



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:35 PM UTC

PDB ID : 3VR6 / pdb_00003vr6
Title : Crystal structure of AMP-PNP bound Enterococcus hirae V1-ATPase [bV1]
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 : 2.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

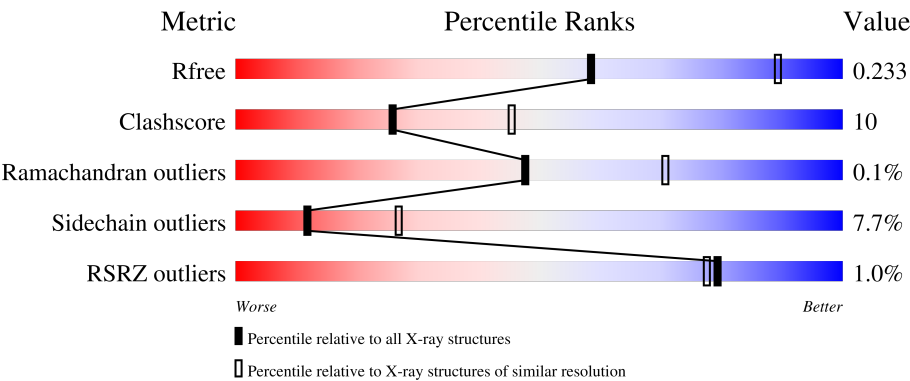
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	600	74%22%..
1	B	600	78%19%..
1	C	600	71%23%..
2	D	465	2% 74%21%..

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Mol	Chain	Length	Quality of chain
2	E	465	78% 17% • •
2	F	465	76% 20% • •
3	G	217	8% 60% 19% • 19%
4	H	115	2% 66% 17% 5% 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27061 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
1	A	587	Total	C	N	O	S	0	0	0
			4566	2868	767	905	26			
1	B	592	Total	C	N	O	S	0	0	0
			4583	2876	770	911	26			
1	C	582	Total	C	N	O	S	0	0	0
			4536	2851	761	898	26			

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
2	D	451	Total	C	N	O	S	0	0	0
			3509	2225	601	669	14			
2	E	452	Total	C	N	O	S	0	0	0
			3549	2250	607	678	14			
2	F	455	Total	C	N	O	S	0	0	0
			3567	2261	610	681	15			

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 a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	176	Total	C	N	O	S	0	0	0
			1412	890	250	262	10			

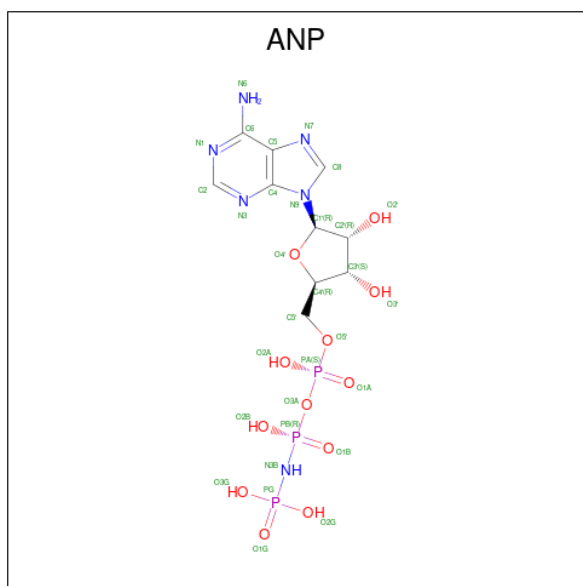
- Molecule 4 is a protein called V-type sodium ATPase subunit G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	102	Total	C	N	O	S	0	0	0
			775	494	127	152	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	expression tag	UNP P43455
H	105	GLY	-	expression tag	UNP P43455
H	106	PRO	-	expression tag	UNP P43455
H	107	SER	-	expression tag	UNP P43455
H	108	SER	-	expression tag	UNP P43455
H	109	GLY	-	expression tag	UNP P43455
H	110	GLU	-	expression tag	UNP P43455
H	111	ASN	-	expression tag	UNP P43455
H	112	LEU	-	expression tag	UNP P43455
H	113	TYR	-	expression tag	UNP P43455
H	114	PHE	-	expression tag	UNP P43455
H	115	GLN	-	expression tag	UNP P43455

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

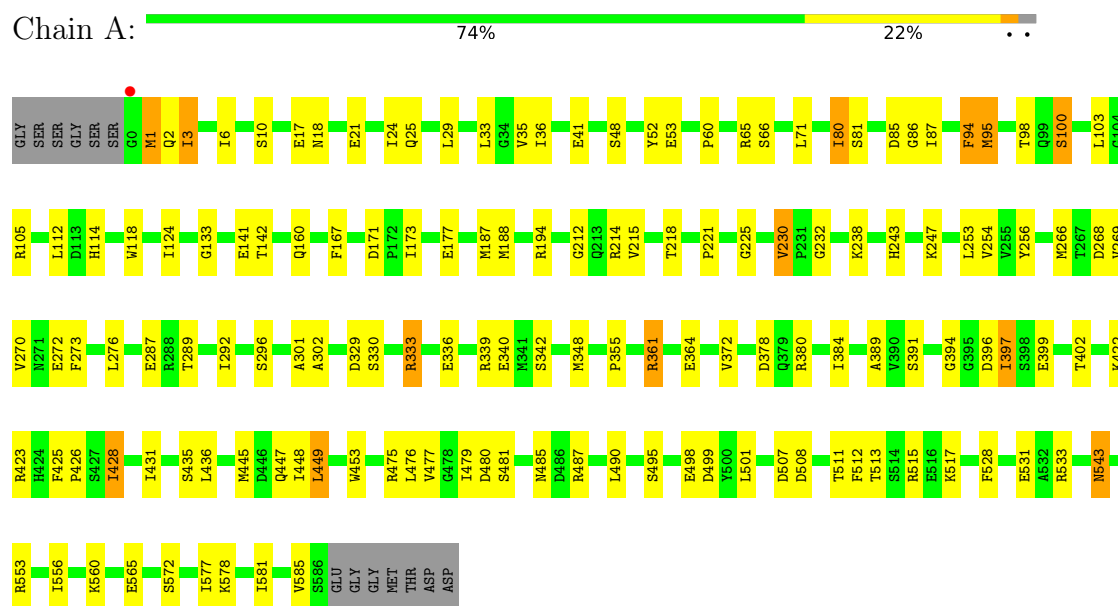
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	78	Total 78	O 78	0	0
7	B	115	Total 115	O 115	0	0
7	C	91	Total 91	O 91	0	0
7	D	46	Total 46	O 46	0	0
7	E	83	Total 83	O 83	0	0
7	F	71	Total 71	O 71	0	0
7	G	11	Total 11	O 11	0	0
7	H	5	Total 5	O 5	0	0

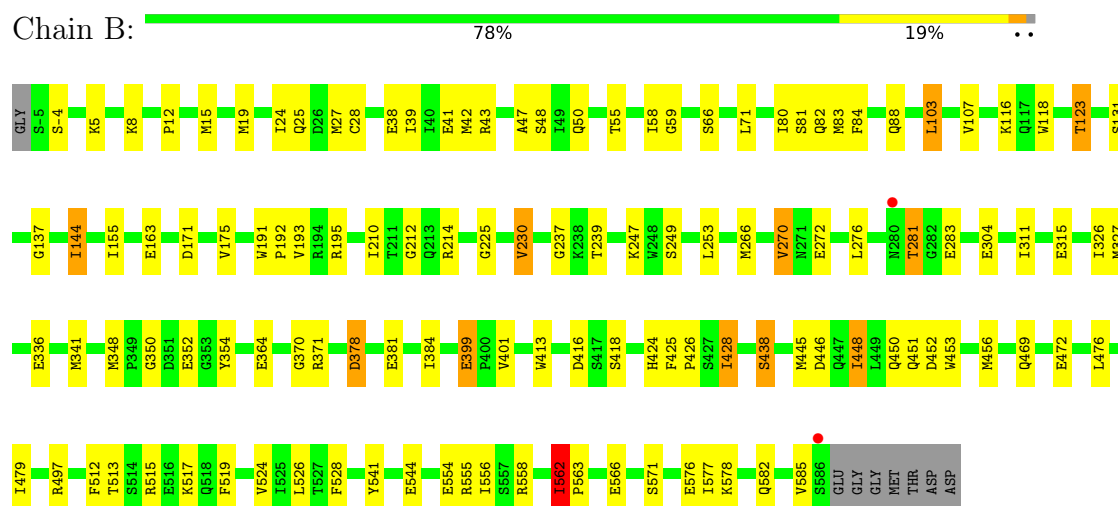
3 Residue-property plots

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.

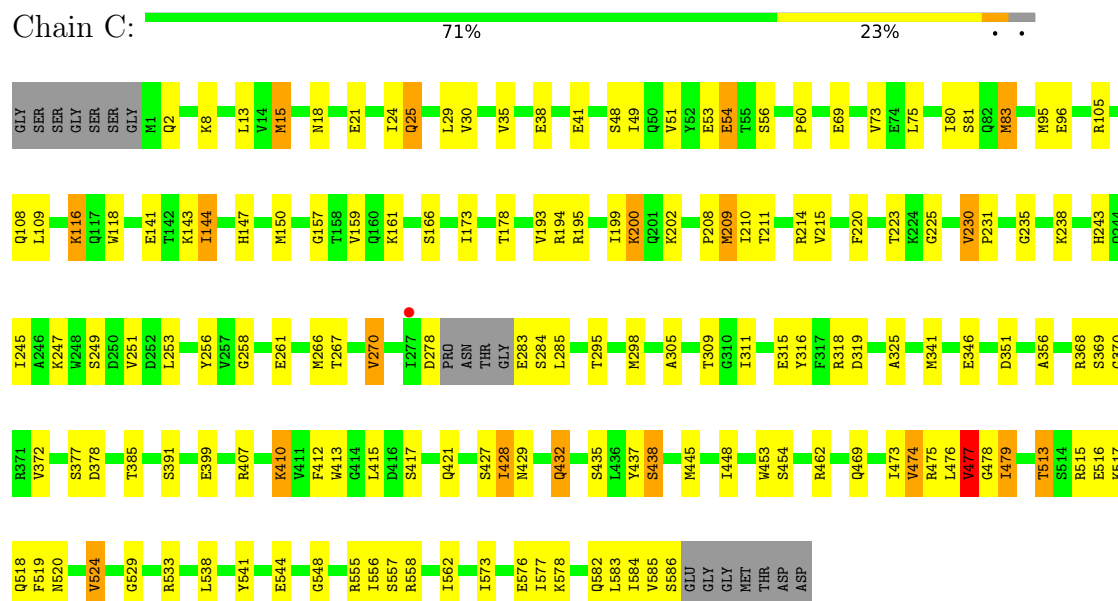
- Molecule 1: V-type sodium ATPase catalytic subunit A



