Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 07:32 PM EST

PDB ID	:	4KLN
Title	:	Structure of p97 N-D1 A232E mutant in complex with ATPgS
Authors	:	Xia, D.; Tang, W.K.
Deposited on	:	2013-05-07
Resolution	:	2.62 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

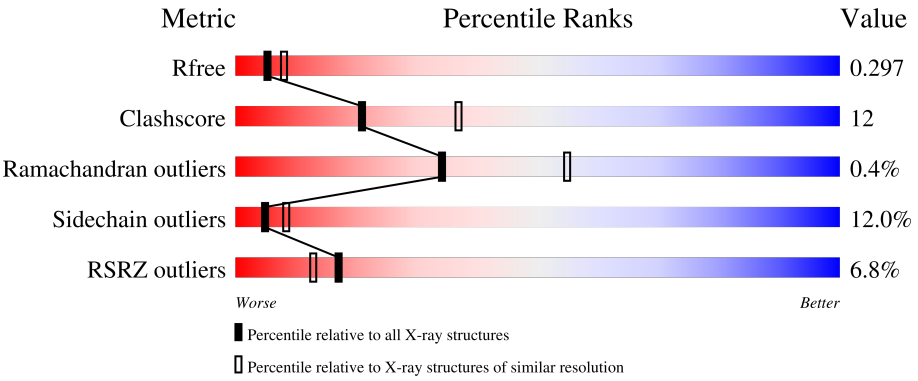
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	489	3% 62% 27% · 8%
1	B	489	2% 65% 24% · 8%
1	C	489	7% 63% 26% · 8%
1	D	489	8% 63% 26% · 8%
1	E	489	11% 61% 28% · 8%

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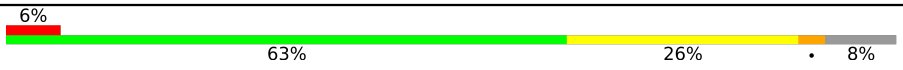
Mol	Chain	Length	Quality of chain
1	F	489	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21556 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	B	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	C	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	D	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	E	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			
1	F	451	Total	C	N	O	S	0	0	0
			3533	2217	626	672	18			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLU	ALA	engineered mutation	UNP P55072
A	482	ARG	-	expression tag	UNP P55072
A	483	SER	-	expression tag	UNP P55072
A	484	HIS	-	expression tag	UNP P55072
A	485	HIS	-	expression tag	UNP P55072
A	486	HIS	-	expression tag	UNP P55072
A	487	HIS	-	expression tag	UNP P55072
A	488	HIS	-	expression tag	UNP P55072
A	489	HIS	-	expression tag	UNP P55072
B	232	GLU	ALA	engineered mutation	UNP P55072
B	482	ARG	-	expression tag	UNP P55072
B	483	SER	-	expression tag	UNP P55072
B	484	HIS	-	expression tag	UNP P55072
B	485	HIS	-	expression tag	UNP P55072
B	486	HIS	-	expression tag	UNP P55072
B	487	HIS	-	expression tag	UNP P55072
B	488	HIS	-	expression tag	UNP P55072

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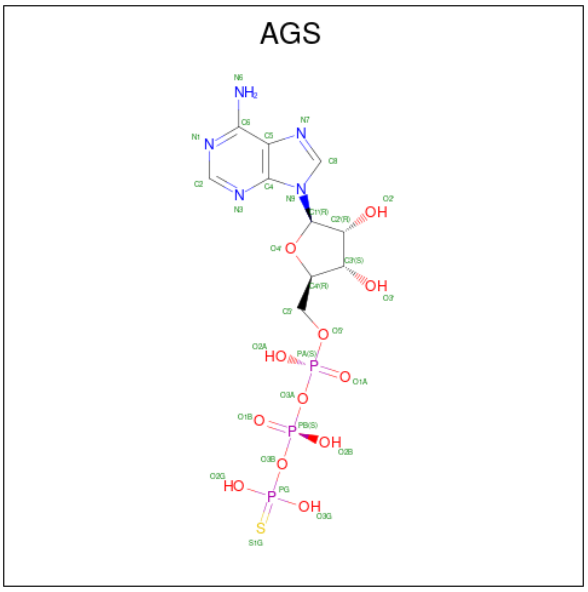
Chain	Residue	Modelled	Actual	Comment	Reference
B	489	HIS	-	expression tag	UNP P55072
C	232	GLU	ALA	engineered mutation	UNP P55072
C	482	ARG	-	expression tag	UNP P55072
C	483	SER	-	expression tag	UNP P55072
C	484	HIS	-	expression tag	UNP P55072
C	485	HIS	-	expression tag	UNP P55072
C	486	HIS	-	expression tag	UNP P55072
C	487	HIS	-	expression tag	UNP P55072
C	488	HIS	-	expression tag	UNP P55072
C	489	HIS	-	expression tag	UNP P55072
D	232	GLU	ALA	engineered mutation	UNP P55072
D	482	ARG	-	expression tag	UNP P55072
D	483	SER	-	expression tag	UNP P55072
D	484	HIS	-	expression tag	UNP P55072
D	485	HIS	-	expression tag	UNP P55072
D	486	HIS	-	expression tag	UNP P55072
D	487	HIS	-	expression tag	UNP P55072
D	488	HIS	-	expression tag	UNP P55072
D	489	HIS	-	expression tag	UNP P55072
E	232	GLU	ALA	engineered mutation	UNP P55072
E	482	ARG	-	expression tag	UNP P55072
E	483	SER	-	expression tag	UNP P55072
E	484	HIS	-	expression tag	UNP P55072
E	485	HIS	-	expression tag	UNP P55072
E	486	HIS	-	expression tag	UNP P55072
E	487	HIS	-	expression tag	UNP P55072
E	488	HIS	-	expression tag	UNP P55072
E	489	HIS	-	expression tag	UNP P55072
F	232	GLU	ALA	engineered mutation	UNP P55072
F	482	ARG	-	expression tag	UNP P55072
F	483	SER	-	expression tag	UNP P55072
F	484	HIS	-	expression tag	UNP P55072
F	485	HIS	-	expression tag	UNP P55072
F	486	HIS	-	expression tag	UNP P55072
F	487	HIS	-	expression tag	UNP P55072
F	488	HIS	-	expression tag	UNP P55072
F	489	HIS	-	expression tag	UNP P55072

- Molecule 2 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
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

