Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:26 AM EDT

PDB ID	:	6QV2
Title	:	Structure of ATPgS-bound outward-facing TM287/288 in complex with nanobody Nb_TM#2
Authors	:	Hutter, C.A.J.; Huerlimann, L.M.; Zimmermann, I.; Egloff, P.; Seeger, M.A.
Deposited on	:	2019-03-01
Resolution	:	4.23 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:

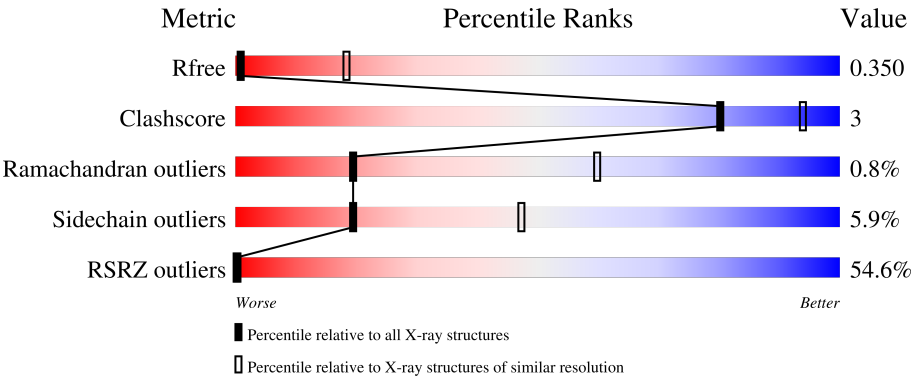
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.23 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	1015 (4.70-3.78)
Clashscore	141614	1051 (4.68-3.80)
Ramachandran outliers	138981	1007 (4.68-3.80)
Sidechain outliers	138945	1016 (4.70-3.78)
RSRZ outliers	127900	1065 (4.76-3.70)

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	587	58% 85% 11% ·
1	C	587	63% 86% 11% ·
2	B	599	36% 82% 12% · 5%
2	D	599	51% 83% 12% · 5%
3	E	132	64% 76% 21% ··

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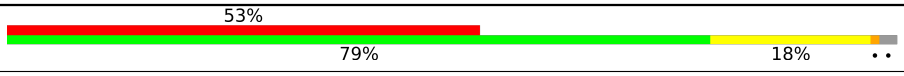
Mol	Chain	Length	Quality of chain
3	F	132	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20086 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 ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			
1	C	568	Total	C	N	O	S	0	0	0
			4464	2879	768	798	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q9WYC3
A	-8	PRO	-	expression tag	UNP Q9WYC3
A	-7	SER	-	expression tag	UNP Q9WYC3
A	-6	GLY	-	expression tag	UNP Q9WYC3
A	-5	SER	-	expression tag	UNP Q9WYC3
A	-4	GLY	-	expression tag	UNP Q9WYC3
A	-3	GLY	-	expression tag	UNP Q9WYC3
A	-2	GLY	-	expression tag	UNP Q9WYC3
A	-1	GLY	-	expression tag	UNP Q9WYC3
A	0	GLY	-	expression tag	UNP Q9WYC3
A	1	SER	-	expression tag	UNP Q9WYC3
A	41	ALA	ASP	engineered mutation	UNP Q9WYC3
C	-9	GLY	-	expression tag	UNP Q9WYC3
C	-8	PRO	-	expression tag	UNP Q9WYC3
C	-7	SER	-	expression tag	UNP Q9WYC3
C	-6	GLY	-	expression tag	UNP Q9WYC3
C	-5	SER	-	expression tag	UNP Q9WYC3
C	-4	GLY	-	expression tag	UNP Q9WYC3
C	-3	GLY	-	expression tag	UNP Q9WYC3
C	-2	GLY	-	expression tag	UNP Q9WYC3
C	-1	GLY	-	expression tag	UNP Q9WYC3
C	0	GLY	-	expression tag	UNP Q9WYC3
C	1	SER	-	expression tag	UNP Q9WYC3
C	41	ALA	ASP	engineered mutation	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			
2	D	570	Total	C	N	O	S	0	0	0
			4541	2936	766	825	14			

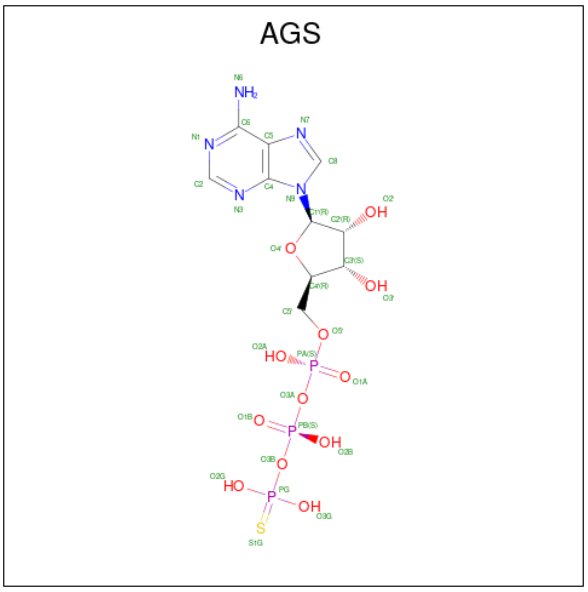
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	ALA	ASP	engineered mutation	UNP Q9WYC4
B	517	ALA	GLU	engineered mutation	UNP Q9WYC4
B	599	ALA	-	expression tag	UNP Q9WYC4
D	65	ALA	ASP	engineered mutation	UNP Q9WYC4
D	517	ALA	GLU	engineered mutation	UNP Q9WYC4
D	599	ALA	-	expression tag	UNP Q9WYC4

- Molecule 3 is a protein called Nb_TM No.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	129	Total	C	N	O	S	0	0	0
			974	611	164	193	6			
3	F	129	Total	C	N	O	S	0	0	0
			974	611	164	193	6			

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

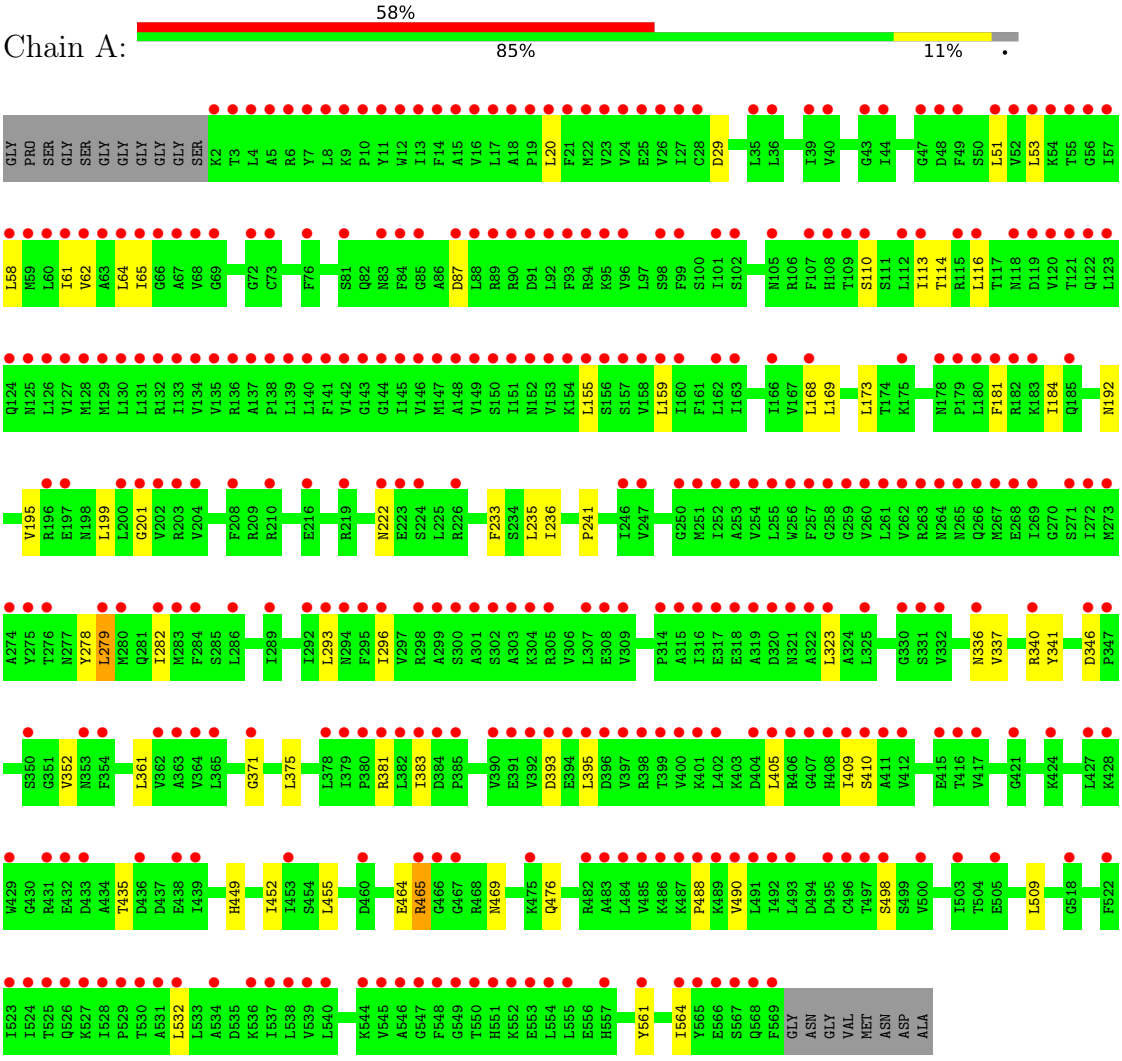
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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.

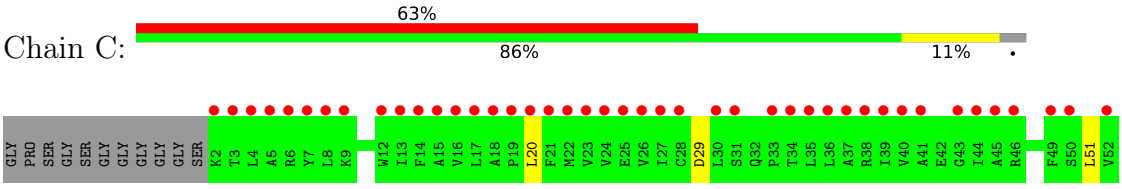
• Molecule 1: ABC transporter, ATP-binding protein

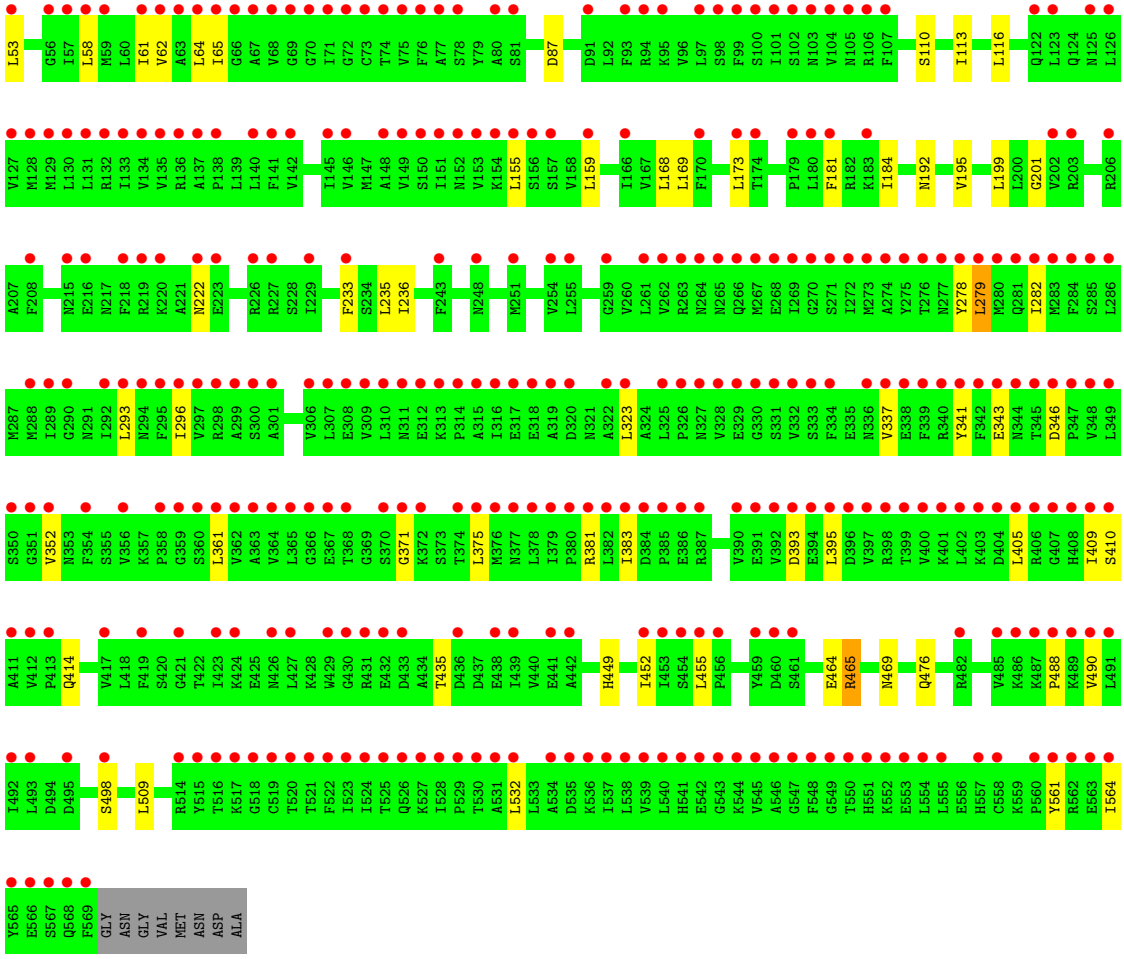
Chain A:



• Molecule 1: ABC transporter, ATP-binding protein

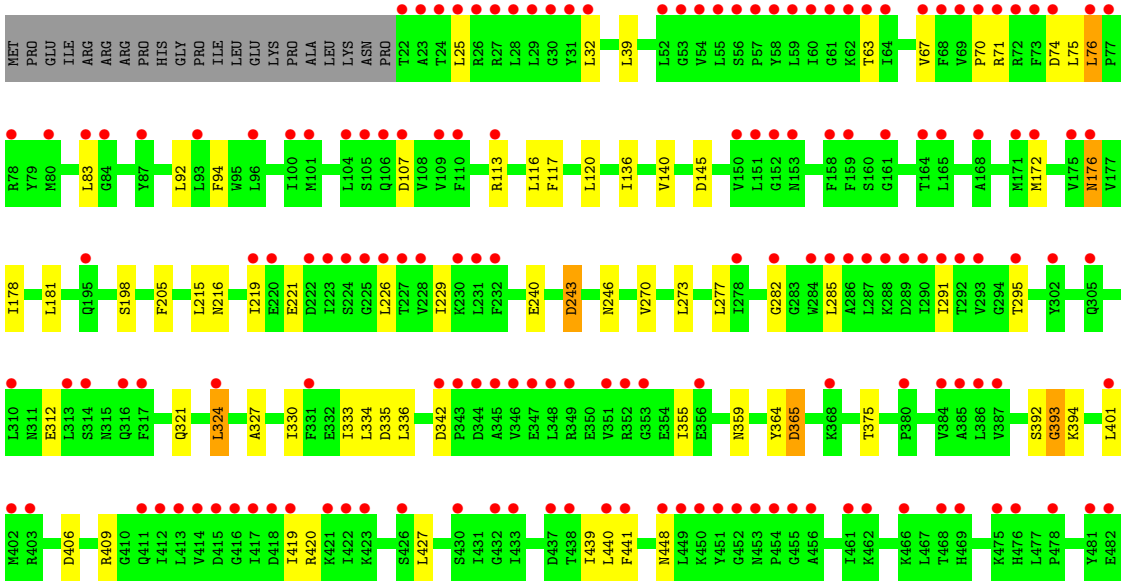
Chain C:

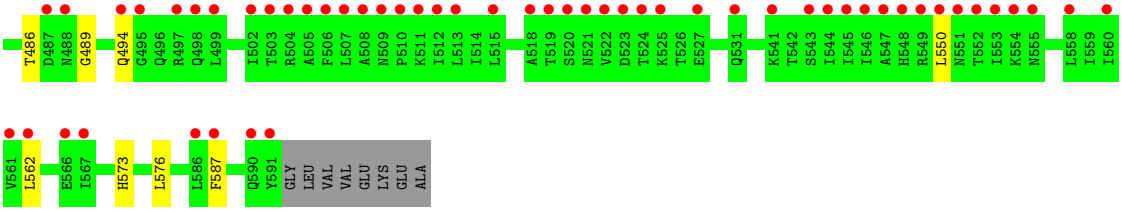




• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

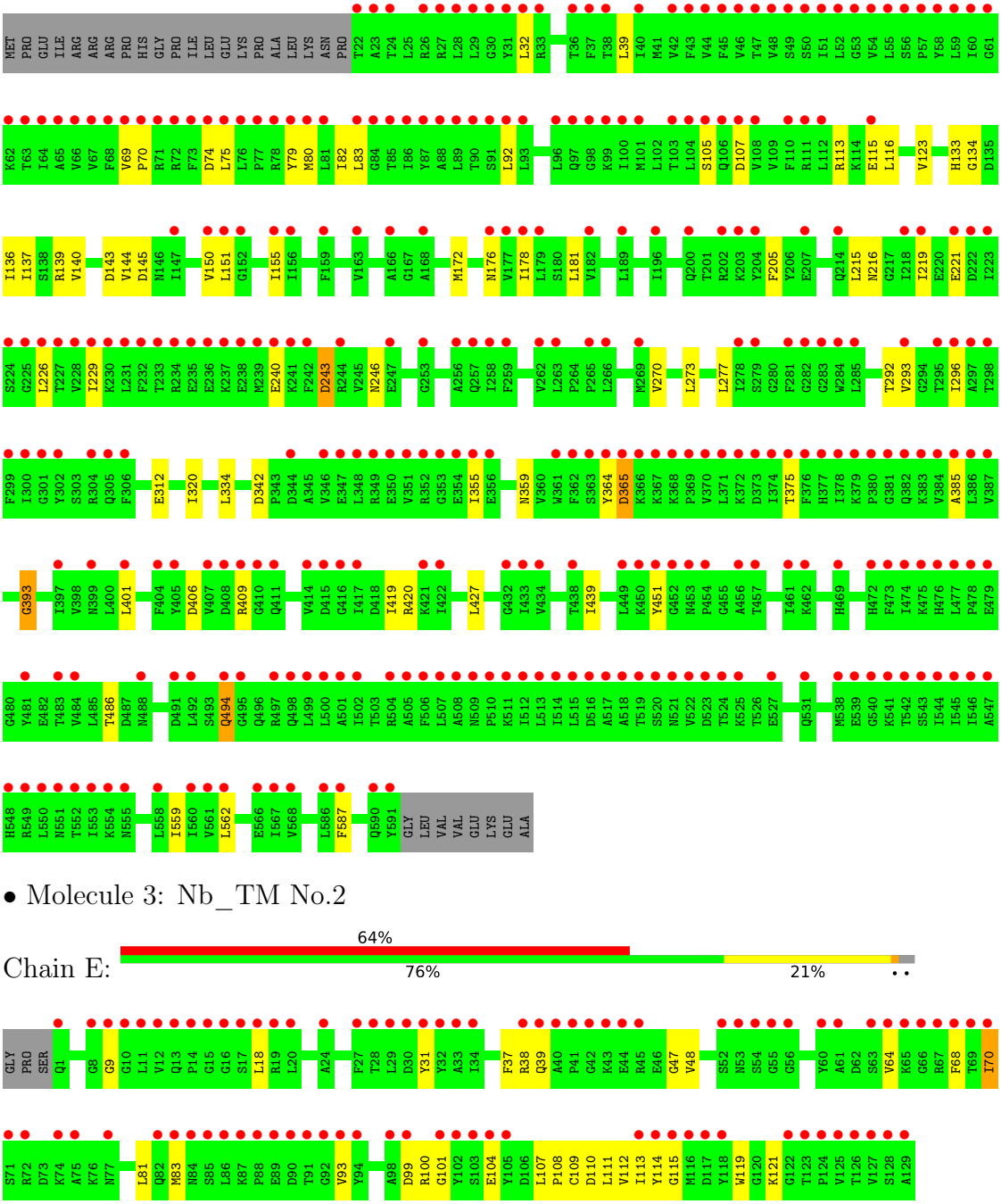
Chain B:





• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288

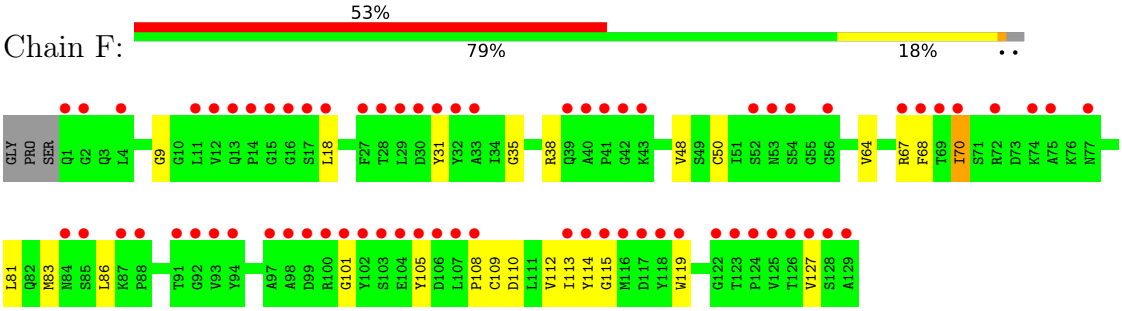
Chain D:



• Molecule 3: Nb_TM No.2

Chain E:

• Molecule 3: Nb_TM No.2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	88.60Å 113.07Å 126.89Å 83.18° 73.00° 67.37°	Depositor
Resolution (Å)	32.59 – 4.23 48.06 – 4.22	Depositor EDS
% Data completeness (in resolution range)	57.9 (32.59-4.23) 57.5 (48.06-4.22)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 4.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.306 , 0.330 0.342 , 0.350	Depositor DCC
R_{free} test set	919 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	129.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 301.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.018 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	20086	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.39	0/4539	0.53	0/6139
1	C	0.40	0/4539	0.53	0/6139
2	B	0.40	0/4619	0.55	0/6245
2	D	0.40	0/4619	0.55	0/6245
3	E	0.38	0/995	0.59	0/1345
3	F	0.40	0/995	0.59	0/1345
All	All	0.40	0/20306	0.55	0/27458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4464	0	4666	21	0
1	C	4464	0	4666	22	0
2	B	4541	0	4724	32	0
2	D	4541	0	4724	31	0
3	E	974	0	934	8	0
3	F	974	0	934	9	0
4	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	2	0
4	C	31	0	12	0	0
4	D	31	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	20086	0	20696	108	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 3.