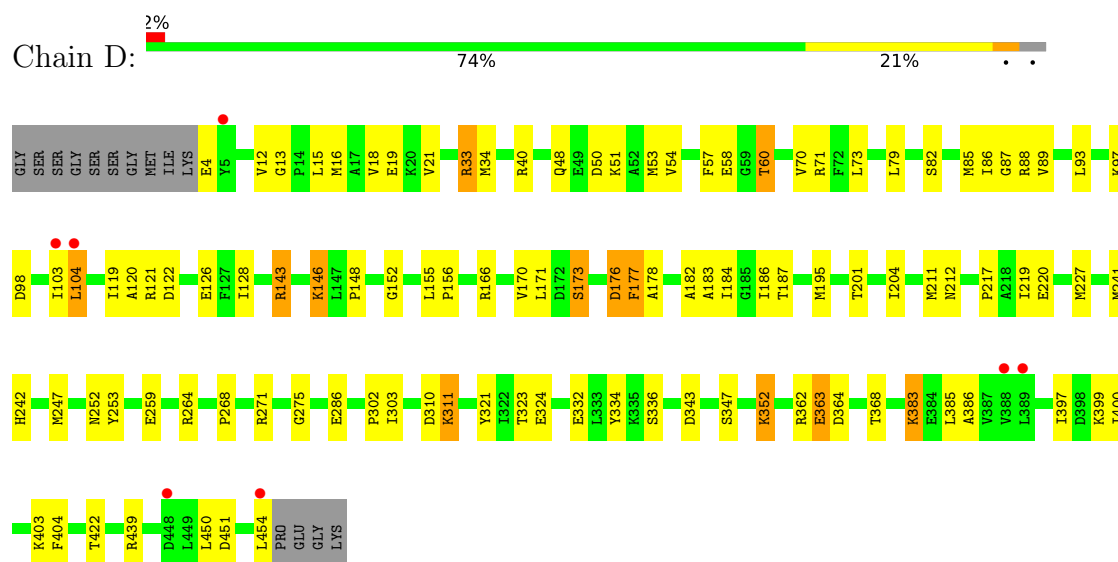
- Molecule 1: V-type sodium ATPase catalytic subunit A



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



• Molecule 2: V-type sodium ATPase subunit B

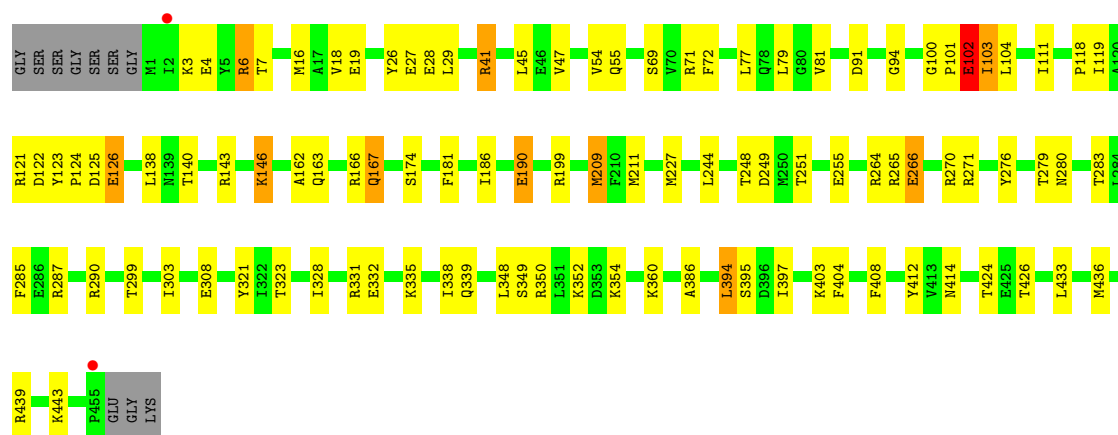


• Molecule 2: V-type sodium ATPase subunit B



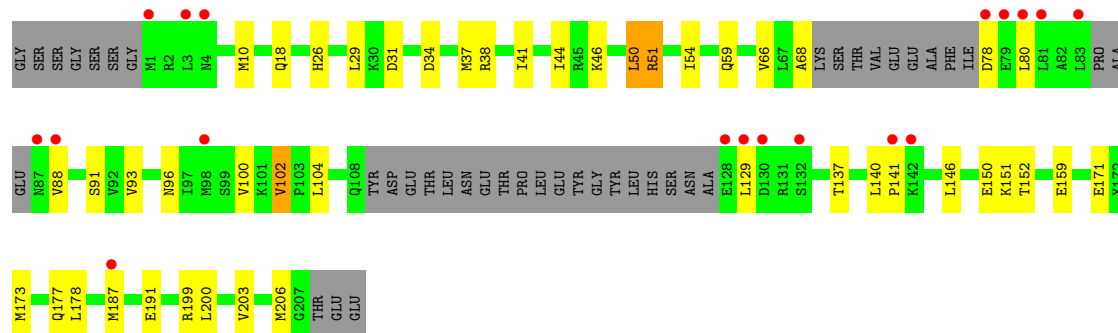
• Molecule 2: V-type sodium ATPase subunit B

Chain F:  76% 20% ..



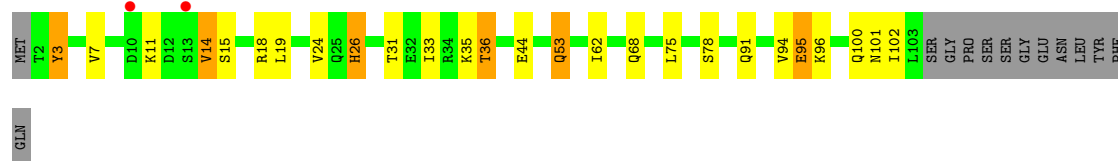
• Molecule 3: V-type sodium ATPase subunit D

Chain G:  8% 60% 19% . 19%



• Molecule 4: V-type sodium ATPase subunit G

Chain H:  2% 66% 17% 5% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.15Å 127.42Å 225.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.68 48.58 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.58-2.68) 95.0 (48.58-2.68)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.182 , 0.246 (Not available) , 0.233	Depositor DCC
R_{free} test set	4864 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27061	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.66	0/4642	0.92	3/6280 (0.0%)
1	B	0.71	0/4659	0.96	8/6304 (0.1%)
1	C	0.70	0/4610	0.93	8/6234 (0.1%)
2	D	0.66	0/3570	0.91	1/4830 (0.0%)
2	E	0.71	0/3612	0.92	4/4884 (0.1%)
2	F	0.72	0/3630	0.91	4/4908 (0.1%)
3	G	0.60	0/1420	0.92	0/1899
4	H	0.58	0/787	0.91	1/1068 (0.1%)
All	All	0.68	0/26930	0.93	29/36407 (0.1%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	399	GLU	CA-C-N	7.31	127.17	119.05
1	C	399	GLU	C-N-CA	7.31	127.17	119.05
1	B	348	MET	CA-C-N	6.34	126.31	119.78
1	B	348	MET	C-N-CA	6.34	126.31	119.78
2	E	289	GLY	N-CA-C	6.23	119.23	110.38
1	B	59	GLY	CA-C-N	6.21	126.18	119.78
1	B	59	GLY	C-N-CA	6.21	126.18	119.78
1	A	431	ILE	N-CA-C	-5.98	106.67	111.81
1	C	562	ILE	CA-C-N	5.52	125.47	119.78
1	C	562	ILE	C-N-CA	5.52	125.47	119.78
1	B	193	VAL	N-CA-C	5.52	117.94	111.05
2	E	352	LYS	N-CA-C	5.40	118.67	111.75
1	C	157	GLY	N-CA-C	5.40	118.14	110.74
2	E	155	LEU	CA-C-N	-5.39	116.21	121.65
2	E	155	LEU	C-N-CA	-5.39	116.21	121.65
1	A	399	GLU	CA-C-N	5.36	124.55	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	GLU	C-N-CA	5.36	124.55	118.97
1	B	562	ILE	CA-C-N	5.23	125.17	119.78
1	B	562	ILE	C-N-CA	5.23	125.17	119.78
1	B	438	SER	N-CA-C	5.21	117.36	111.11
4	H	26	HIS	N-CA-C	5.21	119.14	112.26
2	F	140	THR	N-CA-C	5.18	117.85	110.24
1	C	270	VAL	CB-CA-C	-5.16	104.16	112.16
2	F	102	GLU	N-CA-C	5.07	121.60	110.80
2	F	100	GLY	CA-C-N	5.06	126.16	119.84
2	F	100	GLY	C-N-CA	5.06	126.16	119.84
2	D	126	GLU	N-CA-C	5.04	118.43	109.96
1	C	220	PHE	CA-C-N	5.04	124.94	119.85
1	C	220	PHE	C-N-CA	5.04	124.94	119.85