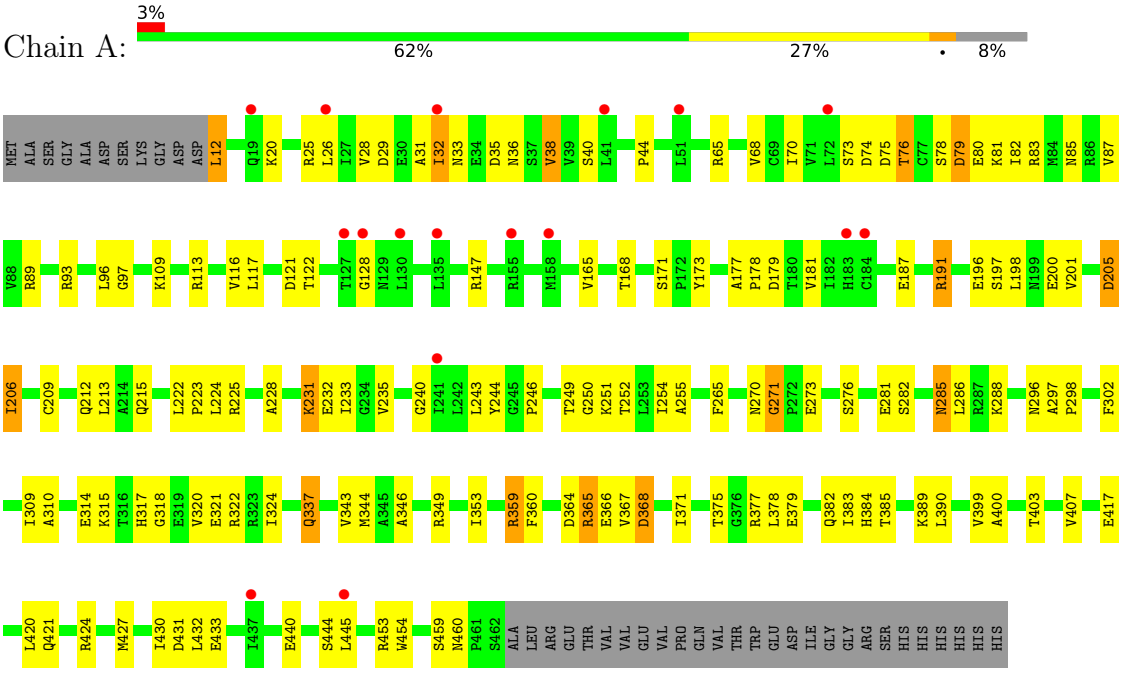
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	28	Total O 28 28	0	0
4	C	30	Total O 30 30	0	0
4	D	26	Total O 26 26	0	0
4	E	25	Total O 25 25	0	0
4	F	24	Total O 24 24	0	0

3 Residue-property plots (i)

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

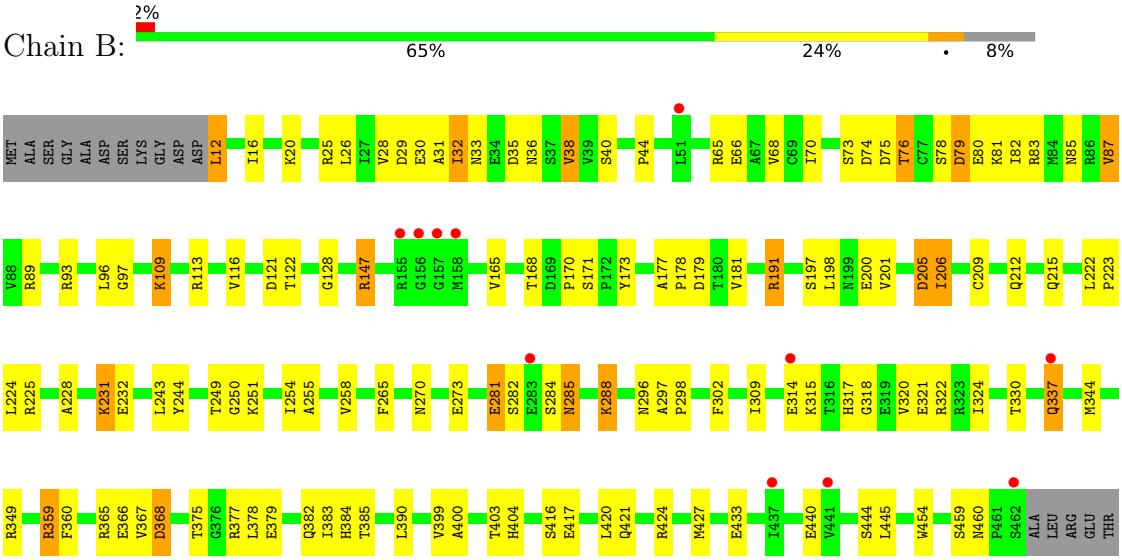
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain A:



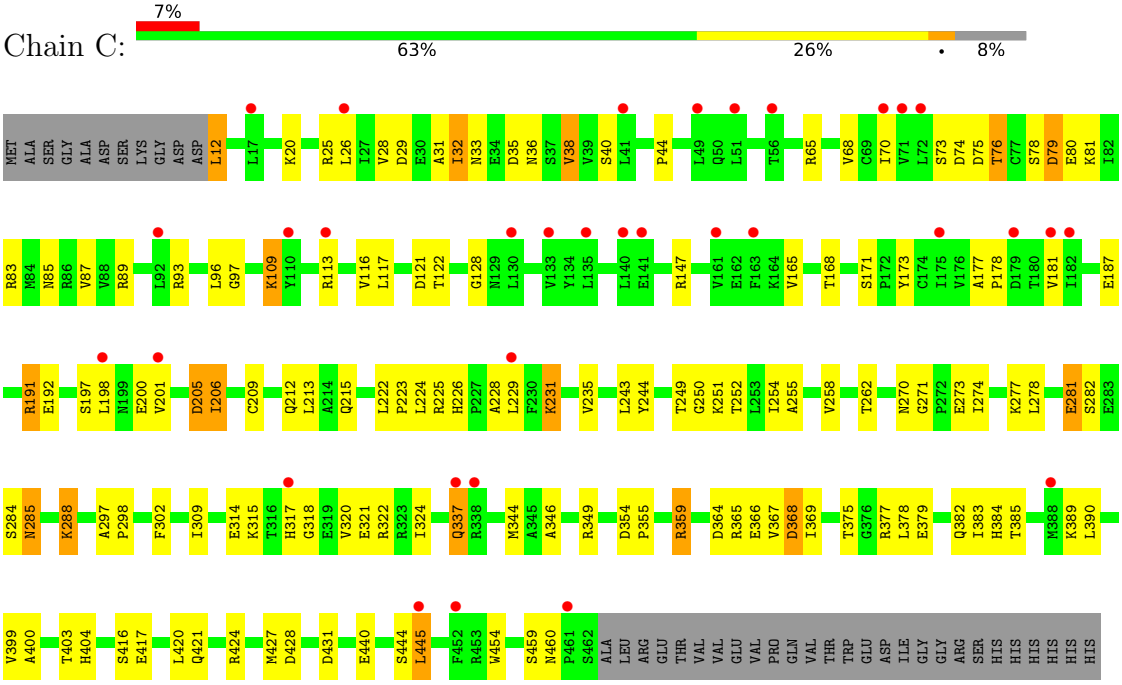
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B:



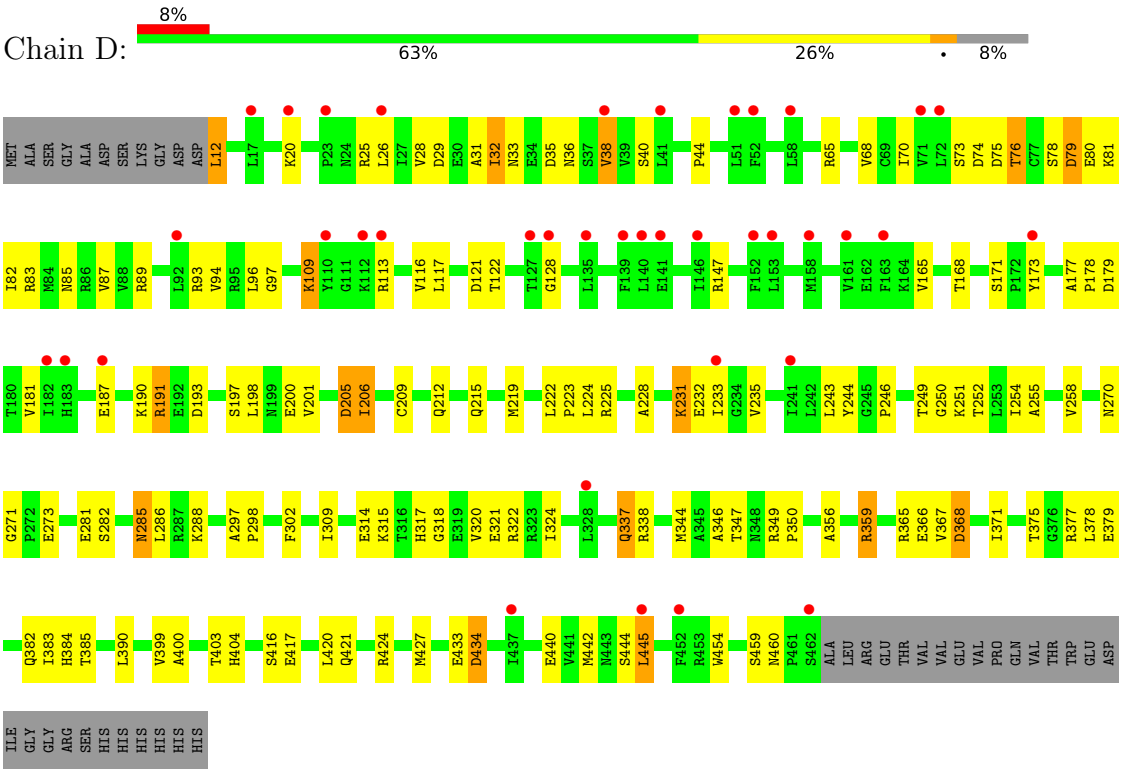
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



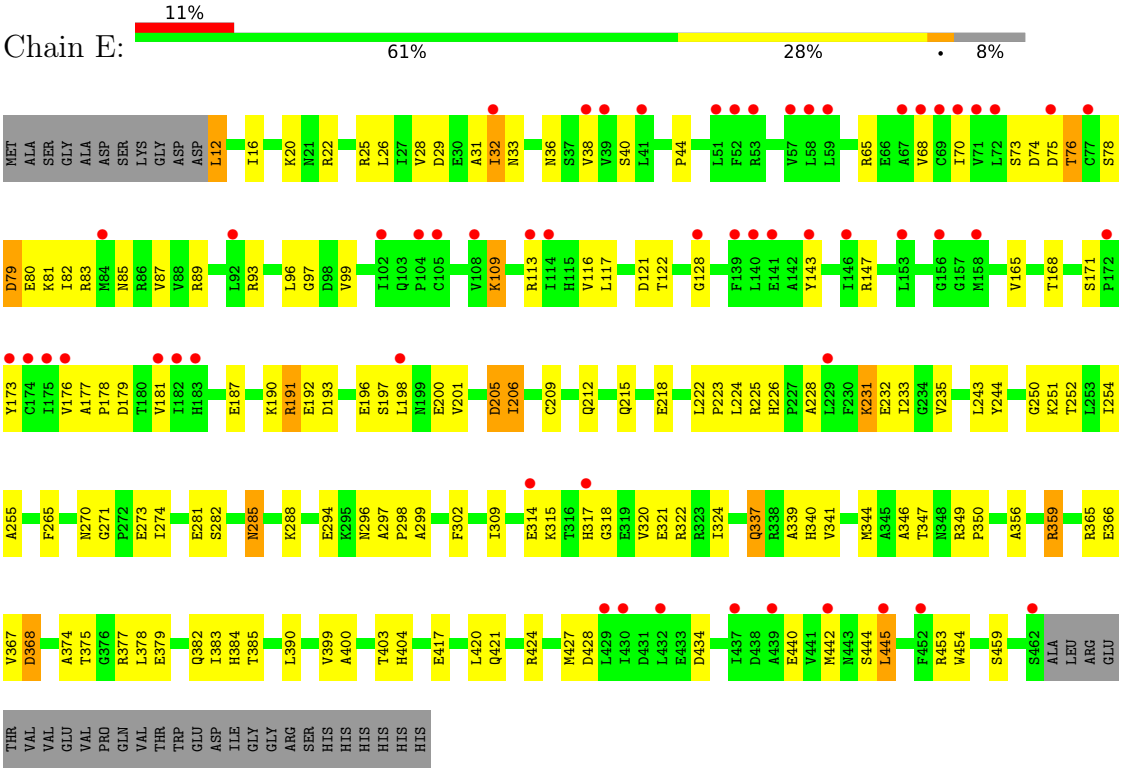
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