All (108) 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)
3:F:38:ARG:HG2	3:F:48:VAL:HG22	1.79	0.64
2:D:216:ASN:HA	2:D:219:ILE:HD12	1.87	0.56
2:B:32:LEU:HB3	2:B:39:LEU:HD11	1.89	0.55
2:D:32:LEU:HB3	2:D:39:LEU:HD11	1.89	0.55
2:B:216:ASN:HA	2:B:219:ILE:HD12	1.89	0.55
3:E:9:GLY:HA2	3:E:18:LEU:HD22	1.89	0.55
2:B:198:SER:HB2	2:B:321:GLN:HG3	1.88	0.54
2:B:117:PHE:HA	2:B:120:LEU:HD12	1.89	0.54
1:C:465:ARG:HG3	2:D:221:GLU:HG3	1.89	0.54
2:B:176:ASN:HD21	2:B:291:ILE:HD13	1.73	0.54
1:C:199:LEU:HB3	2:D:133:HIS:HD2	1.73	0.53
3:F:9:GLY:HA2	3:F:18:LEU:HD22	1.91	0.53
1:A:465:ARG:HG3	2:B:221:GLU:HG3	1.91	0.52
2:B:333:ILE:HA	2:B:336:LEU:HD12	1.91	0.52
3:E:38:ARG:HG2	3:E:48:VAL:HG22	1.92	0.52
1:A:476:GLN:HE22	1:A:498:SER:H	1.58	0.52
2:B:226:LEU:HA	2:B:229:ILE:HD12	1.91	0.52
1:C:561:TYR:HA	1:C:564:ILE:HD12	1.92	0.52
3:E:37:PHE:HA	3:E:47:GLY:HA2	1.92	0.51
1:C:201:GLY:HA3	2:D:439:ILE:HG21	1.92	0.51
1:C:476:GLN:HE22	1:C:498:SER:H	1.58	0.51
1:A:561:TYR:HA	1:A:564:ILE:HD12	1.93	0.51
2:D:226:LEU:HA	2:D:229:ILE:HD12	1.91	0.51
2:D:150:VAL:HG23	2:D:320:ILE:HG22	1.93	0.51
1:A:201:GLY:HA3	2:B:439:ILE:HG21	1.92	0.50
2:D:113:ARG:HG3	2:D:144:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:35:GLY:HA3	3:F:50:CYS:HA	1.93	0.50
1:A:233:PHE:HA	1:A:236:ILE:HD12	1.94	0.50
2:D:365:ASP:HB3	4:D:600:AGS:H2	1.93	0.50
3:E:100:ARG:HB2	3:E:111:LEU:HD23	1.92	0.50
1:A:199:LEU:HD21	2:B:136:ILE:HD13	1.94	0.50
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.94	0.50
2:B:365:ASP:HB3	4:B:600:AGS:H2	1.93	0.50
3:F:70:ILE:HG23	3:F:81:LEU:HD23	1.95	0.49
1:C:181:PHE:HA	1:C:184:ILE:HD12	1.94	0.49
1:A:181:PHE:HA	1:A:184:ILE:HD12	1.94	0.49
3:F:64:VAL:HG13	3:F:67:ARG:HH11	1.78	0.48
3:E:70:ILE:HG23	3:E:81:LEU:HD23	1.96	0.48
1:A:222:ASN:HD21	2:B:113:ARG:HB3	1.77	0.48
1:A:464:GLU:HB2	1:A:469:ASN:HB3	1.95	0.48
1:A:279:LEU:HA	1:A:282:ILE:HD12	1.96	0.48
2:B:355:ILE:HD12	2:B:401:LEU:HD11	1.96	0.48
1:C:279:LEU:HA	1:C:282:ILE:HD12	1.95	0.48
2:D:79:TYR:HA	2:D:82:ILE:HD12	1.95	0.48
2:D:293:VAL:HA	2:D:296:ILE:HD12	1.96	0.48
1:C:464:GLU:HB2	1:C:469:ASN:HB3	1.95	0.47
2:D:355:ILE:HD12	2:D:401:LEU:HD11	1.96	0.47
1:C:337:VAL:HB	1:C:352:VAL:HB	1.96	0.47
1:A:337:VAL:HB	1:A:352:VAL:HB	1.96	0.47
1:C:199:LEU:HD21	2:D:136:ILE:HD13	1.98	0.46
2:D:409:ARG:HD2	3:F:105:TYR:HB2	1.98	0.46
2:D:105:SER:HA	2:D:151:LEU:HD22	1.99	0.45
2:B:67:VAL:HG13	2:B:70:PRO:HG2	1.98	0.45
2:B:441:PHE:H	2:B:448:ASN:HD21	1.64	0.45
1:C:410:SER:HB2	1:C:488:PRO:HG3	1.98	0.45
1:A:195:VAL:HG21	2:B:140:VAL:HG21	1.98	0.45
1:A:62:VAL:HA	1:A:65:ILE:HD12	1.98	0.45
2:D:80:MET:HA	2:D:83:LEU:HD12	1.98	0.45
2:B:327:ALA:HA	2:B:330:ILE:HD12	1.99	0.45
2:B:440:LEU:HD22	2:B:489:GLY:HA3	1.98	0.45
1:A:410:SER:HB2	1:A:488:PRO:HG3	1.98	0.45
3:E:39:GLN:HB2	3:E:93:VAL:O	2.17	0.45
1:A:409:ILE:HG12	1:A:490:VAL:HB	1.98	0.45
1:A:449:HIS:HA	1:A:452:ILE:HD12	1.99	0.45
1:C:293:LEU:HA	1:C:296:ILE:HD12	1.99	0.44
1:C:409:ILE:HG12	1:C:490:VAL:HB	1.98	0.44
1:C:449:HIS:HA	1:C:452:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:VAL:HA	2:D:273:LEU:HD12	1.98	0.44
2:B:419:ILE:HG23	2:B:420:ARG:HD3	2.00	0.44
1:C:62:VAL:HA	1:C:65:ILE:HD12	1.98	0.44
2:D:385:ALA:HB3	2:D:559:ILE:HG12	1.99	0.44
2:B:282:GLY:HA2	2:B:285:LEU:HD12	2.00	0.44
1:C:195:VAL:HG21	2:D:140:VAL:HG21	1.99	0.44
1:C:222:ASN:HD21	2:D:113:ARG:HB3	1.83	0.44
2:D:419:ILE:HG23	2:D:420:ARG:HD3	1.99	0.44
1:A:293:LEU:HA	1:A:296:ILE:HD12	1.99	0.44
2:B:270:VAL:HA	2:B:273:LEU:HD12	1.98	0.44
3:E:64:VAL:HB	3:E:68:PHE:CE2	2.53	0.44
2:B:67:VAL:HG11	2:B:76:LEU:HB2	2.00	0.43
2:B:25:LEU:HB2	2:B:324:LEU:HD21	1.99	0.42
2:B:409:ARG:HD3	3:E:107:LEU:HG	2.00	0.42
2:D:115:GLU:HB3	2:D:334:LEU:HD21	2.01	0.42
2:B:178:ILE:HA	2:B:181:LEU:HD12	2.01	0.42
1:A:452:ILE:HA	1:A:455:LEU:HD12	2.02	0.42
2:D:139:ARG:HA	2:D:143:ASP:HB2	2.00	0.42
2:B:63:THR:HG21	2:B:83:LEU:HD11	2.02	0.42
1:C:452:ILE:HA	1:C:455:LEU:HD12	2.02	0.42
1:C:110:SER:HA	1:C:113:ILE:HD12	2.02	0.42
2:D:178:ILE:HA	2:D:181:LEU:HD12	2.01	0.42
1:A:110:SER:HA	1:A:113:ILE:HD12	2.01	0.41
2:D:151:LEU:HA	2:D:155:ILE:HD12	2.03	0.41
2:D:134:GLY:HA2	2:D:137:ILE:HD12	2.03	0.41
2:B:392:SER:HB3	2:B:394:LYS:HZ3	1.86	0.41
1:C:58:LEU:HA	1:C:61:ILE:HD12	2.01	0.41
2:B:359:ASN:H	2:B:375:THR:HB	1.86	0.41
2:B:573:HIS:HA	2:B:576:LEU:HD12	2.03	0.41
1:A:58:LEU:HA	1:A:61:ILE:HD12	2.01	0.41
2:D:359:ASN:H	2:D:375:THR:HB	1.86	0.41
3:F:38:ARG:HH12	3:F:83:MET:HG2	1.85	0.41
3:F:86:LEU:HD13	3:F:127:VAL:HG11	2.02	0.41
1:C:414:GLN:HB3	2:D:494:GLN:HG3	2.03	0.41
1:A:241:PRO:HB3	2:B:94:PHE:HB3	2.02	0.40
2:D:393:GLY:HA2	4:D:600:AGS:H5'1	2.03	0.40
2:D:69:VAL:HB	2:D:70:PRO:HD3	2.03	0.40
2:D:240:GLU:HA	2:D:243:ASP:HB2	2.03	0.40
2:B:240:GLU:HA	2:B:243:ASP:HB2	2.03	0.40
2:B:393:GLY:HA2	4:B:600:AGS:H5'1	2.04	0.40
3:F:68:PHE:HB3	3:F:81:LEU:HD21	2.04	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	566/587 (96%)	544 (96%)	19 (3%)	3 (0%)	29	68
1	C	566/587 (96%)	542 (96%)	22 (4%)	2 (0%)	34	72
2	B	568/599 (95%)	541 (95%)	24 (4%)	3 (0%)	29	68
2	D	568/599 (95%)	540 (95%)	26 (5%)	2 (0%)	34	72
3	E	127/132 (96%)	93 (73%)	28 (22%)	6 (5%)	2	24
3	F	127/132 (96%)	94 (74%)	28 (22%)	5 (4%)	3	27
All	All	2522/2636 (96%)	2354 (93%)	147 (6%)	21 (1%)	19	60

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	108	PRO
3	F	108	PRO
3	E	101	GLY
2	B	71	ARG
3	F	113	ILE
2	B	74	ASP
2	D	74	ASP
3	E	113	ILE
3	E	121	LYS
3	F	101	GLY
3	F	112	VAL
1	A	336	ASN
1	C	371	GLY
1	A	371	GLY
1	A	381	ARG
1	C	381	ARG
3	E	112	VAL

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Mol	Chain	Res	Type
3	F	115	GLY
2	B	393	GLY
2	D	393	GLY
3	E	115	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/503 (98%)	463 (94%)	31 (6%)	18	45
1	C	494/503 (98%)	464 (94%)	30 (6%)	18	46
2	B	506/531 (95%)	478 (94%)	28 (6%)	21	50
2	D	506/531 (95%)	481 (95%)	25 (5%)	25	52
3	E	102/104 (98%)	93 (91%)	9 (9%)	10	34
3	F	102/104 (98%)	96 (94%)	6 (6%)	19	47
All	All	2204/2276 (97%)	2075 (94%)	129 (6%)	19	47

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	29	ASP
1	A	51	LEU
1	A	53	LEU
1	A	64	LEU
1	A	87	ASP
1	A	114	THR
1	A	116	LEU
1	A	155	LEU
1	A	159	LEU
1	A	168	LEU
1	A	169	LEU
1	A	173	LEU
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	278	TYR
1	A	279	LEU
1	A	323	LEU
1	A	340	ARG
1	A	341	TYR
1	A	346	ASP
1	A	361	LEU
1	A	375	LEU
1	A	383	ILE
1	A	393	ASP
1	A	395	LEU
1	A	405	LEU
1	A	435	THR
1	A	465	ARG
1	A	509	LEU
1	A	532	LEU
2	B	75	LEU
2	B	76	LEU
2	B	92	LEU
2	B	107	ASP
2	B	116	LEU
2	B	145	ASP
2	B	172	MET
2	B	176	ASN
2	B	205	PHE
2	B	215	LEU
2	B	243	ASP
2	B	246	ASN
2	B	277	LEU
2	B	295	THR
2	B	312	GLU
2	B	324	LEU
2	B	334	LEU
2	B	335	ASP
2	B	342	ASP
2	B	364	TYR
2	B	365	ASP
2	B	406	ASP
2	B	427	LEU
2	B	486	THR
2	B	494	GLN

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Mol	Chain	Res	Type
2	B	550	LEU
2	B	562	LEU
2	B	587	PHE
1	C	20	LEU
1	C	29	ASP
1	C	51	LEU
1	C	53	LEU
1	C	64	LEU
1	C	87	ASP
1	C	116	LEU
1	C	155	LEU
1	C	159	LEU
1	C	168	LEU
1	C	169	LEU
1	C	173	LEU
1	C	192	ASN
1	C	235	LEU
1	C	278	TYR
1	C	279	LEU
1	C	323	LEU
1	C	341	TYR
1	C	343	GLU
1	C	346	ASP
1	C	361	LEU
1	C	375	LEU
1	C	383	ILE
1	C	393	ASP
1	C	395	LEU
1	C	405	LEU
1	C	435	THR
1	C	465	ARG
1	C	509	LEU
1	C	532	LEU
2	D	75	LEU
2	D	92	LEU
2	D	107	ASP
2	D	116	LEU
2	D	123	VAL
2	D	145	ASP
2	D	172	MET
2	D	176	ASN
2	D	205	PHE

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Mol	Chain	Res	Type
2	D	215	LEU
2	D	243	ASP
2	D	246	ASN
2	D	277	LEU
2	D	292	THR
2	D	312	GLU
2	D	342	ASP
2	D	364	TYR
2	D	365	ASP
2	D	406	ASP
2	D	427	LEU
2	D	451	TYR
2	D	486	THR
2	D	494	GLN
2	D	562	LEU
2	D	587	PHE
3	E	31	TYR
3	E	70	ILE
3	E	83	MET
3	E	99	ASP
3	E	104	GLU
3	E	109	CYS
3	E	110	ASP
3	E	114	TYR
3	E	119	TRP
3	F	31	TYR
3	F	70	ILE
3	F	109	CYS
3	F	110	ASP
3	F	114	TYR
3	F	119	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN
2	B	176	ASN
2	B	268	ASN
2	B	377	HIS
2	B	448	ASN
2	B	488	ASN
2	B	521	ASN

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Mol	Chain	Res	Type
2	B	551	ASN
2	B	590	GLN
1	C	222	ASN
1	C	474	GLN
1	C	476	GLN
2	D	133	HIS
2	D	176	ASN
2	D	268	ASN
2	D	377	HIS
2	D	448	ASN
2	D	521	ASN
3	F	84	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	AGS	C	600	5	26,33,33	0.60	0	26,52,52	0.68	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	AGS	B	600	5	26,33,33	0.61	0	26,52,52	0.73	1 (3%)
4	AGS	A	600	5	26,33,33	0.60	0	26,52,52	0.71	1 (3%)
4	AGS	D	600	5	26,33,33	0.60	0	26,52,52	0.73	1 (3%)

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
4	AGS	C	600	5	-	0/17/38/38	0/3/3/3
4	AGS	B	600	5	-	4/17/38/38	0/3/3/3
4	AGS	A	600	5	-	3/17/38/38	0/3/3/3
4	AGS	D	600	5	-	4/17/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	600	AGS	C5-C6-N6	2.27	123.80	120.35
4	D	600	AGS	C5-C6-N6	2.25	123.77	120.35
4	B	600	AGS	C5-C6-N6	2.24	123.76	120.35
4	C	600	AGS	C5-C6-N6	2.21	123.72	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	AGS	C5'-O5'-PA-O1A
4	D	600	AGS	C5'-O5'-PA-O1A
4	B	600	AGS	C5'-O5'-PA-O3A
4	D	600	AGS	C5'-O5'-PA-O3A
4	B	600	AGS	C5'-O5'-PA-O2A
4	D	600	AGS	C5'-O5'-PA-O2A
4	A	600	AGS	PB-O3B-PG-O3G
4	B	600	AGS	PA-O3A-PB-O1B
4	D	600	AGS	PA-O3A-PB-O1B
4	A	600	AGS	PG-O3B-PB-O1B
4	A	600	AGS	PG-O3B-PB-O2B

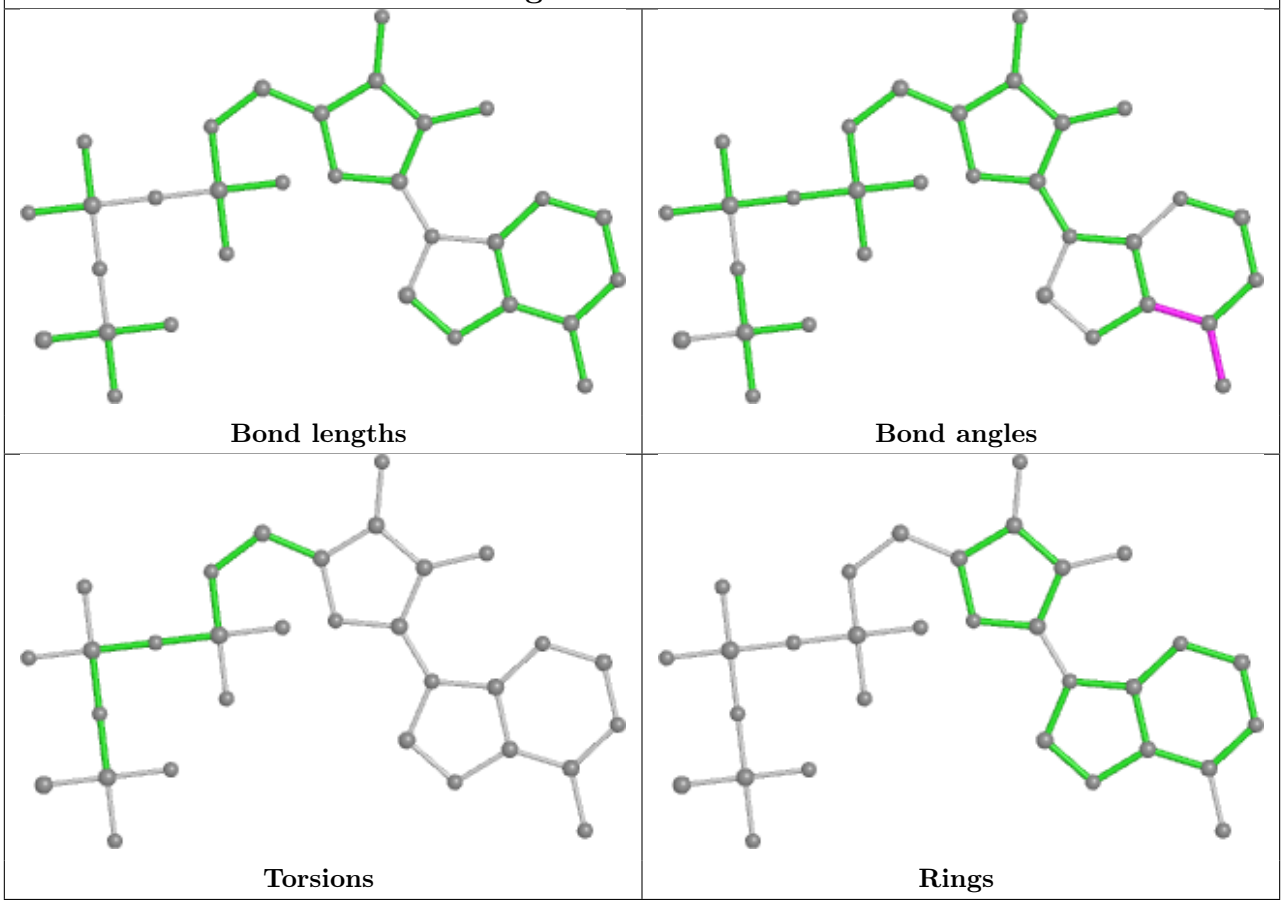
There are no ring outliers.