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	4566	0	4531	103	0
1	B	4583	0	4534	77	0
1	C	4536	0	4503	100	0
2	D	3509	0	3510	69	0
2	E	3549	0	3570	64	0
2	F	3567	0	3586	69	0
3	G	1412	0	1478	32	0
4	H	775	0	772	20	0
5	B	31	0	13	3	0
5	C	31	0	13	3	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	78	0	0	8	0
7	B	115	0	0	13	0
7	C	91	0	0	13	0
7	D	46	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	83	0	0	4	0
7	F	71	0	0	3	0
7	G	11	0	0	2	0
7	H	5	0	0	0	0
All	All	27061	0	26510	505	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 (505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:102:GLU:CB	2:F:103:ILE:HA	1.54	1.28
2:F:102:GLU:HB3	2:F:103:ILE:CA	1.66	1.25
2:E:221:ARG:HG3	2:E:221:ARG:HH11	0.98	1.15
1:A:98:THR:HG22	1:A:100:SER:HB3	1.32	1.06
2:E:41:ARG:HG3	2:E:41:ARG:HH11	1.14	1.04
1:A:98:THR:CG2	1:A:100:SER:HB3	1.88	1.04
1:A:160:GLN:HB3	7:A:711:HOH:O	1.61	1.01
1:A:95:MET:HE1	2:D:120:ALA:HB2	1.41	1.00
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.25	0.99
2:D:34:MET:HE1	2:D:40:ARG:NE	1.79	0.95
1:A:1:MET:HB3	1:A:65:ARG:HH21	1.29	0.95
1:A:94:PHE:O	1:A:98:THR:HB	1.67	0.93
4:H:100:GLN:CB	4:H:101:ASN:HA	1.98	0.92
2:D:34:MET:HE1	2:D:40:ARG:CZ	2.00	0.91
2:F:3:LYS:HG3	7:F:531:HOH:O	1.70	0.90
2:D:362:ARG:HD2	2:D:364:ASP:OD1	1.71	0.90
3:G:51:ARG:NH2	4:H:75:LEU:O	2.05	0.89
1:C:13:LEU:HD13	1:C:341:MET:HE1	1.53	0.88
2:E:221:ARG:HG3	2:E:221:ARG:NH1	1.76	0.88
2:F:181:PHE:CD2	2:F:211:MET:HE1	2.08	0.88
1:A:95:MET:CE	2:D:120:ALA:HB2	2.03	0.88
1:C:267:THR:HG22	2:F:118:PRO:O	1.71	0.88
2:D:146:LYS:NZ	2:D:286:GLU:OE1	2.07	0.88
1:B:237:GLY:HA2	7:B:701:HOH:O	1.73	0.87
1:B:27:MET:HE1	1:B:38:GLU:HB2	1.54	0.86
1:B:27:MET:HE3	1:B:71:LEU:HB2	1.60	0.84
1:A:25:GLN:HG3	2:E:61:SER:HB2	1.60	0.83
2:D:79:LEU:HB2	2:D:227:MET:HE3	1.61	0.82
4:H:91:GLN:HE22	4:H:101:ASN:ND2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLU:OE2	7:B:779:HOH:O	1.99	0.80
1:C:150:MET:SD	7:C:746:HOH:O	2.38	0.80
2:D:146:LYS:HE3	2:D:324:GLU:OE2	1.82	0.79
1:A:348:MET:HE2	2:E:268:PRO:HG3	1.64	0.78
1:B:27:MET:CE	1:B:38:GLU:HB2	2.12	0.78
2:D:93:LEU:HG	2:D:220:GLU:HG2	1.68	0.76
1:C:267:THR:HG21	2:F:121:ARG:HB2	1.68	0.76
2:D:50:ASP:HA	7:D:534:HOH:O	1.86	0.76
1:C:25:GLN:HG2	7:D:539:HOH:O	1.86	0.76
1:C:41:GLU:HB2	1:C:48:SER:HB2	1.68	0.76
1:C:445:MET:HE1	1:C:515:ARG:HD2	1.68	0.75
3:G:51:ARG:NH1	3:G:150:GLU:OE1	2.19	0.75
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.67	0.75
1:A:160:GLN:CB	7:A:711:HOH:O	2.26	0.74
1:C:200:LYS:HD2	7:C:740:HOH:O	1.86	0.74
2:E:41:ARG:HG3	2:E:41:ARG:NH1	1.93	0.74
2:F:181:PHE:HD2	2:F:211:MET:HE1	1.50	0.73
5:B:601:ANP:O2A	7:B:701:HOH:O	2.05	0.73
1:C:295:THR:HG23	1:C:298:MET:HE3	1.71	0.73
1:C:116:LYS:HE2	1:C:118:TRP:CZ2	2.24	0.72
1:A:215:VAL:HG23	1:A:501:LEU:HD22	1.72	0.72
1:B:237:GLY:C	7:B:701:HOH:O	2.33	0.72
1:B:28:CYS:HB3	1:B:66:SER:HA	1.71	0.72
2:F:186:ILE:HD12	2:F:190:GLU:HG2	1.70	0.72
4:H:11:LYS:HA	4:H:26:HIS:CE1	2.26	0.71
1:A:333:ARG:HH11	1:A:333:ARG:CG	2.02	0.71
1:B:554:GLU:O	1:B:558:ARG:HG3	1.91	0.71
2:F:79:LEU:HD13	2:F:227:MET:CE	2.19	0.71
2:D:439:ARG:NH1	2:D:451:ASP:OD1	2.20	0.71
2:F:102:GLU:HB3	2:F:103:ILE:HA	0.76	0.71
1:C:283:GLU:HG3	7:C:765:HOH:O	1.91	0.70
3:G:151:LYS:HE2	4:H:68:GLN:O	1.89	0.70
2:E:362:ARG:HD2	2:E:364:ASP:OD1	1.90	0.70
1:B:451:GLN:HG2	1:B:519:PHE:CE1	2.27	0.70
1:C:478:GLY:C	1:C:479:ILE:HG13	2.17	0.70
2:F:181:PHE:HB3	2:F:209:MET:HG3	1.73	0.70
2:F:338:ILE:HG23	2:F:414:ASN:HB2	1.73	0.70
2:D:166:ARG:HD2	2:D:201:THR:HG21	1.73	0.70
1:C:209:MET:HE3	1:C:385:THR:HG21	1.74	0.69
1:A:477:VAL:HG23	1:A:481:SER:HB3	1.74	0.69
2:D:34:MET:CE	2:D:40:ARG:NE	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:THR:CG2	2:F:118:PRO:O	2.40	0.69
3:G:173:MET:O	3:G:177:GLN:HG3	1.93	0.69
1:B:445:MET:HE1	1:B:515:ARG:CZ	2.23	0.69
1:A:2:GLN:HG3	1:A:21:GLU:HB2	1.74	0.68
2:F:209:MET:HG2	2:F:211:MET:HE3	1.73	0.68
2:D:18:VAL:HG11	2:D:70:VAL:HG11	1.75	0.68
4:H:100:GLN:CB	4:H:101:ASN:CA	2.72	0.68
1:A:142:THR:HB	1:A:287:GLU:OE1	1.93	0.68
1:A:333:ARG:NH2	2:D:321:TYR:O	2.25	0.68
1:C:578:LYS:O	1:C:582:GLN:HB2	1.94	0.68
1:A:133:GLY:O	1:A:380:ARG:NH2	2.26	0.67
1:A:577:ILE:O	1:A:581:ILE:HG12	1.94	0.67
2:D:146:LYS:HE3	2:D:324:GLU:CD	2.18	0.67
2:F:181:PHE:CE2	2:F:211:MET:HE1	2.28	0.67
2:E:362:ARG:NH1	2:E:364:ASP:OD2	2.28	0.67
4:H:15:SER:O	4:H:18:ARG:HB2	1.94	0.67
1:A:2:GLN:HB3	1:A:66:SER:HB3	1.77	0.66
1:A:378:ASP:HB2	1:A:380:ARG:NH1	2.09	0.66
2:E:229:LEU:HD13	2:E:287:ARG:HG3	1.77	0.66
2:D:183:ALA:HB1	2:D:186:ILE:HG12	1.77	0.66
1:A:80:ILE:O	1:A:81:SER:HB2	1.95	0.65
1:B:451:GLN:HG2	1:B:519:PHE:CZ	2.32	0.65
1:A:426:PRO:HB2	1:A:428:ILE:CD1	2.26	0.65
2:E:41:ARG:HH11	2:E:41:ARG:CG	2.00	0.65
1:A:340:GLU:HG3	2:D:275:GLY:O	1.97	0.65
1:B:578:LYS:O	1:B:582:GLN:HG3	1.96	0.65
1:A:342:SER:HB2	1:A:355:PRO:HG3	1.78	0.64
1:B:171:ASP:OD2	7:B:726:HOH:O	2.14	0.64
2:F:102:GLU:CB	2:F:103:ILE:CA	2.41	0.64
1:B:116:LYS:HD3	1:B:118:TRP:CE2	2.33	0.64
1:C:60:PRO:HD3	2:F:47:VAL:HG13	1.80	0.64
2:F:126:GLU:OE2	2:F:143:ARG:NH1	2.31	0.64
1:B:452:ASP:O	1:B:456:MET:HG3	1.98	0.63
2:D:87:GLY:HA2	2:D:204:ILE:O	1.98	0.63
1:A:98:THR:HG22	1:A:100:SER:CB	2.20	0.63
2:E:146:LYS:HE3	2:E:324:GLU:OE2	1.97	0.63
1:A:397:ILE:HD12	1:A:402:THR:HG21	1.81	0.63
1:B:237:GLY:CA	7:B:701:HOH:O	2.38	0.63
2:E:122:ASP:HB3	2:E:290:ARG:HB2	1.80	0.63
2:F:163:GLN:O	2:F:167:GLN:HG3	1.98	0.63
2:E:186:ILE:HB	2:E:190:GLU:OE1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:GLY:HA3	2:F:227:MET:HE2	1.81	0.63
2:F:339:GLN:OE1	7:F:554:HOH:O	2.15	0.63
1:A:543:ASN:OD1	1:A:543:ASN:N	2.31	0.63
1:B:123:THR:HB	1:B:137:GLY:HA2	1.81	0.63
1:C:41:GLU:OE2	2:D:12:VAL:HG13	1.99	0.63
2:F:79:LEU:HD13	2:F:227:MET:HE1	1.81	0.63
2:F:94:GLY:HA3	2:F:227:MET:CE	2.29	0.63
2:F:29:LEU:HD13	2:F:77:LEU:HD13	1.81	0.63
1:C:410:LYS:HG3	1:C:437:TYR:OH	1.98	0.62
4:H:33:ILE:O	4:H:36:THR:HG22	1.98	0.62
2:E:212:ASN:OD1	2:E:221:ARG:HG2	1.99	0.62
1:C:150:MET:HE1	1:C:319:ASP:HB3	1.82	0.62
2:F:181:PHE:HD2	2:F:211:MET:CE	2.13	0.62
3:G:199:ARG:O	3:G:203:VAL:HG23	2.00	0.61
1:A:487:ARG:HD2	7:A:728:HOH:O	1.99	0.61
1:C:477:VAL:HG21	3:G:29:LEU:HD21	1.83	0.61
2:D:82:SER:O	2:D:85:MET:HG2	2.00	0.61
1:A:1:MET:HB3	1:A:65:ARG:NH2	2.09	0.61
1:C:235:GLY:H	5:C:601:ANP:HNB1	1.48	0.61
2:F:6:ARG:HG3	2:F:69:SER:HB3	1.82	0.61
1:A:141:GLU:HG2	1:A:142:THR:HG23	1.82	0.61
1:A:581:ILE:O	1:A:585:VAL:HG23	2.01	0.61
2:F:28:GLU:OE2	2:F:72:PHE:HB3	2.01	0.61
2:F:103:ILE:HD13	2:F:103:ILE:H	1.66	0.60
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.36	0.60
2:E:163:GLN:HE21	2:E:167:GLN:HE22	1.49	0.60
1:C:80:ILE:O	1:C:81:SER:HB2	2.01	0.60
2:E:40:ARG:HD3	2:E:58:GLU:HB2	1.83	0.60
1:C:193:VAL:O	1:C:368:ARG:NH2	2.28	0.60
2:F:79:LEU:HD13	2:F:227:MET:HE3	1.82	0.59
2:D:176:ASP:O	7:D:508:HOH:O	2.15	0.59
2:E:362:ARG:HB3	2:E:364:ASP:OD1	2.03	0.59
1:A:426:PRO:HB2	1:A:428:ILE:HD13	1.84	0.59
1:A:336:GLU:OE1	1:A:339:ARG:NH1	2.35	0.59
2:E:221:ARG:HH11	2:E:221:ARG:CG	1.92	0.59
2:E:397:ILE:HA	2:E:400:ILE:HD12	1.85	0.59
1:A:266:MET:HE3	1:A:269:VAL:HB	1.85	0.59
1:A:194:ARG:NH2	1:A:364:GLU:OE1	2.36	0.58
1:C:513:THR:HG23	1:C:517:LYS:HD2	1.84	0.58
1:B:445:MET:HE1	1:B:515:ARG:NE	2.19	0.58
2:D:352:LYS:HE2	7:D:506:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLN:CG	1:A:21:GLU:HB2	2.33	0.58
1:A:268:ASP:O	1:A:272:GLU:HG3	2.04	0.58
1:C:278:ASP:HB3	7:C:750:HOH:O	2.02	0.58
2:F:94:GLY:CA	2:F:227:MET:HE2	2.33	0.58
3:G:102:VAL:HG21	3:G:152:THR:HG23	1.85	0.58
2:E:125:ASP:O	2:E:126:GLU:HB2	2.02	0.58
2:D:16:MET:HB3	2:D:54:VAL:HG23	1.86	0.57
3:G:102:VAL:CG2	3:G:152:THR:HG23	2.35	0.57
1:C:558:ARG:HH11	1:C:558:ARG:HG2	1.68	0.57
2:D:148:PRO:HA	2:D:302:PRO:HD2	1.87	0.57
2:D:40:ARG:HD3	2:D:58:GLU:HB2	1.85	0.57
1:C:24:ILE:O	1:C:25:GLN:HB2	2.04	0.57
3:G:51:ARG:NH1	3:G:150:GLU:CD	2.63	0.57
1:A:296:SER:OG	2:D:286:GLU:OE2	2.22	0.57
1:C:211:THR:HG22	1:C:245:ILE:HG12	1.87	0.57
1:C:410:LYS:HG3	1:C:437:TYR:CZ	2.39	0.57
1:C:141:GLU:OE2	1:C:147:HIS:ND1	2.29	0.56
2:F:146:LYS:HD3	2:F:285:PHE:O	2.05	0.56
1:B:453:TRP:HZ3	1:B:519:PHE:HA	1.70	0.56
2:E:9:LYS:HB2	2:E:19:GLU:HG2	1.86	0.56
2:E:93:LEU:HA	2:E:227:MET:HE3	1.88	0.56
1:B:247:LYS:NZ	1:B:272:GLU:OE1	2.37	0.56
4:H:91:GLN:NE2	4:H:101:ASN:ND2	2.52	0.56
2:E:40:ARG:NH1	2:E:59:GLY:O	2.39	0.56
3:G:151:LYS:CE	4:H:68:GLN:O	2.53	0.56
2:E:221:ARG:NH1	2:E:221:ARG:CG	2.60	0.56
1:B:24:ILE:O	1:B:25:GLN:HB2	2.06	0.56
1:C:261:GLU:OE1	7:C:741:HOH:O	2.18	0.56
1:C:305:ALA:O	1:C:309:THR:HG23	2.06	0.55
1:B:12:PRO:HB2	1:B:341:MET:HE1	1.87	0.55
1:B:83:MET:CE	1:B:266:MET:HB3	2.36	0.55
1:C:108:GLN:NE2	7:C:714:HOH:O	2.39	0.55
1:C:161:LYS:HE3	7:C:767:HOH:O	2.06	0.55
1:C:582:GLN:O	1:C:585:VAL:HG22	2.06	0.55
2:F:386:ALA:HB2	2:F:394:LEU:HD22	1.87	0.55
1:A:495:SER:OG	1:A:499:ASP:OD2	2.23	0.55
1:C:208:PRO:HA	1:C:223:THR:HA	1.88	0.55
4:H:91:GLN:HA	4:H:91:GLN:OE1	2.07	0.55
1:B:225:GLY:O	1:B:370:GLY:HA2	2.07	0.55
1:A:247:LYS:HD3	1:A:276:LEU:HD22	1.88	0.55
2:F:249:ASP:C	2:F:249:ASP:OD1	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:352:LYS:CE	7:D:506:HOH:O	2.54	0.54
2:F:45:LEU:HD13	2:F:264:ARG:HD2	1.89	0.54
2:F:433:LEU:O	2:F:436:MET:HB2	2.07	0.54
3:G:37:MET:O	3:G:41:ILE:HG13	2.06	0.54
2:E:378:GLN:OE1	7:E:522:HOH:O	2.18	0.54
1:A:95:MET:HE1	2:D:120:ALA:CB	2.26	0.54
1:A:112:LEU:O	1:A:114:HIS:HD2	1.91	0.54
2:E:438:PRO:HB2	2:E:440:THR:HG22	1.89	0.54
1:A:531:GLU:HG3	1:A:578:LYS:HG2	1.88	0.54
2:E:87:GLY:HA2	2:E:204:ILE:O	2.08	0.54
1:C:407:ARG:NH1	7:C:713:HOH:O	2.40	0.54
2:D:156:PRO:HG3	2:D:334:TYR:CE1	2.43	0.54
2:E:229:LEU:O	2:E:233:GLU:HG3	2.09	0.54
2:E:397:ILE:HD12	2:E:397:ILE:H	1.72	0.54
1:A:378:ASP:CB	1:A:380:ARG:NH1	2.71	0.53
3:G:68:ALA:HB1	3:G:129:LEU:HG	1.90	0.53
1:A:333:ARG:HG2	1:A:333:ARG:NH1	2.05	0.53
2:E:103:ILE:O	2:E:105:PRO:HD3	2.09	0.53
4:H:11:LYS:HA	4:H:26:HIS:HE1	1.71	0.53
4:H:91:GLN:HE22	4:H:101:ASN:HD22	1.56	0.53
2:D:13:GLY:O	2:D:60:THR:HG21	2.09	0.53
5:C:601:ANP:HNB1	2:F:350:ARG:HH12	1.57	0.53
2:D:363:GLU:HG2	7:D:529:HOH:O	2.07	0.53
1:C:558:ARG:HG2	1:C:558:ARG:NH1	2.23	0.53
2:E:57:PHE:HA	2:E:219:ILE:HD12	1.91	0.53
2:F:45:LEU:HD11	2:F:55:GLN:HB3	1.89	0.53
1:A:225:GLY:HA2	1:A:384:ILE:O	2.09	0.52
1:A:425:PHE:HA	1:A:426:PRO:C	2.33	0.52
1:B:8:LYS:HE3	2:E:48:GLN:NE2	2.24	0.52
1:C:51:VAL:HG12	1:C:53:GLU:H	1.73	0.52
2:F:126:GLU:OE1	2:F:290:ARG:NE	2.43	0.52
1:B:27:MET:CE	1:B:38:GLU:CB	2.87	0.52
1:B:272:GLU:O	1:B:276:LEU:HD13	2.09	0.52
4:H:14:VAL:CG1	4:H:24:VAL:HG13	2.40	0.52
1:C:247:LYS:HA	1:C:285:LEU:HD21	1.92	0.52
1:C:256:TYR:CD2	1:C:266:MET:HE1	2.45	0.52
2:F:26:TYR:O	2:F:27:GLU:HB2	2.08	0.52
2:F:186:ILE:CD1	2:F:190:GLU:HG2	2.40	0.52
1:A:528:PHE:HA	1:A:577:ILE:HG21	1.92	0.52
1:B:27:MET:SD	1:B:71:LEU:HD13	2.50	0.52
1:C:210:ILE:O	1:C:249:SER:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:VAL:CG2	1:A:481:SER:HB3	2.40	0.52
2:F:279:THR:O	2:F:283:THR:HG23	2.10	0.52
1:A:24:ILE:O	1:A:25:GLN:HB2	2.10	0.51
1:C:407:ARG:HD2	2:D:252:ASN:OD1	2.10	0.51
2:E:28:GLU:OE2	2:E:72:PHE:HB3	2.09	0.51
1:C:150:MET:CE	7:C:746:HOH:O	2.58	0.51
2:F:29:LEU:HD11	2:F:41:ARG:HG2	1.92	0.51
1:A:232:GLY:HA3	1:A:238:LYS:HD3	1.92	0.51
1:C:8:LYS:HB3	1:C:15:MET:HG3	1.91	0.51
1:A:105:ARG:NH1	7:A:758:HOH:O	2.43	0.51
1:A:447:GLN:HB3	7:A:776:HOH:O	2.11	0.51
1:C:143:LYS:HE3	1:C:283:GLU:HA	1.93	0.50
1:B:446:ASP:O	1:B:450:GLN:N	2.42	0.50
2:D:146:LYS:CE	2:D:324:GLU:OE2	2.55	0.50
2:D:271:ARG:NH2	2:D:310:ASP:OD2	2.44	0.50
3:G:78:ASP:HA	7:G:302:HOH:O	2.12	0.50
1:B:416:ASP:OD1	1:B:418:SER:HB3	2.12	0.50
1:B:107:VAL:HA	7:B:788:HOH:O	2.10	0.50
1:C:225:GLY:O	1:C:370:GLY:HA2	2.12	0.50
1:A:214:ARG:NH1	1:A:513:THR:OG1	2.45	0.50
1:B:230:VAL:HG22	1:B:413:TRP:HE3	1.75	0.50
1:C:453:TRP:CZ3	1:C:519:PHE:HA	2.47	0.50
1:C:513:THR:HG22	1:C:517:LYS:HB3	1.94	0.50
2:F:102:GLU:HB2	2:F:103:ILE:HA	1.76	0.50