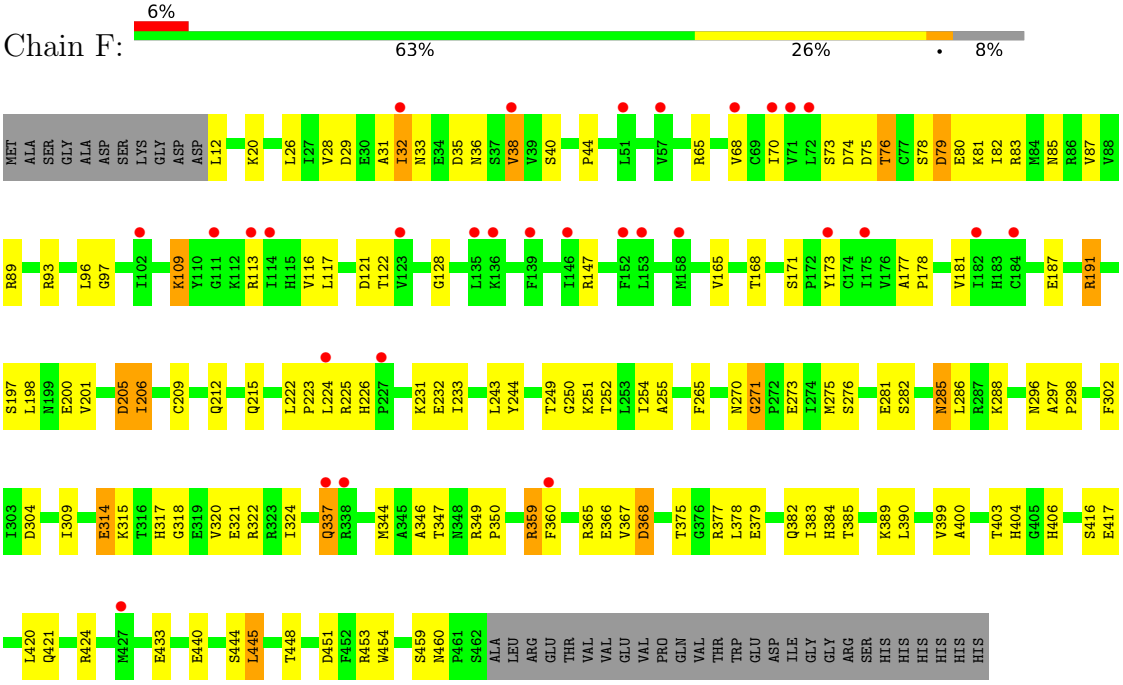
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.15Å 104.51Å 109.53Å 98.11° 90.55° 92.72°	Depositor
Resolution (Å)	46.29 – 2.62 46.24 – 2.62	Depositor EDS
% Data completeness (in resolution range)	83.1 (46.29-2.62) 83.1 (46.24-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.274 , 0.289 0.284 , 0.297	Depositor DCC
R_{free} test set	4959 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21556	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: AGS, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/3587	0.55	1/4846 (0.0%)
1	B	0.31	1/3587 (0.0%)	0.56	1/4846 (0.0%)
1	C	0.30	0/3587	0.55	1/4846 (0.0%)
1	D	0.29	0/3587	0.55	1/4846 (0.0%)
1	E	0.29	0/3587	0.55	1/4846 (0.0%)
1	F	0.31	0/3587	0.55	0/4846
All	All	0.30	1/21522 (0.0%)	0.55	5/29076 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ASN	CG-OD1	-5.75	1.11	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	12	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	12	LEU	CA-CB-CG	5.21	127.28	115.30
1	E	12	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	12	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	12	LEU	CA-CB-CG	5.08	126.98	115.30

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	3533	0	3594	99	0
1	B	3533	0	3594	93	0
1	C	3533	0	3594	97	0
1	D	3533	0	3594	100	0
1	E	3533	0	3594	96	0
1	F	3533	0	3594	89	0
2	A	31	0	12	6	0
2	B	31	0	12	5	0
2	C	31	0	12	4	0
2	D	31	0	12	4	0
2	E	31	0	12	5	0
2	F	31	0	12	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	33	0	0	0	0
4	B	28	0	0	0	0
4	C	30	0	0	0	0
4	D	26	0	0	6	0
4	E	25	0	0	0	0
4	F	24	0	0	0	0
All	All	21556	0	21636	524	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 12.