2 monomers are involved in 4 short contacts:

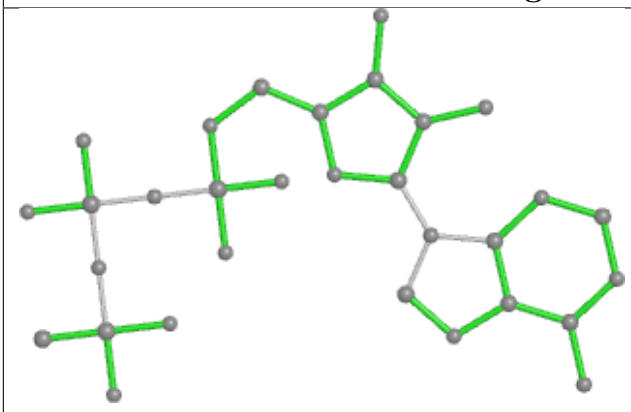
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	AGS	2	0
4	D	600	AGS	2	0

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.

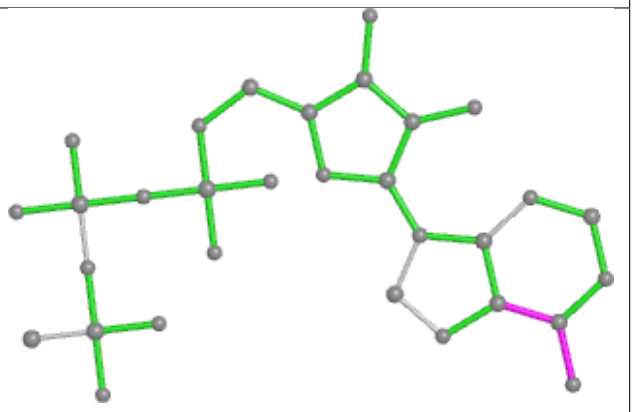
Ligand AGS C 600



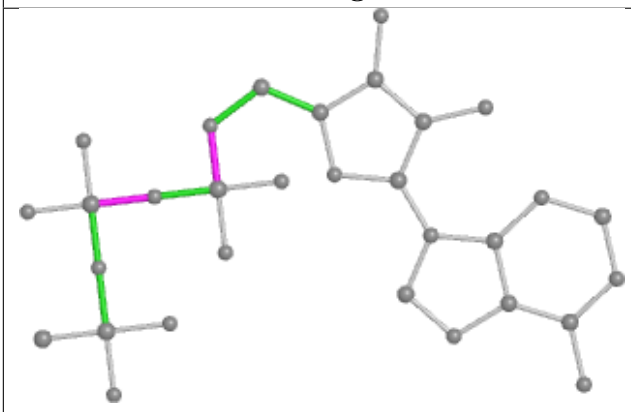
Ligand AGS B 600



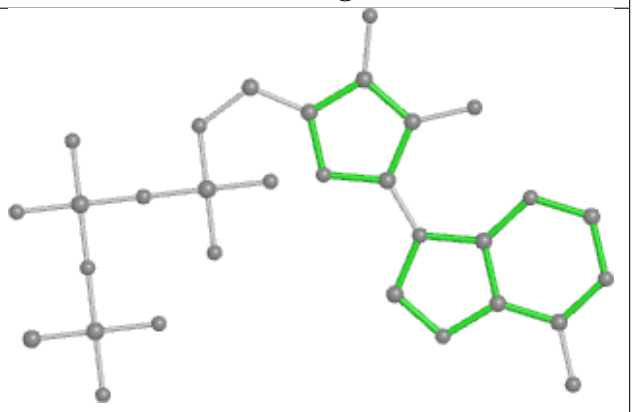
Bond lengths



Bond angles

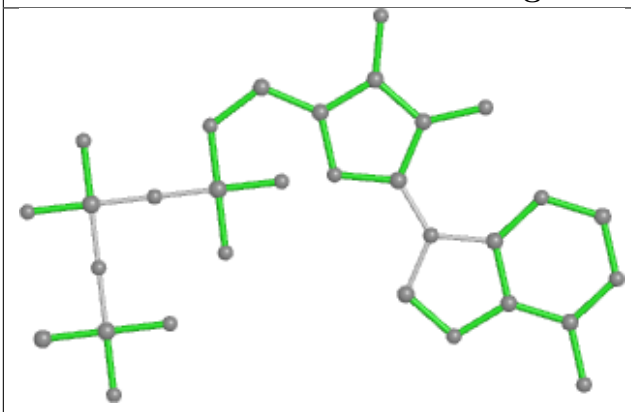


Torsions

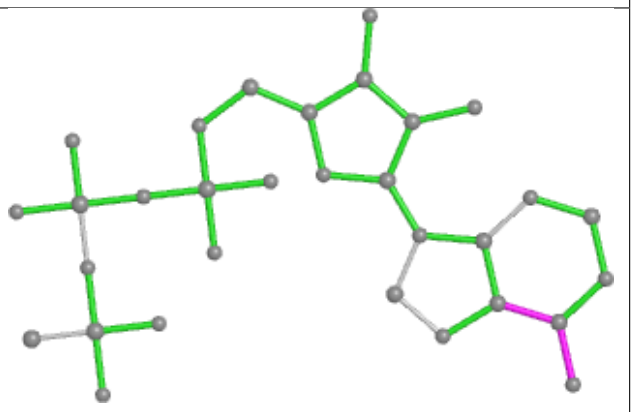


Rings

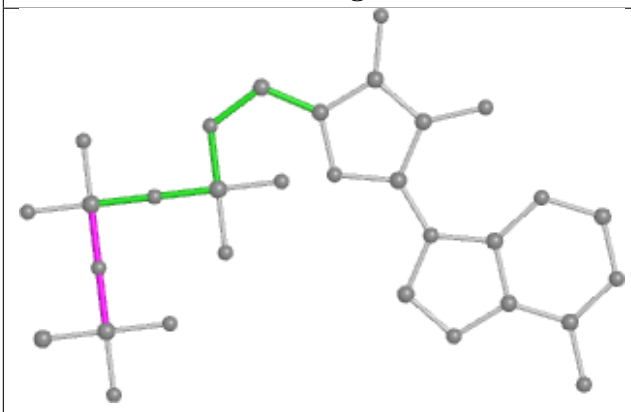
Ligand AGS A 600



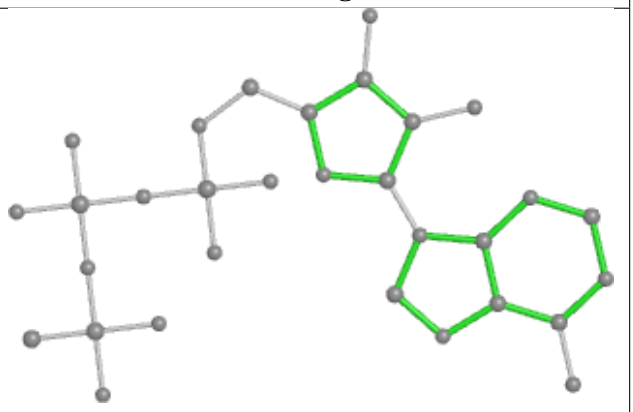
Bond lengths



Bond angles

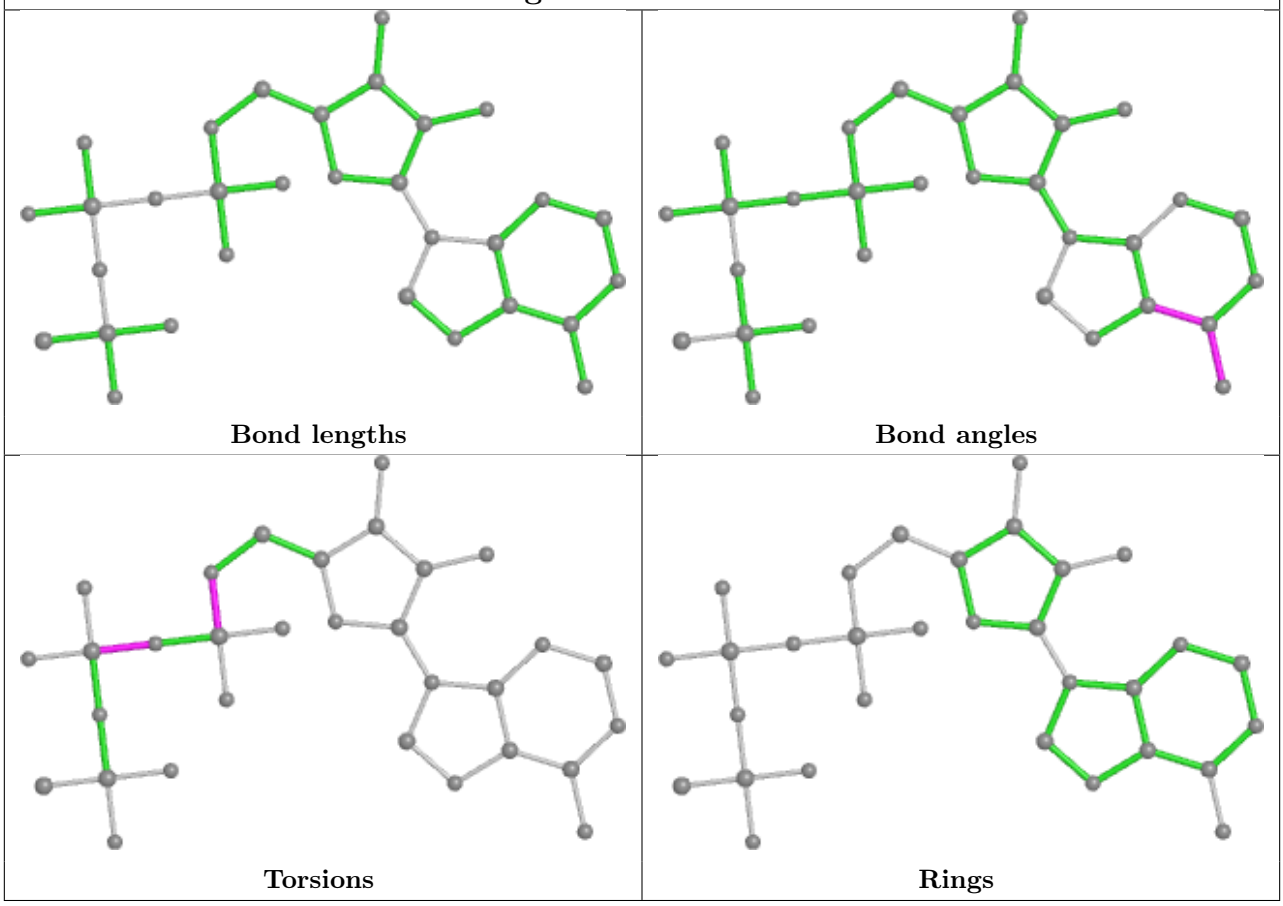


Torsions



Rings

Ligand AGS D 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	568/587 (96%)	3.59	339 (59%) 0 0	36, 173, 288, 300	0
1	C	568/587 (96%)	4.63	371 (65%) 0 0	23, 229, 269, 283	0
2	B	570/599 (95%)	1.85	213 (37%) 0 0	3, 94, 191, 232	0
2	D	570/599 (95%)	3.18	305 (53%) 0 0	19, 193, 267, 289	0
3	E	129/132 (97%)	5.12	85 (65%) 0 0	94, 178, 298, 300	0
3	F	129/132 (97%)	4.20	70 (54%) 0 0	80, 133, 277, 300	0
All	All	2534/2636 (96%)	3.45	1383 (54%) 0 0	3, 180, 276, 300	0

All (1383) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	547	GLY	35.0
1	C	410	SER	24.5
1	C	19	PRO	23.0
1	C	546	ALA	22.2
3	F	14	PRO	22.1
1	A	152	ASN	21.6
3	E	103	SER	21.4
3	E	127	VAL	20.7
3	F	15	GLY	20.6
1	C	23	VAL	20.4
1	C	408	HIS	19.7
1	C	319	ALA	19.4
3	F	115	GLY	19.3
3	F	16	GLY	18.2
1	C	268	GLU	18.0
3	E	91	THR	18.0
1	C	549	GLY	17.9
3	E	92	GLY	17.5
1	C	384	ASP	17.5