1:B:163:GLU:HG2	7:B:773:HOH:O	2.11	0.50
1:B:425:PHE:HA	1:B:426:PRO:C	2.35	0.50
1:C:318:ARG:HD2	1:C:372:VAL:HG21	1.92	0.50
1:C:243:HIS:HE1	7:C:791:HOH:O	1.93	0.49
2:D:57:PHE:HB3	2:D:217:PRO:HG3	1.95	0.49
2:E:362:ARG:HH11	2:E:364:ASP:CG	2.20	0.49
1:C:548:GLY:HA3	1:C:584:ILE:HD11	1.94	0.49
1:B:378:ASP:N	1:B:378:ASP:OD1	2.44	0.49
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.94	0.49
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.93	0.49
2:E:33:ARG:HH21	2:E:71:ARG:NH2	2.10	0.49
2:E:200:GLN:O	2:E:200:GLN:NE2	2.45	0.49
3:G:199:ARG:HD2	7:G:308:HOH:O	2.11	0.49
4:H:53:GLN:NE2	4:H:78:SER:OG	2.46	0.49
1:B:8:LYS:HD2	2:E:48:GLN:HE21	1.78	0.49
2:F:91:ASP:OD1	2:F:91:ASP:C	2.56	0.49
3:G:140:LEU:HB2	3:G:141:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CB	1:A:65:ARG:HH21	2.14	0.48
1:C:24:ILE:O	1:C:25:GLN:CB	2.61	0.48
2:E:183:ALA:HB1	2:E:186:ILE:CD1	2.44	0.48
1:C:30:VAL:HB	1:C:35:VAL:HG23	1.96	0.48
2:E:328:ILE:HG13	2:E:346:PRO:HB2	1.95	0.48
3:G:34:ASP:O	3:G:38:ARG:HG3	2.14	0.48
1:A:35:VAL:HB	1:A:53:GLU:HB2	1.96	0.48
2:D:19:GLU:O	2:D:21:VAL:HG13	2.13	0.48
1:A:378:ASP:OD2	1:A:380:ARG:NH1	2.47	0.48
1:A:475:ARG:NH2	3:G:31:ASP:OD2	2.46	0.48
2:D:128:ILE:HD11	2:D:143:ARG:HG2	1.94	0.48
2:E:166:ARG:NH1	2:E:197:ASP:OD2	2.47	0.48
2:E:397:ILE:HD12	2:E:397:ILE:N	2.28	0.48
1:A:528:PHE:CD2	1:A:528:PHE:C	2.91	0.48
1:C:318:ARG:HD2	1:C:372:VAL:CG2	2.44	0.48
1:B:541:TYR:N	1:B:544:GLU:OE2	2.45	0.48
1:C:513:THR:HG23	1:C:517:LYS:CD	2.44	0.48
2:E:107:LYS:HD2	2:E:109:LEU:HD21	1.94	0.48
3:G:46:LYS:O	3:G:50:LEU:HB2	2.13	0.48
1:A:485:ASN:O	1:A:533:ARG:NH2	2.47	0.48
2:E:383:LYS:O	2:E:387:VAL:HG23	2.13	0.48
2:F:248:THR:HB	2:F:303:ILE:HB	1.96	0.48
1:A:3:ILE:HB	1:A:65:ARG:HD2	1.96	0.48
1:B:225:GLY:HA2	1:B:384:ILE:O	2.14	0.48
1:C:524:VAL:CG1	1:C:556:ILE:HG12	2.44	0.48
2:D:88:ARG:NH2	2:D:98:ASP:OD1	2.47	0.48
2:F:266:GLU:OE1	2:F:276:TYR:OH	2.24	0.48
1:A:52:TYR:CD2	1:A:301:ALA:HB2	2.49	0.47
1:A:445:MET:HG2	1:A:453:TRP:CD1	2.48	0.47
1:B:80:ILE:O	1:B:81:SER:HB2	2.14	0.47
4:H:31:THR:O	4:H:35:LYS:HB2	2.13	0.47
1:C:474:VAL:C	1:C:476:LEU:H	2.23	0.47
1:C:193:VAL:HG11	1:C:309:THR:HG22	1.95	0.47
2:E:233:GLU:HB2	7:E:518:HOH:O	2.13	0.47
2:F:16:MET:HB3	2:F:54:VAL:HG22	1.96	0.47
1:A:498:GLU:O	1:A:560:LYS:NZ	2.42	0.47
2:F:199:ARG:HD3	7:F:540:HOH:O	2.14	0.47
2:F:354:LYS:O	2:F:360:LYS:CE	2.62	0.47
3:G:54:ILE:HG21	3:G:146:LEU:HD22	1.95	0.47
1:B:8:LYS:HB3	1:B:15:MET:HG3	1.97	0.47
1:C:18:ASN:HA	7:C:747:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:770:HOH:O	2:D:187:THR:HB	2.14	0.47
1:A:80:ILE:HG13	1:A:141:GLU:CD	2.40	0.47
2:D:383:LYS:O	2:D:386:ALA:HB3	2.13	0.47
1:B:27:MET:CE	1:B:71:LEU:HB2	2.38	0.47
1:A:378:ASP:HB2	1:A:380:ARG:HH12	1.77	0.47
1:B:239:THR:HB	5:B:601:ANP:O2A	2.15	0.47
1:A:238:LYS:HB3	1:A:238:LYS:HE3	1.57	0.46
1:C:311:ILE:O	1:C:315:GLU:HG3	2.15	0.46
2:F:251:THR:O	2:F:255:GLU:HG2	2.15	0.46
2:E:385:LEU:HD23	2:E:394:LEU:HD23	1.96	0.46
2:F:162:ALA:O	2:F:166:ARG:HB2	2.15	0.46
1:A:333:ARG:CG	1:A:333:ARG:NH1	2.68	0.46
1:C:346:GLU:HG2	3:G:206:MET:HE3	1.96	0.46
3:G:44:ILE:HD12	3:G:44:ILE:HA	1.84	0.46
2:E:242:HIS:HD2	2:E:297:SER:OG	1.97	0.46
1:C:478:GLY:O	1:C:479:ILE:HG13	2.15	0.46
2:D:87:GLY:HA2	2:D:204:ILE:HG13	1.98	0.46
2:E:436:MET:HE2	2:E:436:MET:HB3	1.79	0.46
2:D:148:PRO:HD3	2:D:323:THR:HB	1.97	0.46
3:G:100:VAL:HG22	3:G:159:GLU:HG2	1.97	0.46
1:A:1:MET:HA	1:A:66:SER:O	2.16	0.46
1:C:391:SER:HB3	2:F:321:TYR:CE1	2.51	0.46
1:A:33:LEU:HD21	1:A:105:ARG:HD2	1.98	0.46
1:B:497:ARG:NH2	7:B:787:HOH:O	2.49	0.46
1:C:83:MET:HE2	1:C:266:MET:HB3	1.98	0.46
1:C:417:SER:O	1:C:421:GLN:HG3	2.16	0.46
2:E:9:LYS:HD3	2:E:10:GLU:HG3	1.98	0.46
2:E:48:GLN:O	2:E:48:GLN:HG2	2.15	0.46
2:F:354:LYS:O	2:F:360:LYS:HE2	2.16	0.45
2:F:408:PHE:O	2:F:412:TYR:HB3	2.16	0.45
1:A:256:TYR:C	1:A:256:TYR:CD2	2.93	0.45
1:B:41:GLU:OE1	1:B:43:ARG:NH1	2.44	0.45
2:F:94:GLY:N	2:F:227:MET:HE2	2.31	0.45
1:A:445:MET:SD	1:A:515:ARG:HD3	2.56	0.45
1:A:86:GLY:HA3	1:A:302:ALA:O	2.17	0.45
1:A:221:PRO:O	1:A:435:SER:OG	2.25	0.45
1:C:2:GLN:OE1	1:C:21:GLU:HB2	2.16	0.45
1:C:445:MET:CE	1:C:515:ARG:HD2	2.43	0.45
1:C:555:ARG:NH1	1:C:576:GLU:OE1	2.50	0.45
1:C:202:LYS:NZ	1:C:369:SER:O	2.44	0.45
2:D:34:MET:CE	2:D:40:ARG:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:343:ASP:O	2:D:347:SER:OG	2.25	0.45
1:C:143:LYS:HE3	1:C:283:GLU:CB	2.46	0.45
1:C:258:GLY:HA3	1:C:266:MET:HE3	1.99	0.45
1:C:429:ASN:CG	1:C:432:GLN:HB2	2.42	0.45
2:D:171:LEU:C	2:D:173:SER:H	2.23	0.45
1:B:191:TRP:CD2	1:B:192:PRO:HD2	2.51	0.45
1:C:477:VAL:O	1:C:477:VAL:HG22	2.15	0.45
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.99	0.45
1:B:144:ILE:HG21	1:B:283:GLU:OE2	2.17	0.45
1:C:143:LYS:HE3	1:C:283:GLU:HB3	1.99	0.45
2:D:104:LEU:H	2:D:104:LEU:HG	1.59	0.45
1:B:50:GLN:HG3	1:B:341:MET:HE3	1.99	0.45
1:B:247:LYS:HZ1	1:B:272:GLU:CD	2.25	0.45
1:B:555:ARG:NH1	1:B:576:GLU:OE2	2.44	0.45
1:A:243:HIS:O	1:A:247:LYS:HG2	2.17	0.44
1:A:448:ILE:HG23	1:A:449:LEU:HD13	1.98	0.44
1:A:422:LYS:O	1:A:423:ARG:HB2	2.17	0.44
1:C:230:VAL:HG13	1:C:413:TRP:HB2	1.99	0.44
2:D:268:PRO:HD2	3:G:200:LEU:HD13	1.99	0.44
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.98	0.44
1:C:238:LYS:NZ	5:C:601:ANP:OI1G	2.50	0.44
1:C:477:VAL:HB	3:G:29:LEU:HD11	1.98	0.44
1:C:541:TYR:HB2	1:C:544:GLU:HG3	1.98	0.44
2:E:174:SER:HB3	7:E:541:HOH:O	2.16	0.44
2:E:174:SER:HA	2:E:175:ASP:HA	1.63	0.44
2:F:348:LEU:HG	2:F:349:SER:N	2.33	0.44
1:C:477:VAL:O	1:C:477:VAL:CG2	2.65	0.44
1:A:118:TRP:HB2	1:A:187:MET:HE1	2.00	0.44
1:B:55:THR:HA	1:B:58:ILE:HD12	2.00	0.44
1:B:558:ARG:HE	1:B:558:ARG:HB3	1.61	0.44
1:C:214:ARG:HG2	1:C:518:GLN:HG2	2.00	0.44
2:F:119:ILE:O	2:F:119:ILE:HG22	2.16	0.44
1:A:479:ILE:HG23	1:A:480:ASP:OD1	2.18	0.44
1:B:42:MET:HE2	1:B:42:MET:HB2	1.66	0.44
1:B:472:GLU:HG2	3:G:173:MET:HE1	2.00	0.44
3:G:187:MET:O	3:G:191:GLU:HG2	2.18	0.44
1:A:17:GLU:O	1:A:18:ASN:HB2	2.17	0.44
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.53	0.44
1:C:38:GLU:O	1:C:49:ILE:HA	2.18	0.44
2:E:41:ARG:NH1	2:E:41:ARG:CG	2.68	0.44
1:C:200:LYS:HB2	1:C:200:LYS:HE2	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:GLU:O	1:C:520:ASN:ND2	2.50	0.44
1:A:71:LEU:HD21	1:A:87:ILE:HG22	2.00	0.43
1:B:281:THR:OG1	1:B:283:GLU:OE1	2.33	0.43
2:F:227:MET:HE3	2:F:227:MET:HB3	1.93	0.43
1:A:6:ILE:HG22	1:A:60:PRO:HA	2.00	0.43
1:A:507:ASP:O	1:A:511:THR:HB	2.18	0.43
1:A:553:ARG:HA	1:A:556:ILE:HD12	2.00	0.43
1:B:19:MET:HE3	1:B:39:ILE:HD11	2.00	0.43
1:B:212:GLY:HA3	1:B:512:PHE:CD1	2.53	0.43
3:G:51:ARG:NH1	3:G:150:GLU:OE2	2.51	0.43
3:G:78:ASP:C	3:G:80:LEU:H	2.25	0.43
1:A:218:THR:HG23	1:A:453:TRP:CZ2	2.53	0.43
1:C:231:PRO:HG2	1:C:412:PHE:HE1	1.83	0.43
2:F:4:GLU:OE2	2:F:71:ARG:HG2	2.19	0.43
1:A:230:VAL:O	1:A:389:ALA:HA	2.18	0.43
1:A:517:LYS:NZ	7:A:754:HOH:O	2.42	0.43
1:B:266:MET:O	1:B:270:VAL:HG22	2.17	0.43
2:E:163:GLN:HE21	2:E:167:GLN:NE2	2.15	0.43
1:A:426:PRO:HB2	1:A:428:ILE:HD12	1.98	0.43
2:E:46:GLU:HB3	2:E:53:MET:HB2	2.00	0.43
2:E:58:GLU:OE1	2:E:58:GLU:N	2.43	0.43
1:A:396:ASP:HA	7:A:752:HOH:O	2.18	0.43
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.78	0.43
2:D:79:LEU:CB	2:D:227:MET:HE3	2.39	0.43
2:D:152:GLY:N	2:D:155:LEU:HD12	2.33	0.43
2:D:183:ALA:O	2:D:212:ASN:HB3	2.19	0.43
2:E:249:ASP:OD2	2:E:304:LEU:HA	2.18	0.43
2:F:7:THR:OG1	2:F:19:GLU:O	2.34	0.43
4:H:3:TYR:N	4:H:3:TYR:CD1	2.87	0.43
1:C:413:TRP:HB3	1:C:428:ILE:HD13	2.00	0.43
1:B:524:VAL:CG1	1:B:556:ILE:HG12	2.49	0.42
1:B:528:PHE:HA	1:B:577:ILE:HG21	2.00	0.42
1:C:238:LYS:HE2	1:C:238:LYS:HB2	1.83	0.42
2:F:331:ARG:O	2:F:335:LYS:HG2	2.19	0.42
1:A:394:GLY:C	1:A:396:ASP:H	2.26	0.42
1:B:82:GLN:HG2	1:B:84:PHE:CZ	2.54	0.42
1:C:283:GLU:N	1:C:283:GLU:OE1	2.52	0.42
1:B:214:ARG:NH1	1:B:513:THR:OG1	2.52	0.42
1:B:558:ARG:HD3	7:B:757:HOH:O	2.20	0.42
5:B:601:ANP:PA	7:B:701:HOH:O	2.73	0.42
2:E:125:ASP:OD2	2:E:354:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:146:LYS:NZ	2:E:286:GLU:OE2	2.53	0.42
2:F:270:ARG:O	2:F:271:ARG:HB2	2.19	0.42
1:B:562:ILE:HA	1:B:563:PRO:HD3	1.83	0.42
1:B:39:ILE:HG12	1:B:47:ALA:HB1	2.02	0.42
1:B:350:GLY:N	1:B:354:TYR:O	2.49	0.42
2:F:248:THR:HA	2:F:249:ASP:HA	1.80	0.42
1:A:329:ASP:HA	1:A:330:SER:HA	1.75	0.42
1:A:448:ILE:HD12	1:A:448:ILE:HA	1.90	0.42
2:E:407:ARG:NE	2:E:411:GLU:OE2	2.40	0.42
1:B:426:PRO:HB2	1:B:428:ILE:HG13	2.01	0.42
1:C:529:GLY:O	1:C:533:ARG:HB2	2.20	0.42
2:E:83:GLU:CD	2:E:239:LYS:HD2	2.45	0.42
1:A:10:SER:OG	2:D:264:ARG:HD2	2.20	0.42
1:C:56:SER:O	1:C:105:ARG:NH2	2.42	0.42
1:C:415:LEU:HA	1:C:427:SER:O	2.20	0.42
2:F:125:ASP:N	2:F:125:ASP:OD1	2.51	0.42
4:H:14:VAL:HG13	4:H:14:VAL:O	2.19	0.42
2:D:89:VAL:HG11	2:D:195:MET:SD	2.60	0.41
2:D:93:LEU:CG	2:D:220:GLU:HG2	2.46	0.41
2:E:198:PHE:HB3	2:E:204:ILE:HB	2.02	0.41
2:F:111:ILE:O	2:F:287:ARG:NH2	2.53	0.41
1:B:424:HIS:HE1	7:B:733:HOH:O	2.02	0.41
2:D:33:ARG:HH12	2:D:71:ARG:NH1	2.17	0.41
2:F:404:PHE:HA	2:F:436:MET:HE1	2.02	0.41
1:C:144:ILE:HG21	7:C:765:HOH:O	2.20	0.41
1:C:346:GLU:HG2	3:G:206:MET:CE	2.50	0.41
2:F:244:LEU:HD12	2:F:299:THR:HB	2.01	0.41
7:A:770:HOH:O	2:D:121:ARG:HD3	2.20	0.41
1:B:41:GLU:HB2	1:B:48:SER:HB2	2.02	0.41
1:C:54:GLU:OE2	1:C:56:SER:HB3	2.20	0.41
4:H:95:GLU:HG3	4:H:96:LYS:N	2.36	0.41
1:C:251:VAL:HG11	1:C:325:ALA:HB2	2.03	0.41
1:B:336:GLU:HG3	7:B:764:HOH:O	2.20	0.41
2:D:148:PRO:CA	2:D:302:PRO:HD2	2.50	0.41
2:D:311:LYS:H	2:D:311:LYS:HG3	1.71	0.41
2:E:21:VAL:HB	2:E:24:VAL:HG21	2.03	0.41
2:E:41:ARG:NE	7:E:504:HOH:O	2.35	0.41
1:A:270:VAL:HG11	2:D:119:ILE:HG22	2.03	0.41
1:B:210:ILE:O	1:B:249:SER:HA	2.20	0.41
1:C:75:LEU:HD13	1:C:316:TYR:CD1	2.56	0.41
1:C:435:SER:O	1:C:438:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:399:LYS:O	2:D:403:LYS:HG3	2.21	0.41
2:D:422:THR:HB	7:D:536:HOH:O	2.20	0.41
2:F:123:TYR:HA	2:F:124:PRO:HD3	1.84	0.41
1:C:356:ALA:HB1	2:D:259:GLU:HA	2.02	0.41
1:C:573:ILE:O	1:C:577:ILE:HG13	2.21	0.41
1:B:311:ILE:HD12	1:B:311:ILE:HA	1.94	0.40
2:D:88:ARG:HH21	2:D:98:ASP:CG	2.29	0.40
2:D:177:PHE:HD2	2:D:242:HIS:O	2.04	0.40
2:D:184:ILE:HG21	2:D:253:TYR:HB2	2.03	0.40
1:B:399:GLU:OE2	1:B:401:VAL:HB	2.20	0.40
1:B:445:MET:HA	1:B:448:ILE:HG22	2.03	0.40
1:C:513:THR:CG2	1:C:517:LYS:CD	2.99	0.40
3:G:151:LYS:HA	3:G:151:LYS:HD2	1.86	0.40
1:A:95:MET:HE3	2:D:120:ALA:HB2	1.94	0.40
2:D:404:PHE:CD2	2:D:404:PHE:C	3.00	0.40
3:G:41:ILE:HA	3:G:44:ILE:HG22	2.03	0.40
4:H:91:GLN:O	4:H:94:VAL:HG12	2.22	0.40
1:A:85:ASP:OD1	1:A:85:ASP:C	2.65	0.40
1:A:254:VAL:O	1:A:289:THR:HA	2.22	0.40
1:A:361:ARG:HD3	1:A:361:ARG:HA	1.47	0.40
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.95	0.40
2:D:178:ALA:HB2	2:D:241:MET:HE2	2.03	0.40
2:E:17:ALA:HB2	2:E:53:MET:HE3	2.04	0.40
2:F:146:LYS:HD2	2:F:323:THR:HA	2.03	0.40
3:G:26:HIS:NE2	3:G:171:GLU:HB2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/600 (98%)	574 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	590/600 (98%)	576 (98%)	14 (2%)	0	100	100
1	C	578/600 (96%)	566 (98%)	10 (2%)	2 (0%)	36	57
2	D	449/465 (97%)	437 (97%)	12 (3%)	0	100	100
2	E	450/465 (97%)	437 (97%)	13 (3%)	0	100	100
2	F	453/465 (97%)	441 (97%)	10 (2%)	2 (0%)	30	51
3	G	168/217 (77%)	163 (97%)	5 (3%)	0	100	100
4	H	100/115 (87%)	95 (95%)	5 (5%)	0	100	100
All	All	3373/3527 (96%)	3289 (98%)	80 (2%)	4 (0%)	48	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	102	GLU
1	C	477	VAL
2	F	101	PRO
1	C	159	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	502/511 (98%)	472 (94%)	30 (6%)	17	38
1	B	503/511 (98%)	470 (93%)	33 (7%)	15	33
1	C	499/511 (98%)	452 (91%)	47 (9%)	8	19
2	D	369/387 (95%)	335 (91%)	34 (9%)	8	19
2	E	378/387 (98%)	355 (94%)	23 (6%)	17	37
2	F	379/387 (98%)	350 (92%)	29 (8%)	12	27
3	G	155/198 (78%)	141 (91%)	14 (9%)	9	20
4	H	84/99 (85%)	74 (88%)	10 (12%)	5	11
All	All	2869/2991 (96%)	2649 (92%)	220 (8%)	12	27