All (524) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:VAL:O	1:C:403:THR:HG23	1.42	1.14
1:D:399:VAL:O	1:D:403:THR:HG23	1.47	1.11
2:E:800:AGS:S1G	1:F:359:ARG:HG2	2.04	0.97
2:B:800:AGS:S1G	1:C:359:ARG:CG	2.55	0.95
2:B:800:AGS:S1G	1:C:359:ARG:HG2	2.05	0.95
1:F:399:VAL:O	1:F:403:THR:HG23	1.69	0.93
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.50	0.93
1:C:428:ASP:HA	1:D:20:LYS:HE2	1.50	0.92
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.52	0.92
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.52	0.91
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.52	0.91
2:E:800:AGS:S1G	1:F:359:ARG:CG	2.59	0.90
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.51	0.90
1:D:433:GLU:HG3	1:E:25:ARG:HH21	1.36	0.89
1:A:359:ARG:CG	2:F:800:AGS:S1G	2.63	0.87
1:B:399:VAL:O	1:B:403:THR:HG23	1.73	0.87
1:C:251:LYS:HE3	2:C:800:AGS:O2B	1.75	0.87
1:A:359:ARG:HG2	2:F:800:AGS:S1G	2.16	0.86
1:D:251:LYS:HE3	2:D:800:AGS:O2B	1.77	0.85
1:B:32:ILE:HG23	1:B:83:ARG:HH11	1.42	0.82
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.62	0.82
2:C:800:AGS:S1G	1:D:359:ARG:HG2	2.21	0.81
1:C:250:GLY:O	1:C:254:ILE:HG13	1.81	0.80
1:D:206:ILE:HD11	1:D:209:CYS:HB2	1.63	0.80
1:F:31:ALA:HA	1:F:83:ARG:HB3	1.64	0.80
1:E:206:ILE:HD11	1:E:209:CYS:HB2	1.64	0.80
1:C:206:ILE:HD11	1:C:209:CYS:HB2	1.65	0.79
1:E:399:VAL:O	1:E:403:THR:HG23	1.81	0.79
1:B:32:ILE:HG23	1:B:83:ARG:NH1	1.96	0.79
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.63	0.79
1:B:206:ILE:HD11	1:B:209:CYS:HB2	1.62	0.79
1:E:31:ALA:HA	1:E:83:ARG:HB3	1.63	0.79
1:A:206:ILE:HD11	1:A:209:CYS:HB2	1.66	0.79
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.65	0.78
1:C:249:THR:OG1	1:C:251:LYS:HE2	1.83	0.78
2:A:800:AGS:S1G	1:B:359:ARG:HG2	2.24	0.78
1:D:31:ALA:HA	1:D:83:ARG:HB3	1.64	0.77
1:F:206:ILE:HD11	1:F:209:CYS:HB2	1.64	0.77
2:C:800:AGS:S1G	1:D:359:ARG:CG	2.73	0.77
2:A:800:AGS:S1G	1:B:359:ARG:CG	2.72	0.76
1:C:399:VAL:O	1:C:403:THR:CG2	2.30	0.76
1:B:251:LYS:HE3	2:B:800:AGS:O2B	1.86	0.74
1:C:377:ARG:HD2	1:C:403:THR:OG1	1.87	0.74
2:D:800:AGS:S1G	1:E:359:ARG:HG2	2.29	0.73
1:D:244:TYR:CZ	1:D:368:ASP:HB2	2.23	0.73
1:D:433:GLU:HG3	1:E:25:ARG:NH2	2.02	0.73
1:A:244:TYR:CZ	1:A:368:ASP:HB2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:HIS:HB2	1:F:322:ARG:HH22	1.54	0.73
1:E:243:LEU:HD22	1:E:367:VAL:HB	1.71	0.73
1:F:244:TYR:CZ	1:F:368:ASP:HB2	2.24	0.72
1:A:251:LYS:HE3	2:A:800:AGS:O2B	1.90	0.71
1:D:89:ARG:HD3	4:D:917:HOH:O	1.89	0.71
1:A:25:ARG:HH21	1:F:433:GLU:HG3	1.54	0.71
2:B:800:AGS:S1G	1:C:359:ARG:HG3	2.30	0.71
1:C:377:ARG:CD	1:C:403:THR:OG1	2.38	0.70
2:D:800:AGS:S1G	1:E:359:ARG:CG	2.79	0.70
1:D:109:LYS:H	1:D:109:LYS:HD2	1.57	0.70
1:B:244:TYR:CZ	1:B:368:ASP:HB2	2.29	0.68
1:E:109:LYS:H	1:E:109:LYS:HD2	1.59	0.68
1:F:109:LYS:H	1:F:109:LYS:HD2	1.59	0.68
1:A:399:VAL:O	1:A:403:THR:HG23	1.94	0.68
1:B:416:SER:HA	1:C:235:VAL:HG21	1.76	0.68
1:E:337:GLN:HA	1:E:337:GLN:HE21	1.59	0.68
1:C:109:LYS:H	1:C:109:LYS:HD2	1.58	0.67
1:F:252:THR:O	1:F:255:ALA:HB3	1.95	0.67
1:F:302:PHE:CE2	1:F:344:MET:HE2	2.28	0.67
1:C:277:LYS:HB3	1:C:281:GLU:HB3	1.76	0.67
1:B:109:LYS:H	1:B:109:LYS:HD2	1.60	0.67
1:A:196:GLU:OE2	1:B:337:GLN:HB2	1.94	0.66
1:E:243:LEU:CD2	1:E:367:VAL:HB	2.25	0.66
1:F:377:ARG:NH1	1:F:400:ALA:O	2.28	0.66
1:E:244:TYR:CZ	1:E:368:ASP:HB2	2.30	0.66
1:B:243:LEU:HD22	1:B:367:VAL:HB	1.78	0.66
1:D:377:ARG:HD2	1:D:403:THR:OG1	1.95	0.66
1:E:377:ARG:NH2	1:E:404:HIS:HA	2.10	0.65
1:F:243:LEU:HD22	1:F:367:VAL:HB	1.79	0.65
1:A:337:GLN:HE21	1:A:337:GLN:HA	1.61	0.65
1:F:337:GLN:HA	1:F:337:GLN:HE21	1.62	0.65
1:A:433:GLU:HG3	1:B:25:ARG:HH21	1.62	0.65
1:C:278:LEU:O	1:C:281:GLU:HB2	1.97	0.65
1:D:337:GLN:HE21	1:D:337:GLN:HA	1.62	0.64
1:B:317:HIS:HB2	1:C:322:ARG:HH22	1.60	0.64
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.60	0.64
1:B:433:GLU:HG3	1:C:25:ARG:NH2	2.12	0.64
1:E:385:THR:HB	1:E:390:LEU:HD11	1.80	0.64
1:B:377:ARG:HD2	1:B:403:THR:OG1	1.97	0.64
1:D:317:HIS:HB2	1:E:322:ARG:HH22	1.63	0.64