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Mol	Chain	Res	Type	RSRZ
1	C	518	GLY	17.4
2	D	370	VAL	17.2
3	E	14	PRO	17.2
1	C	406	ARG	17.0
2	D	54	VAL	16.8
3	F	101	GLY	16.6
1	A	260	VAL	16.5
1	C	401	LYS	16.5
3	E	87	LYS	16.4
1	C	407	GLY	16.2
1	C	526	GLN	16.1
3	E	125	VAL	16.0
1	A	14	PHE	16.0
1	C	551	HIS	15.7
1	C	568	GLN	15.6
1	C	519	CYS	15.5
1	C	545	VAL	15.5
1	C	550	THR	15.5
1	C	330	GLY	15.3
1	C	3	THR	15.3
1	C	404	ASP	15.2
1	A	150	SER	15.1
1	C	18	ALA	15.0
3	E	128	SER	14.9
1	C	543	GLY	14.9
3	E	41	PRO	14.5
1	A	25	GLU	14.4
1	C	527	LYS	14.4
3	F	41	PRO	14.3
3	E	126	THR	14.3
1	C	525	THR	14.2
3	E	55	GLY	14.2
1	C	381	ARG	14.1
2	D	56	SER	14.0
3	F	13	GLN	14.0
1	A	526	GLN	14.0
1	C	489	LYS	14.0
3	E	115	GLY	13.9
1	C	364	VAL	13.9
1	A	21	PHE	13.8
1	C	380	PRO	13.7
2	D	369	PRO	13.7

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Mol	Chain	Res	Type	RSRZ
2	D	521	ASN	13.7
2	D	408	ASP	13.6
1	C	151	ILE	13.6
1	A	9	LYS	13.5
1	A	266	GLN	13.4
1	C	351	GLY	13.3
1	A	399	THR	13.3
3	E	89	GLU	13.3
1	C	411	ALA	13.2
1	A	144	GLY	13.2
1	C	274	ALA	13.2
2	D	363	SER	13.1
2	D	57	PRO	13.0
3	F	103	SER	13.0
1	A	155	LEU	12.8
1	A	263	ARG	12.8
2	D	77	PRO	12.8
1	C	383	ILE	12.8
1	A	22	MET	12.7
2	D	365	ASP	12.6
1	C	530	THR	12.6
1	A	319	ALA	12.5
1	A	10	PRO	12.5
1	C	363	ALA	12.5
1	C	70	GLY	12.5
2	B	72	ARG	12.4
1	C	66	GLY	12.4
1	C	531	ALA	12.4
1	C	24	VAL	12.3
1	A	151	ILE	12.3
2	D	549	ARG	12.3
1	C	73	CYS	12.3
2	D	65	ALA	12.3
2	D	230	LYS	12.2
1	A	262	VAL	12.2
1	A	7	TYR	12.2
1	C	278	TYR	12.1
1	A	5	ALA	12.1
2	D	523	ASP	12.0
1	C	341	TYR	12.0
1	A	317	GLU	12.0
2	D	352	ARG	12.0

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Mol	Chain	Res	Type	RSRZ
2	D	72	ARG	12.0
2	D	522	VAL	12.0
1	C	528	ILE	12.0
2	D	552	THR	12.0
1	C	22	MET	11.9
3	E	88	PRO	11.9
1	C	314	PRO	11.9
1	C	267	MET	11.9
3	E	33	ALA	11.8
1	C	317	GLU	11.8
1	C	67	ALA	11.8
1	C	264	ASN	11.8
1	C	400	VAL	11.8
3	F	125	VAL	11.8
1	A	322	ALA	11.8
2	D	368	LYS	11.7
1	C	490	VAL	11.7
1	C	25	GLU	11.7
1	A	146	VAL	11.7
1	C	370	SER	11.7
2	D	232	PHE	11.7
3	E	102	TYR	11.7
3	F	126	THR	11.7
1	C	69	GLY	11.6
1	C	338	GLU	11.6
1	C	135	VAL	11.6
1	A	11	TYR	11.6
1	C	541	HIS	11.6
1	A	568	GLN	11.6
1	A	265	ASN	11.5
3	E	56	GLY	11.5
1	C	20	LEU	11.4
3	F	106	ASP	11.4
1	A	264	ASN	11.3
1	C	74	THR	11.3
2	B	57	PRO	11.2
2	D	551	ASN	11.2
1	C	548	PHE	11.1
2	D	71	ARG	11.1
1	C	488	PRO	11.1
1	C	402	LEU	11.1
1	A	19	PRO	11.0

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Mol	Chain	Res	Type	RSRZ
2	D	233	THR	11.0
1	A	259	GLY	11.0
1	A	23	VAL	10.9
1	C	366	GLY	10.9
2	B	56	SER	10.9
1	C	542	GLU	10.9
1	C	339	PHE	10.9
1	C	271	SER	10.8
2	D	50	SER	10.8
1	C	150	SER	10.7
1	C	316	ILE	10.7
1	C	409	ILE	10.7
1	C	520	THR	10.7
3	E	84	ASN	10.6
2	D	78	ARG	10.6
1	A	401	LYS	10.6
2	D	234	ARG	10.6
1	A	8	LEU	10.6
3	F	29	LEU	10.6
1	C	536	LYS	10.6
2	D	409	ARG	10.6
1	A	128	MET	10.5
1	C	318	GLU	10.5
1	A	383	ILE	10.5
3	E	13	GLN	10.4
1	C	393	ASP	10.4
3	F	116	MET	10.4
1	A	537	ILE	10.4
1	C	17	LEU	10.4
2	D	73	PHE	10.4
1	A	147	MET	10.3
2	B	58	TYR	10.3
2	D	225	GLY	10.3
1	C	405	LEU	10.3
1	C	263	ARG	10.2
2	D	366	LYS	10.2
1	A	135	VAL	10.2
2	B	453	ASN	10.2
2	D	70	PRO	10.2
2	B	455	GLY	10.1
3	F	42	GLY	10.1
1	C	397	VAL	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	142	VAL	10.1
1	C	529	PRO	10.1
3	F	17	SER	10.1
2	D	53	GLY	10.0
1	A	318	GLU	10.0
3	F	74	LYS	10.0
2	D	64	ILE	10.0
3	E	12	VAL	9.9
2	B	345	ALA	9.9
1	A	525	THR	9.9
1	A	538	LEU	9.9
2	D	235	GLU	9.9
1	C	280	MET	9.9
1	C	569	PHE	9.8
1	C	277	ASN	9.8
3	E	54	SER	9.8
1	A	149	VAL	9.8
1	C	266	GLN	9.8
3	E	32	TYR	9.8
3	F	117	ASP	9.7
1	C	62	VAL	9.7
1	A	489	LYS	9.7
2	D	63	THR	9.7
1	A	18	ALA	9.7
1	C	350	SER	9.6
2	D	22	THR	9.6
3	E	90	ASP	9.6
2	B	290	ILE	9.6
2	B	54	VAL	9.5
1	C	544	LYS	9.5
1	A	153	VAL	9.5
2	D	58	TYR	9.5
2	B	521	ASN	9.5
2	B	53	GLY	9.5
3	F	99	ASP	9.5
2	B	452	GLY	9.4
2	B	510	PRO	9.4
2	D	478	PRO	9.4
1	A	148	ALA	9.4
1	C	270	GLY	9.4
2	B	344	ASP	9.4
1	C	539	VAL	9.3

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Mol	Chain	Res	Type	RSRZ
2	D	80	MET	9.3
1	A	275	TYR	9.3
2	D	62	LYS	9.3
1	A	145	ILE	9.3
3	E	68	PHE	9.3
2	B	289	ASP	9.3
1	C	5	ALA	9.2
1	A	6	ARG	9.2
1	A	268	GLU	9.2
1	C	290	GLY	9.2
3	F	102	TYR	9.2
2	D	282	GLY	9.2
3	E	31	TYR	9.2
1	A	24	VAL	9.1
2	D	74	ASP	9.1
2	D	231	LEU	9.1
2	B	454	PRO	9.1
1	A	124	GLN	9.1
3	F	43	LYS	9.1
1	C	275	TYR	9.1
1	A	129	MET	9.0
2	B	509	ASN	9.0
3	E	10	GLY	9.0
2	D	302	TYR	9.0
1	A	397	VAL	9.0
2	D	550	LEU	9.0
2	B	522	VAL	8.9
2	B	590	GLN	8.9
3	E	18	LEU	8.9
2	D	364	TYR	8.9
1	A	91	ASP	8.9
1	A	141	PHE	8.9
3	F	32	TYR	8.8
2	D	66	VAL	8.8
1	A	119	ASP	8.8
1	A	549	GLY	8.8
1	C	367	GLU	8.8
1	C	13	ILE	8.7
1	A	396	ASP	8.7
1	C	28	CYS	8.7
1	C	315	ALA	8.7
1	C	136	ARG	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	8.7
2	D	87	TYR	8.7
1	C	521	THR	8.7
1	A	261	LEU	8.7
1	C	16	VAL	8.6
2	D	367	LYS	8.6
1	C	538	LEU	8.6
1	C	137	ALA	8.6
1	A	182	ARG	8.5
1	C	349	LEU	8.5
1	C	537	ILE	8.5
1	C	398	ARG	8.5
1	C	320	ASP	8.5
3	F	28	THR	8.5
1	A	272	ILE	8.4
1	C	382	LEU	8.4
2	D	372	LYS	8.4
1	C	403	LYS	8.4
1	A	536	LYS	8.4
2	D	361	TRP	8.3
3	E	30	ASP	8.3
2	D	567	ILE	8.3
1	C	134	VAL	8.2
1	A	13	ILE	8.2
3	F	92	GLY	8.2
2	B	71	ARG	8.2
1	C	6	ARG	8.2
2	D	237	LYS	8.2
1	C	14	PHE	8.2
3	E	117	ASP	8.1
1	A	140	LEU	8.1
2	D	67	VAL	8.1
1	C	26	VAL	8.1
1	A	551	HIS	8.1
3	E	53	ASN	8.1
2	D	301	GLY	8.0
2	D	519	THR	8.0
1	A	136	ARG	8.0
1	C	432	GLU	8.0
1	C	265	ASN	8.0
1	A	553	GLU	8.0
1	C	152	ASN	8.0

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Mol	Chain	Res	Type	RSRZ
3	F	128	SER	8.0
1	A	26	VAL	8.0
1	C	63	ALA	8.0
2	B	347	GLU	7.9
2	D	305	GLN	7.9
2	B	342	ASP	7.9
3	E	85	SER	7.9
3	E	86	LEU	7.9
1	C	76	PHE	7.9
1	C	4	LEU	7.9
2	B	591	TYR	7.9
3	F	104	GLU	7.9
1	A	527	LYS	7.9
3	F	100	ARG	7.9
2	D	76	LEU	7.9
1	A	17	LEU	7.9
2	D	176	ASN	7.9
2	D	371	LEU	7.9
2	B	549	ARG	7.8
1	A	316	ILE	7.8
3	E	74	LYS	7.8
3	F	91	THR	7.8
1	C	553	GLU	7.8
3	F	105	TYR	7.8
3	F	30	ASP	7.8
3	E	42	GLY	7.8
1	A	20	LEU	7.8
1	A	320	ASP	7.8
1	A	132	ARG	7.8
1	A	154	LYS	7.8
3	F	27	PHE	7.8
1	C	342	PHE	7.8
1	C	102	SER	7.7
1	C	132	ARG	7.7
1	A	406	ARG	7.7
1	C	15	ALA	7.7
2	D	548	HIS	7.7
3	F	40	ALA	7.7
1	C	72	GLY	7.7
2	D	55	LEU	7.7
1	C	375	LEU	7.6
2	D	75	LEU	7.6

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Mol	Chain	Res	Type	RSRZ
2	D	377	HIS	7.6
2	D	362	PHE	7.6
2	B	418	ASP	7.6
3	E	15	GLY	7.6
1	C	133	ILE	7.6
1	A	59	MET	7.6
1	C	390	VAL	7.6
1	C	129	MET	7.6
1	C	45	ALA	7.6
1	A	411	ALA	7.5
3	F	88	PRO	7.5
1	A	363	ALA	7.5
2	D	416	GLY	7.5
3	E	72	ARG	7.5
2	D	510	PRO	7.5
3	E	43	LYS	7.5
1	A	156	SER	7.5
2	D	61	GLY	7.5
2	B	55	LEU	7.5
1	C	552	LYS	7.4
2	D	238	GLU	7.4
1	C	371	GLY	7.4
1	A	400	VAL	7.4
1	A	529	PRO	7.4
1	A	273	MET	7.4
3	E	29	LEU	7.4
2	D	476	HIS	7.4
1	C	540	LEU	7.4
2	D	380	PRO	7.3
1	A	546	ALA	7.3
2	D	226	LEU	7.3
1	A	15	ALA	7.3
1	C	396	ASP	7.3
2	D	222	ASP	7.3
3	E	65	LYS	7.3
2	D	107	ASP	7.3
1	C	21	PHE	7.3
2	D	229	ILE	7.3
1	C	392	VAL	7.2
2	D	298	THR	7.2
3	E	116	MET	7.2
1	A	125	ASN	7.2