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	29	LEU
1	A	36	ILE
1	A	80	ILE
1	A	94	PHE
1	A	95	MET
1	A	100	SER
1	A	103	LEU
1	A	124	ILE
1	A	173	ILE
1	A	177	GLU
1	A	188	MET
1	A	230	VAL
1	A	253	LEU
1	A	273	PHE
1	A	292	ILE
1	A	333	ARG
1	A	361	ARG
1	A	372	VAL
1	A	391	SER
1	A	397	ILE
1	A	428	ILE
1	A	436	LEU
1	A	449	LEU
1	A	476	LEU
1	A	508	ASP
1	A	543	ASN
1	A	565	GLU
1	A	572	SER
1	B	-4	SER
1	B	5	LYS
1	B	88	GLN
1	B	103	LEU
1	B	123	THR
1	B	131	SER
1	B	144	ILE
1	B	155	ILE
1	B	175	VAL
1	B	195	ARG
1	B	230	VAL
1	B	253	LEU

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Mol	Chain	Res	Type
1	B	270	VAL
1	B	281	THR
1	B	326	ILE
1	B	327	MET
1	B	352	GLU
1	B	364	GLU
1	B	371	ARG
1	B	378	ASP
1	B	381	GLU
1	B	399	GLU
1	B	428	ILE
1	B	438	SER
1	B	448	ILE
1	B	469	GLN
1	B	476	LEU
1	B	479	ILE
1	B	526	LEU
1	B	562	ILE
1	B	566	GLU
1	B	571	SER
1	B	585	VAL
1	C	15	MET
1	C	25	GLN
1	C	29	LEU
1	C	54	GLU
1	C	69	GLU
1	C	73	VAL
1	C	83	MET
1	C	95	MET
1	C	96	GLU
1	C	109	LEU
1	C	116	LYS
1	C	144	ILE
1	C	166	SER
1	C	173	ILE
1	C	178	THR
1	C	194	ARG
1	C	195	ARG
1	C	199	ILE
1	C	200	LYS
1	C	209	MET
1	C	215	VAL