1:E:222:LEU:HB3	1:E:223:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:CD1	1:B:209:CYS:HB2	2.28	0.63
1:C:378:LEU:HG	1:C:382:GLN:NE2	2.14	0.63
1:E:377:ARG:HD2	1:E:403:THR:OG1	1.98	0.63
1:C:243:LEU:HD22	1:C:367:VAL:HB	1.80	0.63
1:C:385:THR:HB	1:C:390:LEU:HD11	1.81	0.63
1:D:378:LEU:HG	1:D:382:GLN:NE2	2.14	0.63
1:F:378:LEU:HG	1:F:382:GLN:NE2	2.13	0.63
1:B:222:LEU:HB3	1:B:223:PRO:HD3	1.81	0.63
1:B:385:THR:HB	1:B:390:LEU:HD11	1.80	0.62
1:B:337:GLN:HE21	1:B:337:GLN:HA	1.64	0.62
1:C:416:SER:HA	1:D:235:VAL:HG21	1.81	0.62
1:D:206:ILE:CD1	1:D:209:CYS:HB2	2.29	0.62
1:E:378:LEU:HG	1:E:382:GLN:NE2	2.13	0.62
1:A:206:ILE:CD1	1:A:209:CYS:HB2	2.29	0.62
1:D:377:ARG:CD	1:D:403:THR:OG1	2.47	0.62
1:A:359:ARG:HG3	2:F:800:AGS:S1G	2.39	0.62
1:A:385:THR:HB	1:A:390:LEU:HD11	1.82	0.62
1:B:74:ASP:OD1	1:B:76:THR:HG23	1.99	0.62
1:B:378:LEU:HG	1:B:382:GLN:NE2	2.14	0.62
1:E:318:GLY:HA3	1:E:321:GLU:HG3	1.81	0.62
1:F:251:LYS:HE3	2:F:800:AGS:O2B	2.00	0.62
1:C:206:ILE:CD1	1:C:209:CYS:HB2	2.29	0.61
1:E:206:ILE:CD1	1:E:209:CYS:HB2	2.30	0.61
1:D:28:VAL:HG21	4:D:917:HOH:O	2.00	0.61
1:F:249:THR:OG1	1:F:251:LYS:HE2	2.00	0.61
1:D:219:MET:O	1:D:223:PRO:HG2	1.99	0.61
1:B:36:ASN:HA	1:B:85:ASN:HD21	1.65	0.61
1:E:285:ASN:N	1:E:285:ASN:HD22	1.99	0.61
1:D:243:LEU:HD22	1:D:367:VAL:HB	1.82	0.61
1:D:250:GLY:O	1:D:254:ILE:HG13	2.01	0.61
1:F:385:THR:HB	1:F:390:LEU:HD11	1.82	0.61
1:F:403:THR:O	1:F:406:HIS:ND1	2.34	0.60
1:A:222:LEU:HB3	1:A:223:PRO:HD3	1.81	0.60
1:C:428:ASP:HA	1:D:20:LYS:CE	2.27	0.60
1:C:201:VAL:HG13	1:C:205:ASP:HB2	1.82	0.60
1:D:320:VAL:O	1:D:324:ILE:HD12	2.02	0.60
1:A:378:LEU:HG	1:A:382:GLN:NE2	2.16	0.60
1:B:29:ASP:O	1:B:83:ARG:HA	2.01	0.59
1:C:222:LEU:HB3	1:C:223:PRO:HD3	1.82	0.59
1:A:431:ASP:HB2	1:B:20:LYS:HD3	1.84	0.59
1:B:201:VAL:HG13	1:B:205:ASP:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:LYS:HD2	1:E:20:LYS:N	2.17	0.59
1:F:222:LEU:HB3	1:F:223:PRO:HD3	1.83	0.59
1:A:25:ARG:NH2	1:F:433:GLU:HG3	2.18	0.59
1:A:285:ASN:HD22	1:A:285:ASN:N	2.00	0.59
1:C:320:VAL:O	1:C:324:ILE:HD12	2.03	0.59
1:F:201:VAL:HG13	1:F:205:ASP:HB2	1.84	0.59
1:B:20:LYS:HD2	1:B:20:LYS:N	2.18	0.58
1:F:206:ILE:CD1	1:F:209:CYS:HB2	2.31	0.58
1:D:243:LEU:CD2	1:D:367:VAL:HB	2.34	0.58
1:D:385:THR:HB	1:D:390:LEU:HD11	1.85	0.58
1:F:243:LEU:CD2	1:F:367:VAL:HB	2.33	0.58
1:F:377:ARG:HD2	1:F:403:THR:OG1	2.03	0.58
2:E:800:AGS:S1G	1:F:359:ARG:HG3	2.44	0.58
1:A:201:VAL:HG13	1:A:205:ASP:HB2	1.85	0.58
2:A:800:AGS:S1G	1:B:359:ARG:HG3	2.43	0.57
1:E:192:GLU:O	1:E:196:GLU:HG3	2.04	0.57
1:C:244:TYR:CZ	1:C:368:ASP:HB2	2.38	0.57
1:A:32:ILE:HG23	1:A:83:ARG:NH1	2.19	0.57
1:C:32:ILE:HG23	1:C:83:ARG:NH1	2.20	0.57
1:A:431:ASP:CB	1:B:20:LYS:HD3	2.35	0.57
1:D:399:VAL:O	1:D:403:THR:CG2	2.38	0.57
1:F:250:GLY:HA2	2:F:800:AGS:O1A	2.05	0.57
1:F:318:GLY:HA3	1:F:321:GLU:HG3	1.86	0.57
1:E:29:ASP:O	1:E:83:ARG:HA	2.04	0.57
1:B:320:VAL:O	1:B:324:ILE:HD12	2.05	0.57
1:C:417:GLU:OE2	1:C:454:TRP:HZ3	1.87	0.57
1:F:74:ASP:OD1	1:F:76:THR:HG23	2.05	0.57
1:F:285:ASN:N	1:F:285:ASN:HD22	2.02	0.57
1:A:250:GLY:O	1:A:254:ILE:HG13	2.05	0.57
1:A:417:GLU:OE2	1:A:454:TRP:HZ3	1.87	0.57
1:C:285:ASN:N	1:C:285:ASN:HD22	2.03	0.57
1:D:32:ILE:HG23	1:D:83:ARG:NH1	2.20	0.57
1:C:428:ASP:CA	1:D:20:LYS:HE2	2.30	0.56
1:C:302:PHE:CE2	1:C:344:MET:HE2	2.40	0.56
1:D:285:ASN:N	1:D:285:ASN:HD22	2.02	0.56
1:E:377:ARG:CZ	1:E:404:HIS:HA	2.34	0.56
1:E:428:ASP:HA	1:F:20:LYS:HE2	1.86	0.56
1:B:255:ALA:HB2	1:B:302:PHE:CZ	2.41	0.56
1:A:320:VAL:O	1:A:324:ILE:HD12	2.05	0.56
1:E:32:ILE:HG23	1:E:83:ARG:NH1	2.20	0.56
1:B:243:LEU:CD2	1:B:367:VAL:HB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:800:AGS:S1G	1:D:359:ARG:HG3	2.45	0.56
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.88	0.56
1:E:442:MET:HG3	1:F:232:GLU:HG2	1.87	0.56
1:A:74:ASP:OD1	1:A:76:THR:HG23	2.06	0.56
1:D:417:GLU:OE2	1:D:454:TRP:HZ3	1.88	0.56
1:E:320:VAL:O	1:E:324:ILE:HD12	2.06	0.56
1:F:32:ILE:HG23	1:F:83:ARG:NH1	2.21	0.56
1:A:377:ARG:NH1	1:A:400:ALA:O	2.38	0.56
1:B:212:GLN:HA	1:B:215:GLN:HG3	1.88	0.56