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Mol	Chain	Res	Type	RSRZ
2	B	456	ALA	7.2
1	A	254	VAL	7.2
1	C	331	SER	7.2
1	C	322	ALA	7.1
2	B	77	PRO	7.1
2	D	23	ALA	7.1
1	A	87	ASP	7.1
1	C	251	MET	7.1
1	C	283	MET	7.1
3	F	31	TYR	7.1
3	F	77	ASN	7.1
2	D	353	GLY	7.1
2	B	73	PHE	7.1
2	D	381	GLY	7.0
2	D	31	TYR	7.0
1	C	262	VAL	7.0
1	A	158	VAL	7.0
1	A	302	SER	7.0
1	C	379	ILE	7.0
1	A	3	THR	7.0
2	D	227	THR	7.0
2	D	407	VAL	7.0
1	A	547	GLY	7.0
2	D	236	GLU	7.0
1	C	98	SER	7.0
2	D	296	ILE	7.0
3	F	114	TYR	6.9
1	A	4	LEU	6.9
1	A	123	LEU	6.9
1	C	430	GLY	6.9
3	E	129	ALA	6.9
1	C	105	ASN	6.9
1	C	561	TYR	6.9
1	C	64	LEU	6.9
1	C	307	LEU	6.9
1	A	569	PHE	6.9
2	B	291	ILE	6.8
2	D	553	ILE	6.8
2	D	97	GLN	6.8
1	C	565	TYR	6.8
2	D	454	PRO	6.8
1	C	378	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	62	VAL	6.8
1	C	77	ALA	6.8
2	D	540	GLY	6.8
1	C	566	GLU	6.8
1	C	65	ILE	6.8
1	C	71	ILE	6.7
1	A	65	ILE	6.7
2	B	22	THR	6.7
1	C	35	LEU	6.7
1	C	254	VAL	6.7
1	A	486	LYS	6.7
1	A	98	SER	6.7
3	F	75	ALA	6.7
1	C	75	VAL	6.7
3	E	44	GLU	6.7
2	D	415	ASP	6.7
1	C	138	PRO	6.6
2	D	495	GLY	6.6
1	C	269	ILE	6.6
3	F	124	PRO	6.5
1	C	255	LEU	6.5
1	C	298	ARG	6.5
2	D	179	LEU	6.5
2	D	541	LYS	6.5
3	E	67	ARG	6.5
1	C	343	GLU	6.5
1	C	309	VAL	6.5
2	D	300	ILE	6.5
1	C	181	PHE	6.5
1	C	491	LEU	6.5
1	A	251	MET	6.5
1	A	122	GLN	6.5
3	E	114	TYR	6.5
3	E	66	GLY	6.4
1	C	329	GLU	6.4
1	C	344	ASN	6.4
2	B	224	SER	6.4
2	B	70	PRO	6.4
3	E	99	ASP	6.4
2	B	346	VAL	6.4
2	D	494	GLN	6.3
1	C	289	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
3	E	11	LEU	6.3
2	D	518	ALA	6.3
1	A	485	VAL	6.3
1	C	346	ASP	6.3
1	C	532	LEU	6.3
1	C	131	LEU	6.3
2	D	33	ARG	6.3
1	A	548	PHE	6.3
1	C	36	LEU	6.3
2	D	520	SER	6.3
1	C	328	VAL	6.3
1	A	12	TRP	6.2
2	D	561	VAL	6.2
2	D	49	SER	6.2
1	C	365	LEU	6.2
1	A	255	LEU	6.2
1	A	528	ILE	6.2
2	D	373	ASP	6.2
1	C	68	VAL	6.2
2	D	481	TYR	6.2
1	C	362	VAL	6.2
1	C	128	MET	6.2
1	C	130	LEU	6.2
1	A	298	ARG	6.2
1	C	517	LYS	6.2
1	A	269	ILE	6.2
2	B	24	THR	6.1
1	A	565	TYR	6.1
1	A	530	THR	6.1
2	B	288	LYS	6.1
2	B	352	ARG	6.1
1	C	222	ASN	6.1
2	D	472	HIS	6.1
2	D	547	ALA	6.1
1	A	66	GLY	6.1
1	A	276	THR	6.1
2	B	59	LEU	6.1
1	A	567	SER	6.1
1	C	276	THR	6.1
2	D	511	LYS	6.1
3	F	127	VAL	6.1
2	B	60	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	554	LEU	6.0
2	B	76	LEU	6.0
2	D	104	LEU	6.0
2	B	83	LEU	6.0
1	A	16	VAL	6.0
1	C	203	ARG	6.0
1	A	381	ARG	6.0
1	C	354	PHE	6.0
3	E	118	TYR	6.0
2	D	527	GLU	6.0
2	D	240	GLU	5.9
1	A	84	PHE	5.9
2	B	548	HIS	5.9
2	B	417	ILE	5.9
1	C	59	MET	5.9
1	A	35	LEU	5.9
1	C	368	THR	5.9
2	B	551	ASN	5.9
1	C	348	VAL	5.9
1	C	456	PRO	5.9
2	B	547	ALA	5.8
1	A	134	VAL	5.8
1	C	106	ARG	5.8
3	E	45	ARG	5.8
3	E	17	SER	5.8
1	C	352	VAL	5.8
3	E	101	GLY	5.8
2	B	481	TYR	5.8
1	A	120	VAL	5.8
1	A	258	GLY	5.8
1	C	395	LEU	5.8
2	D	60	ILE	5.8
3	F	84	ASN	5.8
2	D	91	SER	5.8
1	C	97	LEU	5.8
2	B	84	GLY	5.7
1	A	402	LEU	5.7
2	D	542	THR	5.7
1	A	179	PRO	5.7
2	D	411	GLN	5.7
1	A	160	ILE	5.7
2	D	506	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
2	B	421	LYS	5.7
1	C	7	TYR	5.7
1	A	408	HIS	5.7
1	A	410	SER	5.7
1	C	310	LEU	5.7
2	D	106	GLN	5.7
1	C	41	ALA	5.7
2	B	168	ALA	5.7
1	A	159	LEU	5.6
2	B	343	PRO	5.6
1	C	358	PRO	5.6
1	C	454	SER	5.6
1	A	139	LEU	5.6
1	C	216	GLU	5.5
2	B	478	PRO	5.5
1	C	34	THR	5.5
1	C	399	THR	5.5
2	D	351	VAL	5.5
1	A	495	ASP	5.5
1	C	281	GLN	5.5
2	B	27	ARG	5.5
1	A	552	LYS	5.5
1	A	380	PRO	5.5
3	F	98	ALA	5.5
1	C	567	SER	5.5
1	A	307	LEU	5.5
2	B	176	ASN	5.5
1	C	557	HIS	5.4
2	B	282	GLY	5.4
3	E	83	MET	5.4
2	B	415	ASP	5.4
2	B	508	ALA	5.4
2	D	105	SER	5.4
3	E	52	SER	5.4
3	E	105	TYR	5.4
2	D	452	GLY	5.4
1	A	43	GLY	5.4
1	A	393	ASP	5.4
2	D	46	VAL	5.4
3	E	75	ALA	5.4
3	E	64	VAL	5.4
1	C	523	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	73	CYS	5.3
1	A	138	PRO	5.3
2	D	27	ARG	5.3
2	B	285	LEU	5.3
1	C	372	LYS	5.3
2	D	524	THR	5.3
2	B	26	ARG	5.3
1	A	157	SER	5.3
2	B	498	GLN	5.3
1	A	566	GLU	5.3
2	B	482	GLU	5.3
3	F	87	LYS	5.3
2	B	28	LEU	5.3
1	A	409	ILE	5.2
1	A	52	VAL	5.2
1	A	131	LEU	5.2
2	B	305	GLN	5.2
2	D	68	PHE	5.2
1	C	292	ILE	5.2
2	D	37	PHE	5.2
1	A	39	ILE	5.2
1	C	286	LEU	5.2
2	D	453	ASN	5.2
1	A	382	LEU	5.2
1	C	555	LEU	5.2
2	D	285	LEU	5.2
1	C	140	LEU	5.2
1	A	69	GLY	5.2
1	C	33	PRO	5.2
2	D	101	MET	5.2
1	C	311	ASN	5.1
2	B	23	ALA	5.1
1	A	432	GLU	5.1
2	D	241	LYS	5.1
1	A	133	ILE	5.1
1	C	2	LYS	5.1
2	D	45	PHE	5.1
2	D	590	GLN	5.1
1	A	127	VAL	5.1
1	A	364	VAL	5.1
1	A	115	ARG	5.1
1	C	61	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
2	D	379	LYS	5.1
1	A	539	VAL	5.1
1	A	439	ILE	5.1
1	C	429	TRP	5.1
1	A	271	SER	5.0
1	A	109	THR	5.0
1	C	285	SER	5.0
1	A	295	PHE	5.0
2	D	477	LEU	5.0
2	D	83	LEU	5.0
1	C	31	SER	5.0
1	C	78	SER	5.0
3	F	118	TYR	5.0
1	A	416	THR	5.0
2	D	513	LEU	5.0
2	D	239	MET	5.0
1	A	61	ILE	5.0
2	D	568	VAL	5.0
1	C	455	LEU	5.0
1	C	433	ASP	4.9
2	D	177	VAL	4.9
2	D	473	PHE	4.9
2	D	509	ASN	4.9
2	D	79	TYR	4.9
1	A	113	ILE	4.9
1	C	141	PHE	4.9
2	D	88	ALA	4.9
2	B	558	LEU	4.8
2	D	228	VAL	4.8
1	C	273	MET	4.8
2	D	278	ILE	4.8
1	A	292	ILE	4.8
1	C	219	ARG	4.8
1	C	522	PHE	4.8
2	B	488	ASN	4.8
2	D	591	TYR	4.8
1	A	294	ASN	4.8
1	A	405	LEU	4.8
2	D	26	ARG	4.8
1	C	460	ASP	4.8
2	D	36	THR	4.8
2	B	525	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	4.8
2	B	284	TRP	4.8
1	A	55	THR	4.8
2	B	29	LEU	4.8
3	F	70	ILE	4.8
1	C	361	LEU	4.7
2	D	84	GLY	4.7
2	B	286	ALA	4.7
2	B	524	THR	4.7
2	D	48	VAL	4.7
2	D	32	LEU	4.7
2	B	519	THR	4.7
1	A	56	GLY	4.7
1	C	323	LEU	4.7
1	A	384	ASP	4.7
2	D	538	MET	4.7
1	A	379	ILE	4.7
2	D	223	ILE	4.7
2	B	62	LYS	4.7
1	A	49	PHE	4.7
1	A	181	PHE	4.7
1	A	137	ALA	4.7
2	B	553	ILE	4.7
2	D	224	SER	4.7
3	F	107	LEU	4.7
2	B	462	LYS	4.7
1	A	58	LEU	4.6
2	D	178	ILE	4.6
1	C	101	ILE	4.6
1	A	398	ARG	4.6
2	D	499	LEU	4.6
1	C	284	PHE	4.6
2	D	47	THR	4.6
2	B	106	GLN	4.6
3	F	69	THR	4.6
3	E	93	VAL	4.6
2	D	375	THR	4.6
2	B	222	ASP	4.6
2	B	523	ASP	4.6
1	C	148	ALA	4.6
2	D	479	GLU	4.6
2	B	507	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	507	LEU	4.6
1	A	308	GLU	4.5
1	A	488	PRO	4.5
1	A	223	GLU	4.5
1	A	126	LEU	4.5
1	C	155	LEU	4.5
3	E	104	GLU	4.5
1	A	314	PRO	4.5
1	C	347	PRO	4.5
2	D	438	THR	4.5
2	D	281	PHE	4.5
2	D	554	LYS	4.5
1	A	392	VAL	4.5
1	A	67	ALA	4.5
2	D	59	LEU	4.5
2	D	374	ILE	4.5
1	C	438	GLU	4.5
2	B	450	LYS	4.5
1	A	490	VAL	4.5
1	A	564	ILE	4.5
1	C	12	TRP	4.5
1	C	293	LEU	4.5
2	D	258	ILE	4.5
2	D	385	ALA	4.5
2	D	299	PHE	4.4
3	E	19	ARG	4.4
1	A	175	LYS	4.4
1	C	334	PHE	4.4
1	C	486	LYS	4.4
2	D	69	VAL	4.4
1	A	200	LEU	4.4
2	D	498	GLN	4.4
1	A	201	GLY	4.4
1	A	256	TRP	4.4
1	A	523	ILE	4.4
2	B	64	ILE	4.4
1	A	267	MET	4.4
3	E	77	ASN	4.4
3	E	34	ILE	4.4
2	D	404	PHE	4.3
2	D	433	ILE	4.4
1	C	95	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	226	ARG	4.3
2	D	100	ILE	4.3
1	C	94	ARG	4.3
1	A	166	ILE	4.3
1	C	142	VAL	4.3
2	D	378	ILE	4.3
1	A	299	ALA	4.3
2	D	207	GLU	4.3
2	D	51	ILE	4.3
1	A	487	LYS	4.3
3	E	40	ALA	4.3
3	F	54	SER	4.3
2	D	92	LEU	4.3
1	C	183	LYS	4.3
2	B	550	LEU	4.2
2	D	475	LYS	4.2
1	A	246	ILE	4.2
2	B	385	ALA	4.2
2	B	561	VAL	4.2
3	F	85	SER	4.2
2	B	356	GLU	4.2
3	F	12	VAL	4.2
1	A	99	PHE	4.2
1	A	274	ALA	4.2
2	D	555	ASN	4.2
2	D	30	GLY	4.2
2	B	432	GLY	4.1
3	F	97	ALA	4.1
1	C	294	ASN	4.1
1	C	377	ASN	4.1
1	A	289	ILE	4.1
2	D	417	ILE	4.1
1	A	280	MET	4.1
2	B	25	LEU	4.1
3	E	9	GLY	4.1
1	A	304	LYS	4.1
1	A	203	ARG	4.1
1	C	359	GLY	4.1
2	D	497	ARG	4.1
1	A	323	LEU	4.1
1	C	166	ILE	4.1
1	A	257	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	351	VAL	4.1
2	D	348	LEU	4.0
1	A	524	ILE	4.0
1	A	550	THR	4.0
2	D	546	ILE	4.0
1	C	145	ILE	4.0
2	D	566	GLU	4.0
1	A	108	HIS	4.0
3	F	39	GLN	4.0
2	D	108	VAL	4.0
2	B	61	GLY	4.0
1	A	92	LEU	4.0
1	A	404	ASP	4.0
1	A	283	MET	4.0
2	B	317	PHE	4.0
1	C	332	VAL	4.0
1	C	159	LEU	4.0
2	D	505	ALA	4.0
1	C	40	VAL	4.0
2	D	96	LEU	4.0
2	D	421	LYS	4.0
3	F	33	ALA	4.0
2	D	543	SER	4.0
2	B	414	VAL	4.0
2	D	539	GLU	4.0
2	D	86	ILE	4.0
2	D	525	LYS	4.0
2	D	512	ILE	4.0
2	D	456	ALA	3.9
1	A	57	ILE	3.9
2	D	110	PHE	3.9
2	B	223	ILE	3.9
2	D	90	THR	3.9
2	B	494	GLN	3.9
3	F	123	THR	3.9
2	B	438	THR	3.9
1	A	116	LEU	3.9
1	C	146	VAL	3.9
2	D	434	VAL	3.9
3	F	129	ALA	3.9
1	A	305	ARG	3.9
1	A	365	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
3	E	69	THR	3.8
3	E	70	ILE	3.8
1	C	492	ILE	3.8
1	A	561	TYR	3.8
2	D	355	ILE	3.8
1	C	419	PHE	3.8
2	D	451	TYR	3.8
1	C	360	SER	3.8
1	C	386	GLU	3.8
1	A	178	ASN	3.8
2	D	159	PHE	3.8
2	B	32	LEU	3.8
2	D	52	LEU	3.8
2	D	85	THR	3.8
1	A	183	LYS	3.8
2	D	560	ILE	3.8
2	B	543	SER	3.8
1	A	421	GLY	3.8
2	D	558	LEU	3.8
1	A	465	ARG	3.8
1	C	215	ASN	3.8
2	D	279	SER	3.8
1	C	421	GLY	3.8
1	C	80	ALA	3.8
1	C	223	GLU	3.8
1	A	482	ARG	3.8
1	A	545	VAL	3.8
1	A	433	ASP	3.8
2	B	151	LEU	3.7
2	D	382	GLN	3.7
2	D	386	LEU	3.7
3	E	60	TYR	3.7
1	C	564	ILE	3.7
2	D	257	GLN	3.7
3	F	119	TRP	3.7
1	A	44	ILE	3.7
1	A	247	VAL	3.7
3	F	113	ILE	3.7
1	A	496	CYS	3.7
1	C	279	LEU	3.7
2	D	387	VAL	3.7
2	D	152	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	50	SER	3.7
1	A	226	ARG	3.7
1	A	315	ALA	3.7
1	C	126	LEU	3.7
2	D	262	VAL	3.7
2	B	475	LYS	3.7
1	A	250	GLY	3.6
1	A	293	LEU	3.6
1	A	88	LEU	3.6
1	A	197	GLU	3.6
2	D	219	ILE	3.6
2	B	505	ALA	3.6
2	B	292	THR	3.6
2	D	545	ILE	3.6
1	C	385	PRO	3.6
1	A	415	GLU	3.6
2	B	513	LEU	3.6
1	A	102	SER	3.6
1	A	40	VAL	3.6
1	C	312	GLU	3.6
2	B	302	TYR	3.6
2	B	80	MET	3.6
1	A	522	PHE	3.6
1	A	2	LYS	3.5
1	C	387	ARG	3.5
2	B	422	ILE	3.5
2	B	527	GLU	3.5
2	B	386	LEU	3.5
2	D	492	LEU	3.5
2	D	504	ARG	3.5
2	B	159	PHE	3.5
2	D	24	THR	3.5
2	D	43	PHE	3.5
1	C	524	ILE	3.5
1	A	484	LEU	3.5
1	C	337	VAL	3.5
2	D	346	VAL	3.5
1	C	391	GLU	3.5
1	C	220	LYS	3.5
3	E	27	PHE	3.5
2	D	517	ALA	3.5
1	A	531	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	31	TYR	3.4
2	B	348	LEU	3.4
2	D	28	LEU	3.4
2	B	545	ILE	3.4
1	A	81	SER	3.4
2	B	105	SER	3.4
1	A	101	ILE	3.4
1	A	163	ILE	3.4
2	D	284	TRP	3.4
1	A	121	THR	3.4
2	D	218	ILE	3.4
1	A	216	GLU	3.4
1	C	534	ALA	3.4
2	B	171	MET	3.4
3	F	93	VAL	3.4
1	A	321	ASN	3.4
1	A	303	ALA	3.4
1	A	284	PHE	3.4
1	C	227	ARG	3.4
2	B	225	GLY	3.4
1	A	222	ASN	3.4
2	D	354	GLU	3.4
1	A	85	GLY	3.4
1	C	27	ILE	3.4
2	D	204	TYR	3.4
1	C	424	LYS	3.4
2	B	380	PRO	3.3
2	D	44	VAL	3.3
2	D	450	LYS	3.3
1	A	27	ILE	3.3
3	E	61	ALA	3.3
2	B	107	ASP	3.3
2	B	511	LYS	3.3
1	A	95	LYS	3.3
2	B	416	GLY	3.3
1	C	325	LEU	3.3
1	A	354	PHE	3.3
2	B	541	LYS	3.3
2	D	457	THR	3.3
2	B	461	ILE	3.3
1	A	492	ILE	3.3
2	B	504	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	461	ILE	3.3
1	C	374	THR	3.3
1	A	68	VAL	3.2
2	B	231	LEU	3.2
1	C	170	PHE	3.2
1	C	99	PHE	3.2
2	B	316	GLN	3.2
2	B	468	THR	3.2
2	D	469	HIS	3.2
1	C	453	ILE	3.2
3	F	52	SER	3.2
1	C	431	ARG	3.2
2	B	68	PHE	3.2
2	B	287	LEU	3.2
2	D	474	ILE	3.2
2	B	74	ASP	3.2
1	A	362	VAL	3.2
3	F	68	PHE	3.2
1	A	309	VAL	3.2
1	C	297	VAL	3.2
2	B	384	VAL	3.2
2	D	151	LEU	3.2
2	B	401	LEU	3.2
3	E	8	GLY	3.2
1	C	336	ASN	3.2
1	C	417	VAL	3.2
1	C	107	PHE	3.1
1	C	562	ARG	3.1
2	D	516	ASP	3.1
1	C	37	ALA	3.1
1	A	110	SER	3.1
2	B	437	ASP	3.1
1	C	459	TYR	3.1
2	B	451	TYR	3.1
1	C	516	THR	3.1
2	D	349	ARG	3.1
1	A	112	LEU	3.1
1	C	340	ARG	3.1
2	D	405	TYR	3.1
2	B	402	MET	3.1
2	B	353	GLY	3.1
2	D	111	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	265	PRO	3.1
1	C	127	VAL	3.1
3	F	122	GLY	3.1
1	A	130	LEU	3.1
3	E	16	GLY	3.1
1	C	282	ILE	3.1
1	C	8	LEU	3.1
1	A	196	ARG	3.1
2	B	487	ASP	3.1
2	D	295	THR	3.1
1	C	514	ARG	3.1
1	C	427	LEU	3.0
2	B	195	GLN	3.0
1	A	94	ARG	3.0
2	D	103	THR	3.0
2	D	344	ASP	3.0
1	C	52	VAL	3.0
1	C	39	ILE	3.0
2	B	96	LEU	3.0
2	D	29	LEU	3.0
2	B	87	TYR	3.0
2	D	501	ALA	3.0
2	D	347	GLU	3.0
1	A	385	PRO	3.0
1	C	43	GLY	3.0
1	A	467	GLY	3.0
1	A	279	LEU	3.0
1	C	563	GLU	3.0
3	F	108	PRO	3.0
2	B	506	PHE	3.0
1	C	394	GLU	3.0
2	D	544	ILE	3.0
2	B	164	THR	3.0
2	D	150	VAL	3.0
2	D	376	PHE	3.0
2	D	432	GLY	3.0
1	C	44	ILE	3.0
2	B	228	VAL	3.0
1	C	308	GLU	3.0
1	A	180	LEU	3.0
2	B	113	ARG	2.9
3	F	53	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	587	PHE	2.9
1	A	296	ILE	2.9
2	D	259	PHE	2.9
1	C	313	LYS	2.9
2	B	310	LEU	2.9
2	B	497	ARG	2.9
3	E	124	PRO	2.9
2	D	297	ALA	2.9
1	A	532	LEU	2.9
1	A	60	LEU	2.9
2	D	483	THR	2.9
1	A	90	ARG	2.9
1	C	300	SER	2.9
2	D	502	ILE	2.9
1	A	412	VAL	2.9
2	B	349	ARG	2.9
2	D	42	VAL	2.9
1	C	93	PHE	2.9
3	E	123	THR	2.9
1	C	153	VAL	2.9
2	B	503	THR	2.9
1	C	356	VAL	2.9
1	C	515	TYR	2.8
1	A	498	SER	2.8
2	B	552	THR	2.8
1	A	331	SER	2.8
1	A	491	LEU	2.8
2	B	411	GLN	2.8
1	A	96	VAL	2.8
1	A	407	GLY	2.8
1	A	534	ALA	2.8
2	B	554	LYS	2.8
1	A	89	ARG	2.8
1	A	330	GLY	2.8
1	C	295	PHE	2.8
2	D	350	GLU	2.8
2	D	414	VAL	2.8
1	A	453	ILE	2.8
1	C	326	PRO	2.8
2	B	220	GLU	2.8
2	B	520	SER	2.8
2	B	387	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	544	LYS	2.8
1	C	154	LYS	2.8
2	B	52	LEU	2.8
2	B	544	ILE	2.8
3	E	71	SER	2.8
2	D	99	LYS	2.8
1	A	83	ASN	2.8
2	D	269	MET	2.8
2	D	500	LEU	2.8
1	A	466	GLY	2.8
3	F	67	ARG	2.8
1	A	554	LEU	2.8
1	A	424	LYS	2.8
1	C	535	ASP	2.8
1	C	81	SER	2.8
2	D	356	GLU	2.8
1	C	122	GLN	2.8
2	B	278	ILE	2.8
1	A	325	LEU	2.8
3	F	18	LEU	2.8
1	C	208	PHE	2.8
1	C	272	ILE	2.8
2	D	156	ILE	2.8
2	D	196	ILE	2.8
2	B	555	ASN	2.7
1	A	500	VAL	2.7
3	F	2	GLY	2.7
1	C	104	VAL	2.7
2	B	314	SER	2.7
2	D	81	LEU	2.7
2	D	410	GLY	2.7
1	C	57	ILE	2.7
1	A	417	VAL	2.7
1	C	493	LEU	2.7
2	D	221	GLU	2.7
2	D	242	PHE	2.7
1	A	346	ASP	2.7
1	A	353	ASN	2.7
2	B	368	LYS	2.7
1	A	76	PHE	2.7
3	F	56	GLY	2.7
1	A	253	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	67	VAL	2.7
2	B	331	PHE	2.7
1	A	347	PRO	2.7
2	D	244	ARG	2.7
2	D	98	GLY	2.7
1	A	286	LEU	2.7
1	C	149	VAL	2.7
2	B	562	LEU	2.7
1	A	107	PHE	2.7
1	C	157	SER	2.7
1	C	452	ILE	2.7
1	C	58	LEU	2.7
1	A	185	GLN	2.6
1	C	248	ASN	2.6
3	F	1	GLN	2.6
2	B	172	MET	2.6
2	B	419	ILE	2.6
2	D	155	ILE	2.6
1	C	233	PHE	2.6
2	D	491	ASP	2.6
3	F	4	LEU	2.6
1	C	288	MET	2.6
1	A	28	CYS	2.6
1	C	345	THR	2.6
2	B	586	LEU	2.6
1	A	540	LEU	2.6
1	C	103	ASN	2.6
2	D	166	ALA	2.6
1	A	118	ASN	2.6
2	D	488	ASN	2.6
1	C	259	GLY	2.6
1	C	482	ARG	2.6
2	B	227	THR	2.6
1	A	436	ASP	2.6
1	A	371	GLY	2.6
1	C	156	SER	2.6
1	A	72	GLY	2.6
2	D	266	LEU	2.6
2	D	562	LEU	2.6
2	B	426	SER	2.6
1	C	202	VAL	2.6
2	B	100	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	69	VAL	2.6
1	A	54	LYS	2.6
2	B	469	HIS	2.6
1	C	206	ARG	2.5
2	D	508	ALA	2.5
2	B	423	LYS	2.5
1	C	174	THR	2.5
2	B	63	THR	2.5
1	A	505	GLU	2.5
1	A	204	VAL	2.5
2	B	430	SER	2.5
2	B	433	ILE	2.5
2	B	161	GLY	2.5
2	D	304	ARG	2.5
1	A	378	LEU	2.5
1	A	395	LEU	2.5
1	A	475	LYS	2.5
1	C	560	PRO	2.5
2	D	263	LEU	2.5
1	A	301	ALA	2.5
2	D	515	LEU	2.5
2	B	313	LEU	2.5
2	D	383	LYS	2.5
2	B	93	LEU	2.5
3	E	20	LEU	2.5
1	C	91	ASP	2.5
1	A	431	ARG	2.5
1	A	93	PHE	2.5
1	A	224	SER	2.5
2	D	384	VAL	2.5
1	A	503	ILE	2.4
2	D	531	GLN	2.4
1	A	162	LEU	2.4
1	A	497	THR	2.4
1	A	219	ARG	2.4
1	A	394	GLU	2.4
2	D	168	ALA	2.4
2	D	202	ARG	2.4
1	A	336	ASN	2.4
1	C	125	ASN	2.4
2	D	89	LEU	2.4
2	D	189	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	200	GLN	2.4
1	A	48	ASP	2.4
1	A	390	VAL	2.4
2	B	175	VAL	2.4
2	B	104	LEU	2.4
2	B	566	GLU	2.4
1	A	483	ALA	2.4
2	B	413	LEU	2.4
2	D	163	VAL	2.4
1	C	423	ILE	2.4
3	E	82	GLN	2.4
2	D	293	VAL	2.4
1	A	53	LEU	2.4
2	B	512	ILE	2.4
3	E	113	ILE	2.4
3	E	28	THR	2.4
1	C	299	ALA	2.4
2	D	38	THR	2.4
1	C	412	VAL	2.4
1	C	498	SER	2.4
2	B	449	LEU	2.4
3	E	63	SER	2.4
1	C	426	ASN	2.4
3	E	38	ARG	2.4
3	F	72	ARG	2.3
2	D	247	GLU	2.3
3	E	94	TYR	2.3
3	F	94	TYR	2.3
1	C	376	MET	2.3
2	B	567	ILE	2.3
1	A	63	ALA	2.3
2	B	441	PHE	2.3
2	D	422	ILE	2.3
1	C	261	LEU	2.3
1	C	327	ASN	2.3
2	B	531	GLN	2.3
1	C	229	ILE	2.3
3	E	122	GLY	2.3
1	C	30	LEU	2.3
2	B	295	THR	2.3
1	A	518	GLY	2.3
2	D	112	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	158	PHE	2.3
1	A	555	LEU	2.3
2	B	165	LEU	2.3
1	A	460	ASP	2.3
1	C	53	LEU	2.3
1	A	557	HIS	2.3
2	B	587	PHE	2.3
1	C	413	PRO	2.3
3	E	39	GLN	2.2
1	C	485	VAL	2.2
2	D	397	ILE	2.2
1	A	300	SER	2.2
1	C	333	SER	2.2
1	A	51	LEU	2.2
1	C	9	LYS	2.2
1	C	56	GLY	2.2
2	B	324	LEU	2.2
2	B	466	LYS	2.2
1	C	442	ALA	2.2
2	B	109	VAL	2.2
1	C	46	ARG	2.2
1	C	296	ILE	2.2
2	B	30	GLY	2.2
2	D	182	VAL	2.2
3	F	11	LEU	2.2
2	B	495	GLY	2.2
3	E	98	ALA	2.2
1	A	429	TRP	2.2
1	A	168	LEU	2.2
1	A	105	ASN	2.2
1	A	340	ARG	2.2
2	B	515	LEU	2.2
1	C	495	ASP	2.2
1	A	47	GLY	2.2
1	A	493	LEU	2.2
1	C	558	CYS	2.2
1	A	428	LYS	2.2
1	A	202	VAL	2.2
2	B	412	ILE	2.2
3	E	1	GLN	2.2
2	B	546	ILE	2.2
2	D	40	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	391	GLU	2.2
2	D	399	ASN	2.2
1	C	243	PHE	2.2
2	D	147	ILE	2.2
2	D	484	VAL	2.2
2	B	219	ILE	2.2
2	B	232	PHE	2.2
2	D	256	ALA	2.2
1	C	38	ARG	2.2
1	C	436	ASP	2.2
2	B	152	GLY	2.2
2	B	560	ILE	2.2
1	C	441	GLU	2.1
2	B	110	PHE	2.1
2	B	293	VAL	2.1
2	D	115	GLU	2.1
1	C	461	SER	2.1
1	A	282	ILE	2.1
2	D	203	LYS	2.1
1	A	438	GLU	2.1
2	B	518	ALA	2.1
1	A	208	PHE	2.1
2	D	586	LEU	2.1
1	C	179	PRO	2.1
2	D	214	GLN	2.1
1	C	100	SER	2.1
2	B	78	ARG	2.1
2	B	403	ARG	2.1
2	D	449	LEU	2.1
2	D	514	ILE	2.1
2	D	462	LYS	2.1
1	C	173	LEU	2.1
1	C	180	LEU	2.1
2	D	283	GLY	2.1
1	C	487	LYS	2.1
2	B	230	LYS	2.1
1	C	306	VAL	2.1
2	B	476	HIS	2.1
2	D	306	PHE	2.1
2	B	499	LEU	2.1
2	D	253	GLY	2.1
2	B	101	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	252	ILE	2.1
1	A	332	VAL	2.1
2	B	153	ASN	2.1
1	C	123	LEU	2.1
1	A	64	LEU	2.0
1	A	210	ARG	2.0
2	B	226	LEU	2.0
1	A	350	SER	2.0
2	B	150	VAL	2.0
2	D	93	LEU	2.0
2	D	401	LEU	2.0
2	B	448	ASN	2.0
2	B	502	ILE	2.0
1	C	439	ILE	2.0
2	B	440	LEU	2.0
1	C	49	PHE	2.0
1	C	218	PHE	2.0
1	A	427	LEU	2.0
1	C	301	ALA	2.0
3	E	24	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	C	601	1/1	0.78	0.09	217,217,217,217	0
4	AGS	C	600	31/31	0.88	0.59	187,206,221,225	0
4	AGS	D	600	31/31	0.91	0.25	162,196,218,226	0