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Mol	Chain	Res	Type
1	C	230	VAL
1	C	253	LEU
1	C	270	VAL
1	C	284	SER
1	C	351	ASP
1	C	377	SER
1	C	378	ASP
1	C	410	LYS
1	C	428	ILE
1	C	432	GLN
1	C	438	SER
1	C	448	ILE
1	C	454	SER
1	C	462	ARG
1	C	469	GLN
1	C	473	ILE
1	C	474	VAL
1	C	475	ARG
1	C	477	VAL
1	C	479	ILE
1	C	513	THR
1	C	524	VAL
1	C	538	LEU
1	C	557	SER
1	C	583	LEU
1	C	586	SER
2	D	4	GLU
2	D	15	LEU
2	D	33	ARG
2	D	48	GLN
2	D	51	LYS
2	D	53	MET
2	D	60	THR
2	D	73	LEU
2	D	86	ILE
2	D	97	LYS
2	D	103	ILE
2	D	104	LEU
2	D	122	ASP
2	D	143	ARG
2	D	146	LYS
2	D	170	VAL

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Mol	Chain	Res	Type
2	D	173	SER
2	D	176	ASP
2	D	177	PHE
2	D	211	MET
2	D	219	ILE
2	D	303	ILE
2	D	311	LYS
2	D	332	GLU
2	D	336	SER
2	D	352	LYS
2	D	363	GLU
2	D	368	THR
2	D	383	LYS
2	D	385	LEU
2	D	397	ILE
2	D	400	ILE
2	D	450	LEU
2	D	454	LEU
2	E	15	LEU
2	E	41	ARG
2	E	48	GLN
2	E	53	MET
2	E	61	SER
2	E	83	GLU
2	E	102	GLU
2	E	103	ILE
2	E	104	LEU
2	E	106	GLU
2	E	107	LYS
2	E	119	ILE
2	E	146	LYS
2	E	173	SER
2	E	175	ASP
2	E	221	ARG
2	E	260	ILE
2	E	353	ASP
2	E	362	ARG
2	E	380	LYS
2	E	397	ILE
2	E	452	LYS
2	E	454	LEU
2	F	6	ARG