1:B:318:GLY:HA3	1:B:321:GLU:HG3	1.88	0.56
1:A:20:LYS:N	1:A:20:LYS:HD2	2.21	0.55
1:E:36:ASN:HA	1:E:85:ASN:HD21	1.71	0.55
1:A:29:ASP:O	1:A:83:ARG:HA	2.06	0.55
1:B:302:PHE:CE2	1:B:344:MET:HE2	2.41	0.55
1:C:29:ASP:O	1:C:83:ARG:HA	2.06	0.55
1:F:417:GLU:OE2	1:F:454:TRP:HZ3	1.89	0.55
1:E:298:PRO:HA	1:E:340:HIS:O	2.06	0.55
1:F:252:THR:OG1	1:F:304:ASP:OD2	2.25	0.55
1:B:250:GLY:O	1:B:254:ILE:HG13	2.06	0.55
1:F:320:VAL:O	1:F:324:ILE:HD12	2.07	0.55
1:A:36:ASN:HA	1:A:85:ASN:HD21	1.71	0.55
1:A:235:VAL:HG21	1:F:416:SER:HA	1.89	0.55
1:B:65:ARG:HG3	1:B:93:ARG:CG	2.37	0.55
1:D:29:ASP:O	1:D:83:ARG:HA	2.06	0.55
1:A:273:GLU:HG3	1:B:330:THR:HG23	1.89	0.55
1:E:299:ALA:HB3	1:E:341:VAL:HG22	1.89	0.55
1:A:212:GLN:HA	1:A:215:GLN:HG3	1.89	0.55
1:D:212:GLN:HA	1:D:215:GLN:HG3	1.89	0.54
1:B:65:ARG:HG3	1:B:93:ARG:HG2	1.89	0.54
1:A:243:LEU:HD22	1:A:367:VAL:HB	1.89	0.54
1:A:317:HIS:HB2	1:B:322:ARG:HH22	1.71	0.54
1:D:20:LYS:N	1:D:20:LYS:HD2	2.22	0.54
1:D:74:ASP:OD1	1:D:76:THR:HG23	2.08	0.54
1:E:251:LYS:HE3	2:E:800:AGS:O2B	2.06	0.54
1:F:36:ASN:HA	1:F:85:ASN:HD21	1.73	0.54
1:D:201:VAL:HG13	1:D:205:ASP:HB2	1.89	0.54
1:A:65:ARG:HG3	1:A:93:ARG:CG	2.38	0.54
1:E:250:GLY:O	1:E:254:ILE:HG13	2.08	0.54
1:E:252:THR:O	1:E:255:ALA:HB3	2.08	0.54
1:B:35:ASP:O	1:B:38:VAL:HG12	2.07	0.54
1:C:212:GLN:HA	1:C:215:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:HD2	1:A:403:THR:OG1	2.07	0.54
1:C:74:ASP:OD1	1:C:76:THR:HG23	2.07	0.54
1:F:20:LYS:N	1:F:20:LYS:HD2	2.23	0.53
1:E:417:GLU:OE2	1:E:454:TRP:HZ3	1.90	0.53
1:B:377:ARG:NH2	1:B:404:HIS:HA	2.24	0.53
1:E:116:VAL:HG12	1:E:165:VAL:HA	1.90	0.53
1:F:65:ARG:HG3	1:F:93:ARG:CG	2.38	0.53
1:B:89:ARG:HD3	1:B:96:LEU:HG	1.90	0.53
1:C:20:LYS:HD2	1:C:20:LYS:N	2.23	0.53
1:C:377:ARG:HD3	1:C:403:THR:OG1	2.09	0.53
1:D:35:ASP:O	1:D:38:VAL:HG12	2.09	0.53
1:D:36:ASN:HA	1:D:85:ASN:HD21	1.74	0.53
1:F:212:GLN:HA	1:F:215:GLN:HG3	1.90	0.53
1:C:318:GLY:HA3	1:C:321:GLU:HG3	1.90	0.53
1:E:297:ALA:CB	1:E:339:ALA:O	2.57	0.53
1:F:65:ARG:HG3	1:F:93:ARG:HG2	1.91	0.53
1:F:250:GLY:O	1:F:254:ILE:HG13	2.09	0.53
1:A:35:ASP:O	1:A:38:VAL:HG12	2.09	0.52
1:B:116:VAL:HG12	1:B:165:VAL:HA	1.92	0.52
1:B:377:ARG:NH1	1:B:400:ALA:O	2.43	0.52
1:C:35:ASP:O	1:C:38:VAL:HG12	2.09	0.52
1:E:74:ASP:OD1	1:E:76:THR:HG23	2.10	0.52
1:F:29:ASP:O	1:F:83:ARG:HA	2.08	0.52
1:E:212:GLN:HA	1:E:215:GLN:HG3	1.90	0.52
1:C:243:LEU:CD2	1:C:367:VAL:HB	2.38	0.52
1:A:433:GLU:HB2	1:B:25:ARG:NH2	2.24	0.52
1:B:417:GLU:OE2	1:B:454:TRP:HZ3	1.93	0.52
1:C:116:VAL:HG12	1:C:165:VAL:HA	1.91	0.52
1:C:262:THR:HG23	1:C:262:THR:O	2.09	0.52
1:D:65:ARG:HG3	1:D:93:ARG:CG	2.40	0.51
1:C:36:ASN:HA	1:C:85:ASN:HD21	1.74	0.51
1:F:116:VAL:HG12	1:F:165:VAL:HA	1.91	0.51
1:B:224:LEU:HD22	1:B:298:PRO:HB3	1.92	0.51
1:E:201:VAL:HG13	1:E:205:ASP:HB2	1.92	0.51
1:C:377:ARG:NH1	1:C:400:ALA:O	2.44	0.51
1:C:65:ARG:HG3	1:C:93:ARG:CG	2.41	0.51
1:A:121:ASP:OD2	1:A:191:ARG:HD2	2.11	0.51
1:D:89:ARG:HG2	4:D:917:HOH:O	2.10	0.51
1:D:116:VAL:HG12	1:D:165:VAL:HA	1.91	0.51
1:D:252:THR:O	1:D:255:ALA:HB3	2.11	0.51
1:E:224:LEU:HD22	1:E:298:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HG3	1:A:93:ARG:HG2	1.94	0.50
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.93	0.50
1:A:116:VAL:HG12	1:A:165:VAL:HA	1.91	0.50
1:C:121:ASP:OD2	1:C:191:ARG:HD2	2.11	0.50
1:E:302:PHE:CE2	1:E:344:MET:HE2	2.47	0.50
1:A:379:GLU:O	1:A:383:ILE:HG13	2.11	0.50
1:B:121:ASP:OD2	1:B:191:ARG:HD2	2.11	0.50
1:B:281:GLU:O	1:B:285:ASN:ND2	2.36	0.50
1:D:377:ARG:NH1	1:D:400:ALA:O	2.43	0.50
1:E:445:LEU:HD22	1:F:233:ILE:HD12	1.94	0.50
1:E:32:ILE:HG13	1:E:33:ASN:H	1.76	0.50
1:F:32:ILE:HG13	1:F:33:ASN:H	1.77	0.50
1:B:433:GLU:HG3	1:C:25:ARG:HH21	1.75	0.50
1:F:113:ARG:HG2	1:F:181:VAL:HB	1.94	0.50
1:C:32:ILE:HG23	1:C:83:ARG:HH11	1.77	0.49
1:A:113:ARG:HG2	1:A:181:VAL:HB	1.94	0.49
1:B:30:GLU:O	1:B:83:ARG:HG2	2.12	0.49
1:F:35:ASP:O	1:F:38:VAL:HG12	2.12	0.49
1:D:224:LEU:HD22	1:D:298:PRO:HB3	1.94	0.49
1:A:233:ILE:HD12	1:F:445:LEU:HD22	1.93	0.49
1:C:364:ASP:O	1:C:365:ARG:HD3	2.12	0.49