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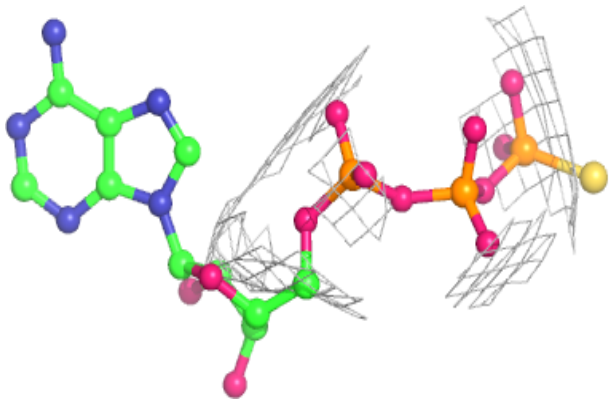
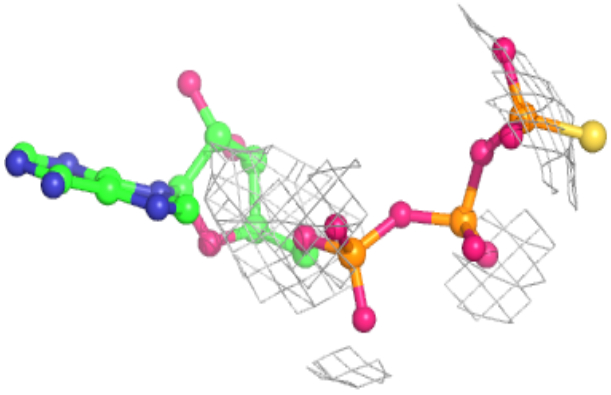
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AGS	A	600	31/31	0.91	0.24	99,135,179,183	0
5	MG	A	601	1/1	0.94	0.18	116,116,116,116	0
4	AGS	B	600	31/31	0.94	0.22	4,26,78,82	0
5	MG	D	601	1/1	0.95	0.10	176,176,176,176	0
5	MG	B	601	1/1	0.98	0.22	70,70,70,70	0