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Mol	Chain	Res	Type
2	F	18	VAL
2	F	41	ARG
2	F	81	VAL
2	F	103	ILE
2	F	104	LEU
2	F	122	ASP
2	F	126	GLU
2	F	138	LEU
2	F	146	LYS
2	F	167	GLN
2	F	174	SER
2	F	190	GLU
2	F	209	MET
2	F	265	ARG
2	F	266	GLU
2	F	280	ASN
2	F	308	GLU
2	F	328	ILE
2	F	332	GLU
2	F	352	LYS
2	F	394	LEU
2	F	395	SER
2	F	397	ILE
2	F	403	LYS
2	F	424	THR
2	F	426	THR
2	F	439	ARG
2	F	443	LYS
3	G	10	MET
3	G	18	GLN
3	G	50	LEU
3	G	51	ARG
3	G	59	GLN
3	G	66	VAL
3	G	88	VAL
3	G	91	SER
3	G	93	VAL
3	G	96	ASN
3	G	102	VAL
3	G	104	LEU
3	G	137	THR
3	G	178	LEU

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Mol	Chain	Res	Type
4	H	3	TYR
4	H	7	VAL
4	H	14	VAL
4	H	19	LEU
4	H	36	THR
4	H	44	GLU
4	H	53	GLN
4	H	62	ILE
4	H	95	GLU
4	H	102	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	B	146	GLN
1	B	153	ASN
1	B	160	GLN
1	B	242	GLN
1	B	404	ASN
1	B	520	ASN
1	B	574	ASN
1	C	108	GLN
1	C	180	GLN
1	C	201	GLN
1	C	582	GLN
2	D	139	ASN
2	E	48	GLN
2	E	112	ASN
2	E	139	ASN
2	E	167	GLN
2	E	242	HIS
2	E	370	ASN
2	E	410	ASN
2	F	43	GLN
2	F	370	ASN
2	F	378	GLN
2	F	381	GLN
3	G	33	GLN
3	G	39	GLN
3	G	48	ASN
3	G	52	GLN

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Mol	Chain	Res	Type
3	G	59	GLN
3	G	177	GLN
4	H	26	HIS
4	H	53	GLN
4	H	91	GLN

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 oligosaccharides 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	$\# Z > 2$
5	ANP	B	601	6	33,33,33	1.93	8 (24%)	45,52,52	1.74	10 (22%)
5	ANP	C	601	6	33,33,33	1.91	8 (24%)	45,52,52	2.11	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	B	601	6	-	5/18/38/38	0/3/3/3
5	ANP	C	601	6	-	4/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	ANP	C5-C4	5.05	1.48	1.39
5	C	601	ANP	C5-C4	4.88	1.47	1.39
5	B	601	ANP	PG-N3B	4.24	1.74	1.63
5	B	601	ANP	PB-N3B	3.98	1.73	1.63
5	C	601	ANP	PG-O1G	3.79	1.51	1.46
5	C	601	ANP	PG-N3B	3.71	1.73	1.63
5	C	601	ANP	PB-N3B	3.62	1.72	1.63
5	B	601	ANP	PG-O1G	3.20	1.51	1.46
5	B	601	ANP	PB-O1B	2.96	1.50	1.46
5	C	601	ANP	PB-O3A	2.83	1.62	1.59
5	C	601	ANP	C5-C6	2.81	1.48	1.41
5	B	601	ANP	C5-C6	2.78	1.48	1.41
5	C	601	ANP	C8-N7	2.72	1.36	1.31
5	C	601	ANP	PB-O1B	2.70	1.50	1.46
5	B	601	ANP	C8-N7	2.53	1.36	1.31
5	B	601	ANP	C5-N7	-2.32	1.34	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	ANP	C5-C4-N3	-5.77	118.77	126.72
5	B	601	ANP	C5-C4-N3	-5.42	119.26	126.72
5	C	601	ANP	N3-C4-N9	4.85	135.41	127.17
5	B	601	ANP	N3-C4-N9	4.53	134.88	127.17
5	C	601	ANP	O1G-PG-N3B	-4.52	105.11	111.77
5	C	601	ANP	O2G-PG-O3G	3.97	118.25	107.59
5	C	601	ANP	C2-N3-C4	3.85	121.23	111.83
5	C	601	ANP	C4-N9-C8	3.57	109.49	105.74
5	C	601	ANP	N3-C2-N1	-3.39	123.45	128.58
5	C	601	ANP	C4-C5-N7	-3.25	106.86	110.58
5	B	601	ANP	O2G-PG-O3G	3.14	116.03	107.59
5	B	601	ANP	C2-N3-C4	3.01	119.19	111.83
5	C	601	ANP	C2'-C1'-N9	-2.80	106.34	113.30
5	B	601	ANP	C3'-C2'-C1'	2.79	106.75	101.46
5	C	601	ANP	C5-N7-C8	2.74	107.75	103.45
5	C	601	ANP	N9-C8-N7	-2.72	110.08	113.94
5	B	601	ANP	O1G-PG-N3B	-2.67	107.83	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	ANP	O2B-PB-O1B	2.63	115.51	109.87
5	B	601	ANP	C4-C5-N7	-2.43	107.80	110.58
5	B	601	ANP	C4-N9-C8	2.27	108.12	105.74
5	B	601	ANP	N3-C2-N1	-2.16	125.31	128.58
5	B	601	ANP	O2'-C2'-C1'	-2.11	102.84	110.10
5	C	601	ANP	C6-C5-N7	2.06	136.06	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

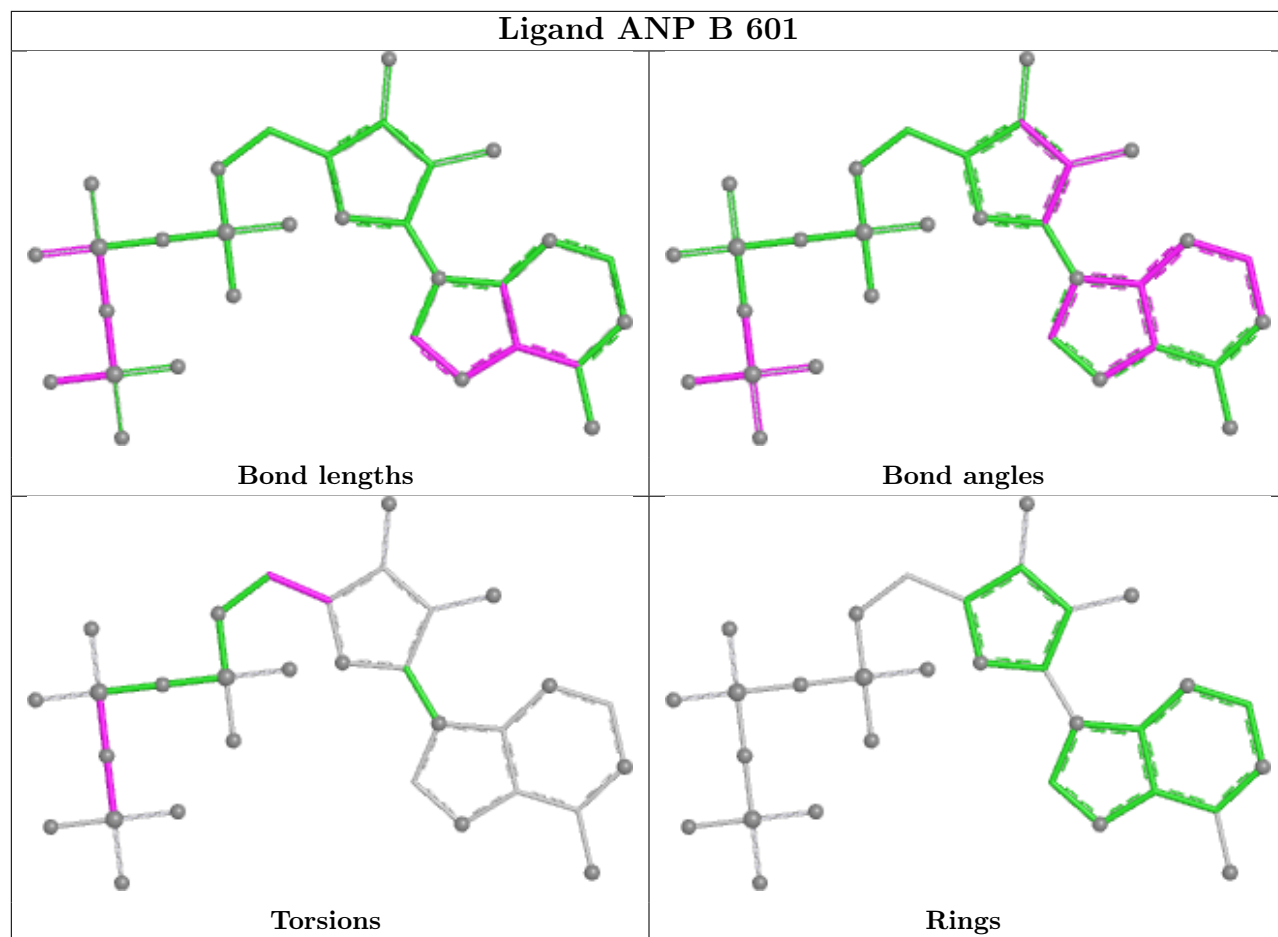
Mol	Chain	Res	Type	Atoms
5	B	601	ANP	PB-N3B-PG-O1G
5	B	601	ANP	PG-N3B-PB-O1B
5	C	601	ANP	PB-N3B-PG-O1G
5	C	601	ANP	PG-N3B-PB-O1B
5	C	601	ANP	PA-O3A-PB-O2B
5	B	601	ANP	O4'-C4'-C5'-O5'
5	B	601	ANP	C3'-C4'-C5'-O5'
5	B	601	ANP	PG-N3B-PB-O3A
5	C	601	ANP	PA-O3A-PB-O1B

