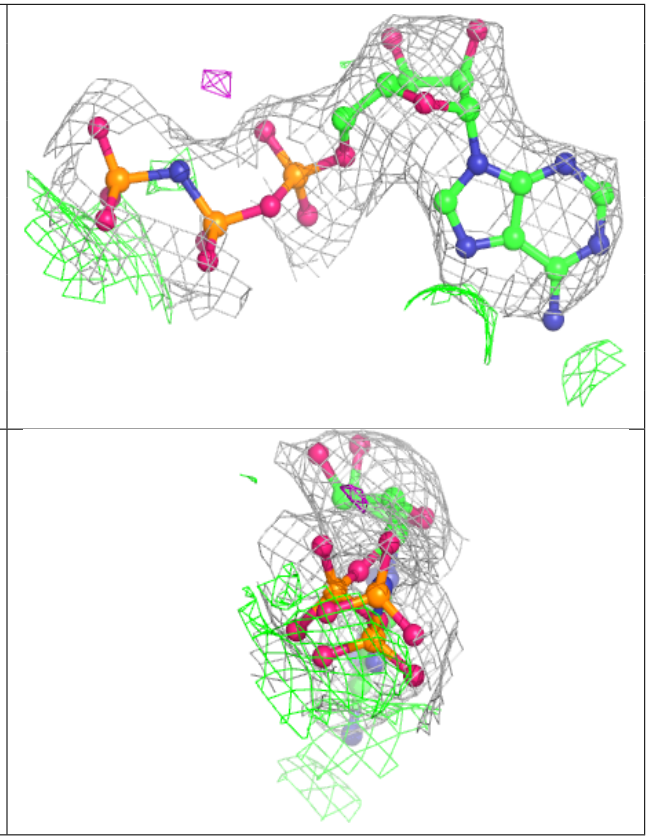
Electron density around ANP B 601:

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 ANP C 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.