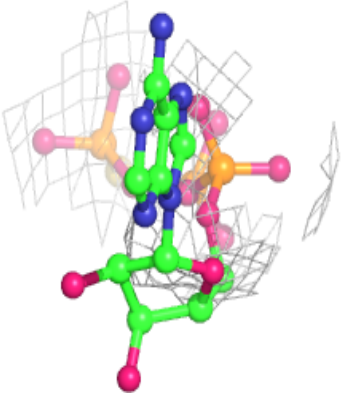
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS C 600:

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

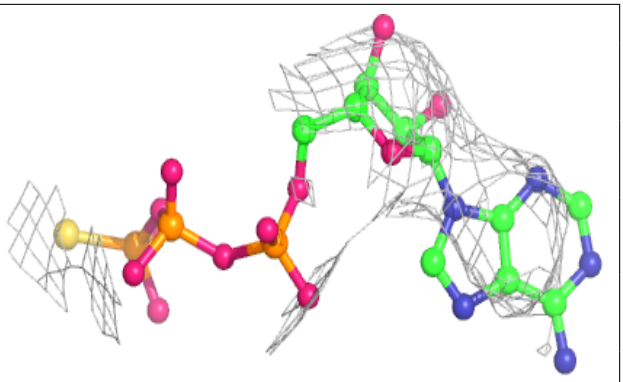


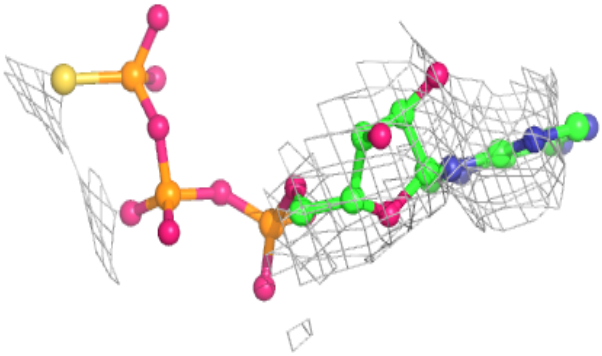


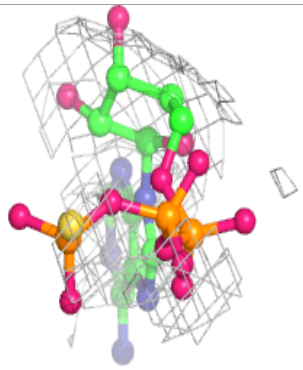


Electron density around AGS D 600:

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

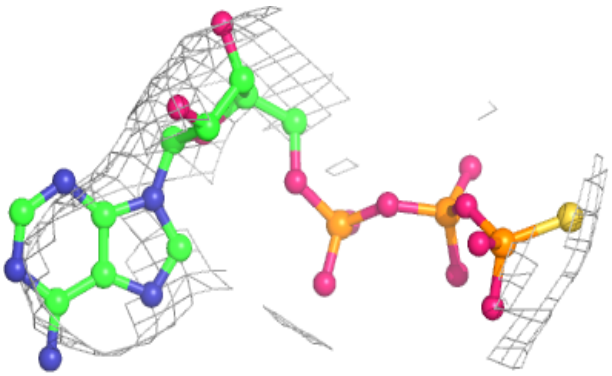


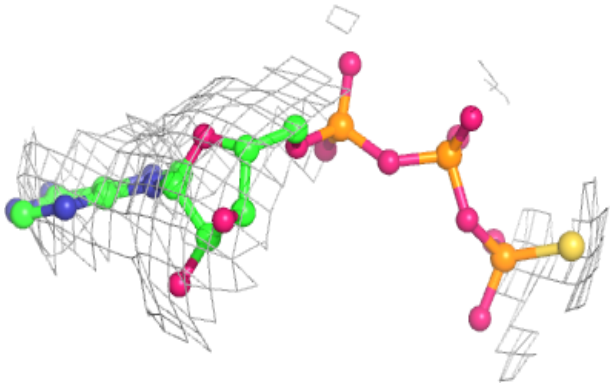


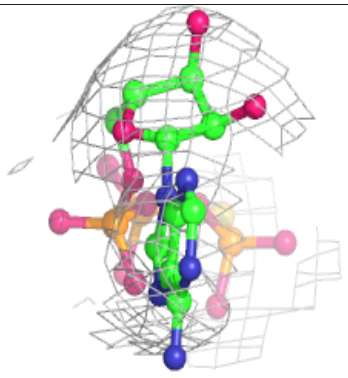


Electron density around AGS A 600:

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

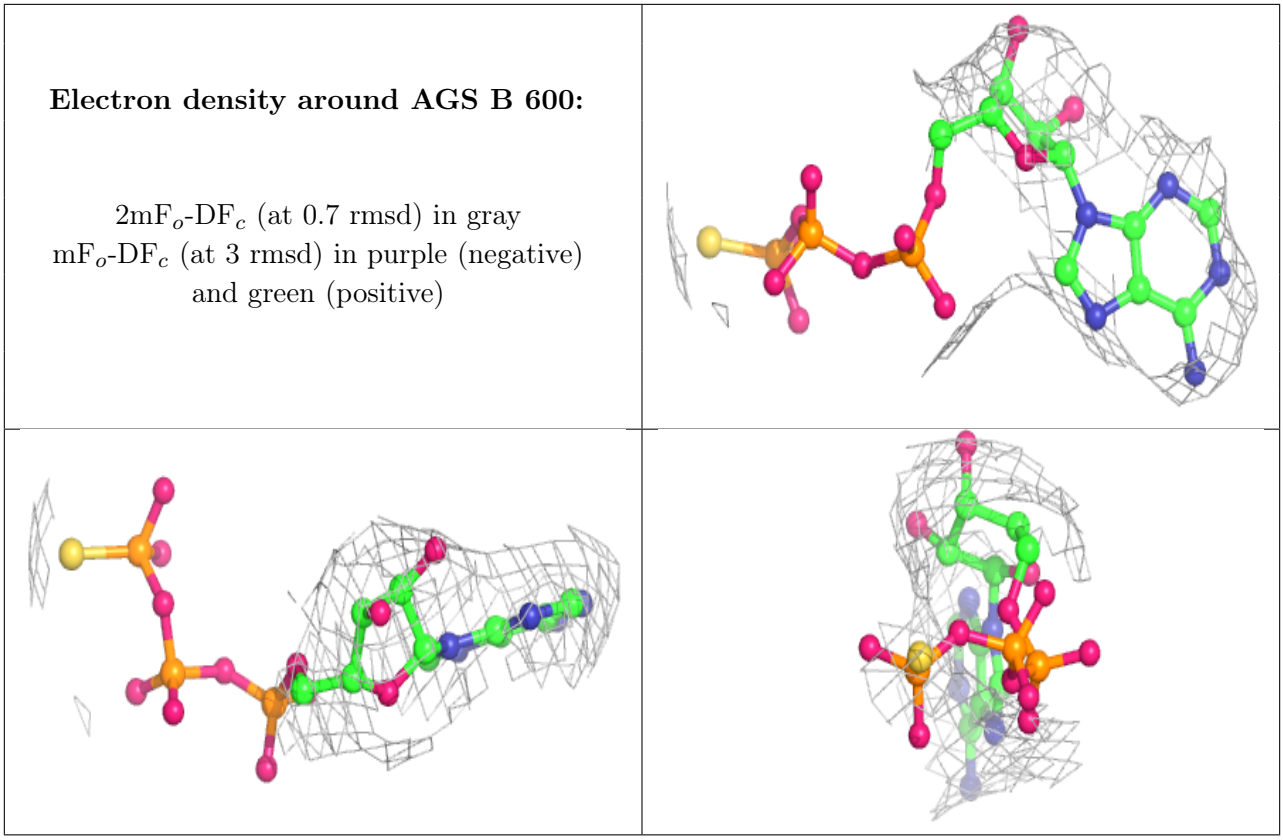






Electron density around AGS B 600:

$2mF_o$-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.