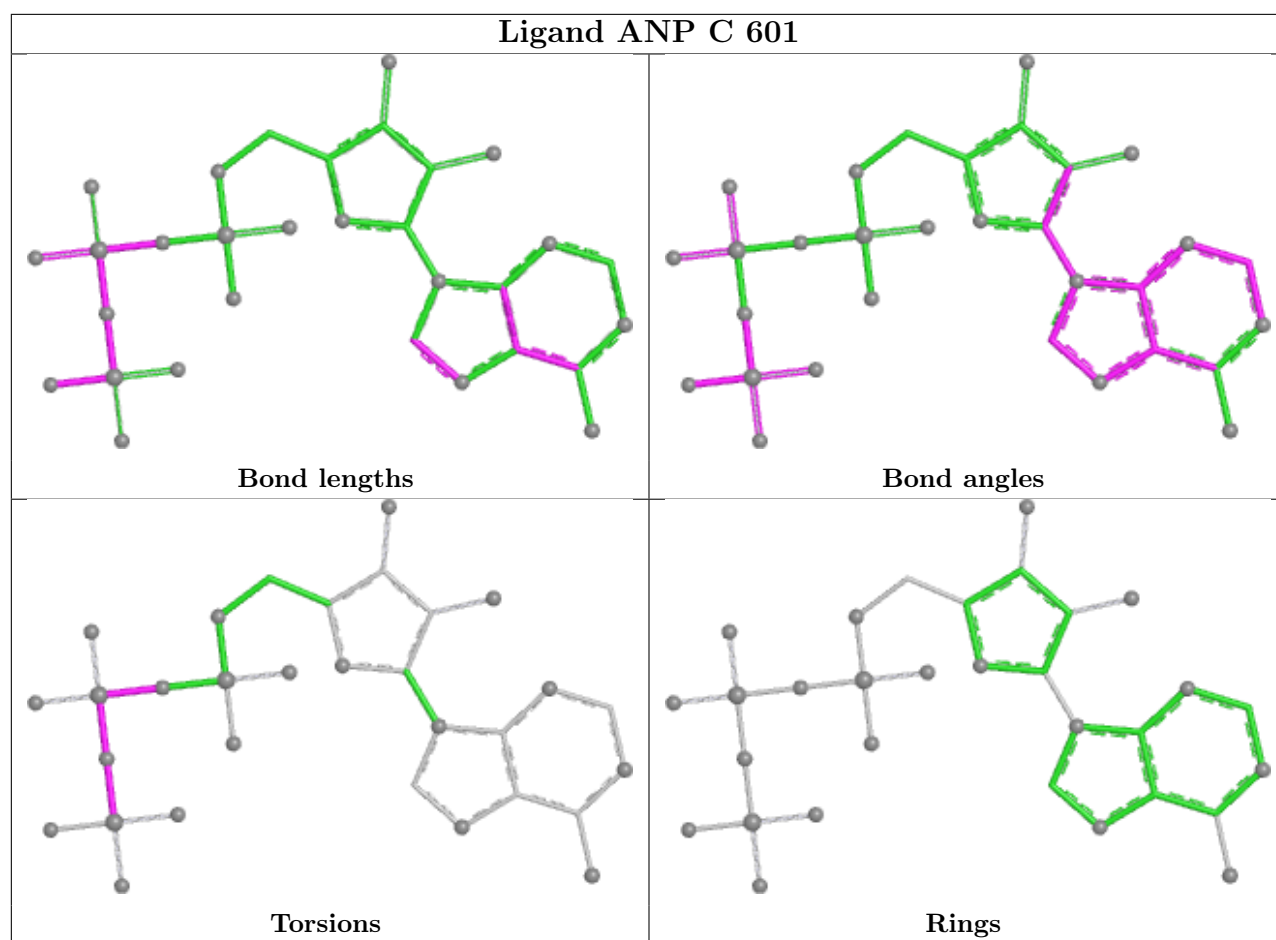
There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	587/600 (97%)	-0.34	1 (0%) 91 90	25, 43, 72, 91	0
1	B	592/600 (98%)	-0.50	2 (0%) 90 89	19, 34, 64, 85	0
1	C	582/600 (97%)	-0.41	1 (0%) 91 90	21, 38, 64, 90	0
2	D	451/465 (96%)	-0.27	7 (1%) 70 68	26, 43, 73, 90	0
2	E	452/465 (97%)	-0.56	1 (0%) 91 90	21, 35, 59, 77	0
2	F	455/465 (97%)	-0.52	2 (0%) 88 87	21, 35, 61, 84	0
3	G	176/217 (81%)	0.43	18 (10%) 12 10	35, 58, 121, 148	0
4	H	102/115 (88%)	0.69	2 (1%) 65 61	36, 80, 112, 126	0
All	All	3397/3527 (96%)	-0.35	34 (1%) 79 77	19, 40, 75, 148	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	83	LEU	4.2
3	G	128	GLU	4.1
3	G	88	VAL	3.8
3	G	80	LEU	3.7
3	G	79	GLU	3.6
1	B	586	SER	3.3
3	G	1	MET	3.2
2	D	454	LEU	3.2
3	G	4	ASN	3.1
3	G	141	PRO	2.9
3	G	78	ASP	2.9
1	B	280	ASN	2.8
3	G	98	MET	2.7
1	A	0	GLY	2.6
3	G	142	LYS	2.6
2	D	104	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	81	LEU	2.6
2	D	388	VAL	2.5
3	G	129	LEU	2.5
3	G	87	ASN	2.5
4	H	13	SER	2.5
3	G	3	LEU	2.4
2	F	455	PRO	2.3
3	G	130	ASP	2.3
2	D	448	ASP	2.2
3	G	187	MET	2.2
2	D	103	ILE	2.1
2	F	2	ILE	2.1
2	D	389	LEU	2.1
4	H	10	ASP	2.1
1	C	277	ILE	2.1
2	D	5	TYR	2.1
3	G	132	SER	2.0
2	E	104	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

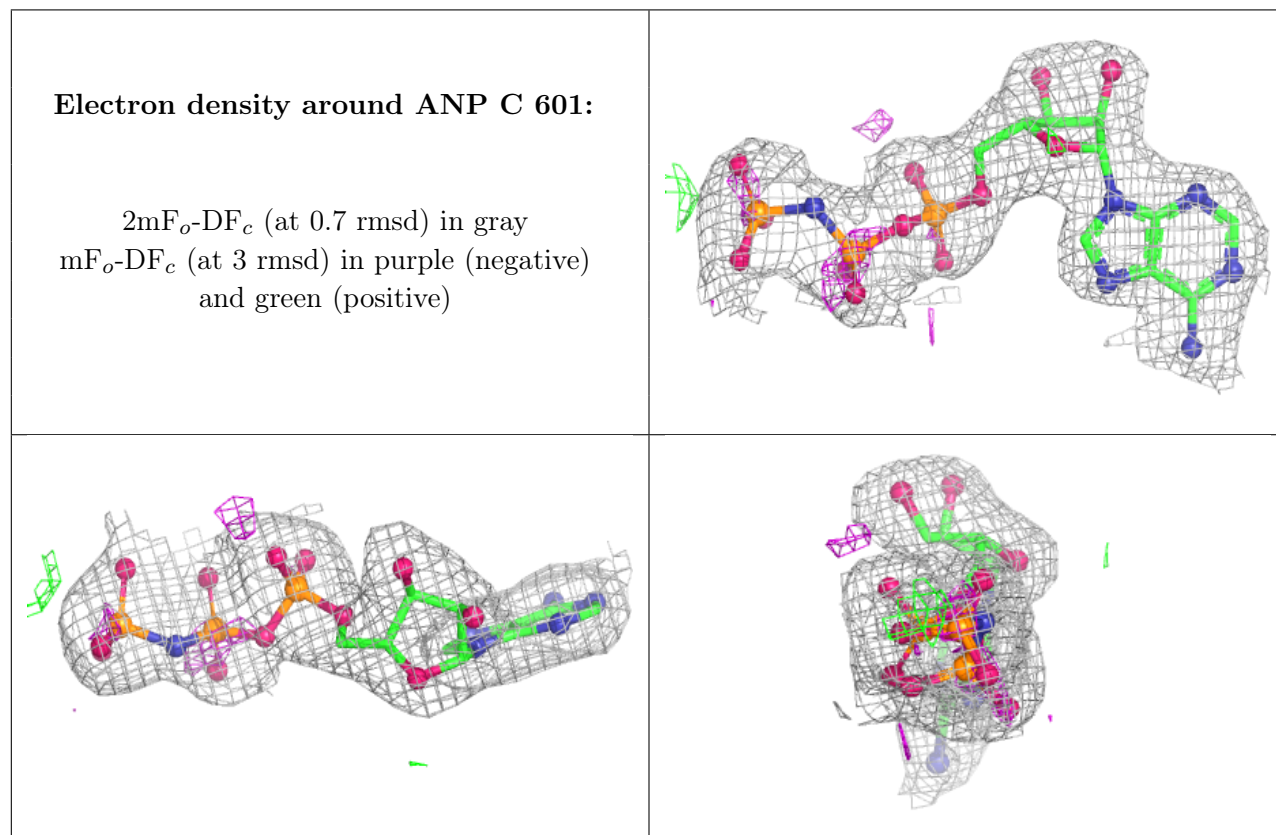
There are no oligosaccharides in this entry.

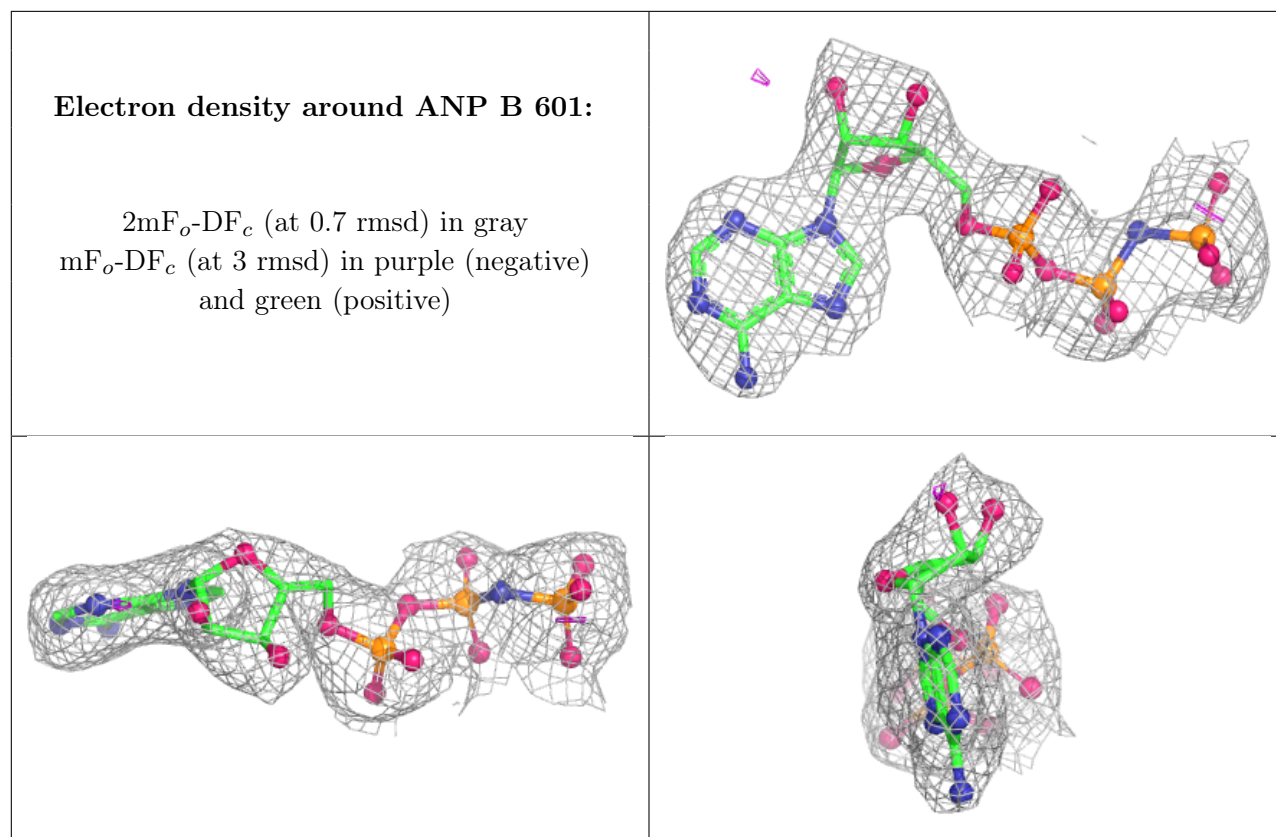
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	C	602	1/1	0.97	0.04	27,27,27,27	0
6	MG	B	602	1/1	0.98	0.04	24,24,24,24	0
5	ANP	C	601	31/31	0.98	0.05	13,21,30,31	0
5	ANP	B	601	31/31	0.99	0.05	12,19,23,26	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.