1:D:421:GLN:HA	1:D:424:ARG:HE	1.78	0.49
1:E:379:GLU:O	1:E:383:ILE:HG13	2.12	0.49
1:A:32:ILE:HG23	1:A:83:ARG:HH11	1.76	0.49
1:D:32:ILE:HG13	1:D:33:ASN:H	1.78	0.49
1:D:243:LEU:O	1:D:346:ALA:HA	2.13	0.49
1:E:113:ARG:HG2	1:E:181:VAL:HB	1.94	0.49
1:A:255:ALA:HB2	1:A:302:PHE:CZ	2.48	0.49
1:A:270:ASN:O	1:A:273:GLU:N	2.43	0.49
1:A:224:LEU:HD22	1:A:298:PRO:HB3	1.95	0.49
1:D:302:PHE:CE2	1:D:344:MET:HE2	2.48	0.49
1:A:32:ILE:HG13	1:A:33:ASN:H	1.77	0.48
1:F:379:GLU:O	1:F:383:ILE:HG13	2.13	0.48
1:C:32:ILE:HG13	1:C:33:ASN:H	1.77	0.48
1:C:243:LEU:O	1:C:346:ALA:HA	2.13	0.48
1:D:113:ARG:HG2	1:D:181:VAL:HB	1.95	0.48
1:D:318:GLY:HA3	1:D:321:GLU:HG3	1.95	0.48
1:C:224:LEU:HD22	1:C:298:PRO:HB3	1.95	0.48
1:E:378:LEU:HG	1:E:382:GLN:HE21	1.78	0.48
1:F:121:ASP:OD2	1:F:191:ARG:HD2	2.13	0.48
1:C:389:LYS:HE2	1:D:232:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:HB2	1:B:25:ARG:HH22	1.79	0.47
1:D:121:ASP:OD2	1:D:191:ARG:HD2	2.14	0.47
1:F:224:LEU:HD22	1:F:298:PRO:HB3	1.95	0.47
1:B:378:LEU:HG	1:B:382:GLN:HE21	1.79	0.47
1:C:252:THR:O	1:C:255:ALA:HB3	2.15	0.47
1:D:32:ILE:HG23	1:D:83:ARG:HH11	1.77	0.47
1:E:349:ARG:HH12	1:F:314:GLU:HG2	1.78	0.47
1:F:378:LEU:HG	1:F:382:GLN:HE21	1.78	0.47
1:B:44:PRO:HB2	1:B:79:ASP:OD2	2.14	0.47
1:E:32:ILE:HG23	1:E:83:ARG:HH11	1.78	0.47
1:E:65:ARG:HG3	1:E:93:ARG:CG	2.45	0.47
1:B:377:ARG:CD	1:B:403:THR:OG1	2.63	0.47
1:A:302:PHE:CE2	1:A:344:MET:HE2	2.50	0.47
1:A:360:PHE:CE1	2:F:800:AGS:H4'	2.50	0.47
1:B:317:HIS:HB2	1:C:322:ARG:NH2	2.29	0.47
1:C:378:LEU:HG	1:C:382:GLN:HE21	1.80	0.47
1:E:344:MET:HE2	1:E:344:MET:HB3	1.64	0.47
1:B:379:GLU:O	1:B:383:ILE:HG13	2.15	0.47
1:F:421:GLN:HA	1:F:424:ARG:HE	1.79	0.47
1:C:421:GLN:HA	1:C:424:ARG:HE	1.80	0.47
1:D:379:GLU:O	1:D:383:ILE:HG13	2.14	0.47
2:D:800:AGS:S1G	1:E:359:ARG:HG3	2.55	0.47
1:F:377:ARG:NH2	1:F:404:HIS:HA	2.29	0.47
1:A:244:TYR:OH	1:A:368:ASP:HB2	2.15	0.47
1:C:113:ARG:HG2	1:C:181:VAL:HB	1.97	0.47
1:A:243:LEU:CD2	1:A:367:VAL:HB	2.44	0.47
1:B:40:SER:O	1:B:82:ILE:HG13	2.15	0.47
1:D:65:ARG:HG3	1:D:93:ARG:HG2	1.96	0.47
1:D:378:LEU:HG	1:D:382:GLN:HE21	1.79	0.47
1:D:249:THR:OG1	1:D:251:LYS:HE2	2.15	0.47
1:E:377:ARG:CD	1:E:403:THR:OG1	2.63	0.47
1:C:379:GLU:O	1:C:383:ILE:HG13	2.14	0.46
1:F:32:ILE:HG23	1:F:83:ARG:HH11	1.79	0.46
1:F:270:ASN:O	1:F:273:GLU:N	2.43	0.46
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.96	0.46
1:B:113:ARG:HG2	1:B:181:VAL:HB	1.95	0.46
1:E:421:GLN:HA	1:E:424:ARG:HE	1.79	0.46
1:D:28:VAL:HG23	1:D:97:GLY:H	1.81	0.46
1:A:318:GLY:HA3	1:A:321:GLU:HG3	1.98	0.46
1:C:337:GLN:HE21	1:C:337:GLN:CA	2.27	0.46
1:B:270:ASN:O	1:B:273:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLN:HA	1:A:424:ARG:HE	1.81	0.46
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.97	0.46
1:E:121:ASP:OD2	1:E:191:ARG:HD2	2.16	0.46
1:A:297:ALA:HA	1:A:298:PRO:C	2.37	0.45
1:E:377:ARG:NH1	1:E:400:ALA:O	2.50	0.45
1:C:270:ASN:O	1:C:273:GLU:N	2.47	0.45
1:D:377:ARG:HD3	1:D:403:THR:OG1	2.16	0.45
1:E:65:ARG:HG3	1:E:93:ARG:HG2	1.98	0.45
1:A:273:GLU:HG3	1:B:330:THR:CG2	2.46	0.45
1:B:89:ARG:CD	1:B:96:LEU:HG	2.45	0.45
1:A:378:LEU:HG	1:A:382:GLN:HE21	1.80	0.45
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.99	0.45
1:B:177:ALA:HB1	1:B:178:PRO:CD	2.46	0.45
1:E:297:ALA:HA	1:E:298:PRO:C	2.36	0.45
1:A:196:GLU:CD	1:B:337:GLN:HB2	2.36	0.45
1:B:421:GLN:HA	1:B:424:ARG:HE	1.82	0.45
1:C:65:ARG:HG3	1:C:93:ARG:HG2	1.99	0.45
1:C:317:HIS:HB2	1:D:322:ARG:HH22	1.82	0.45
1:D:445:LEU:HD22	1:E:233:ILE:HD12	1.99	0.45
1:D:434:ASP:OD1	1:D:434:ASP:N	2.50	0.45
1:E:243:LEU:O	1:E:346:ALA:HA	2.17	0.45
1:A:430:ILE:O	1:B:20:LYS:NZ	2.49	0.45
1:B:284:SER:O	1:B:288:LYS:HB2	2.16	0.45
1:E:28:VAL:HG23	1:E:97:GLY:H	1.81	0.45
1:A:28:VAL:HG23	1:A:96:LEU:HA	1.98	0.45
1:A:44:PRO:HB2	1:A:79:ASP:OD2	2.17	0.45
1:A:360:PHE:CD1	1:A:360:PHE:C	2.90	0.45
1:E:434:ASP:O	1:F:226:HIS:HE1	1.99	0.45
1:C:44:PRO:HB2	1:C:79:ASP:OD2	2.17	0.44
1:C:192:GLU:OE1	1:D:338:ARG:HB2	2.17	0.44
1:F:243:LEU:O	1:F:346:ALA:HA	2.17	0.44
1:C:431:ASP:OD2	1:D:25:ARG:NH2	2.49	0.44
1:D:434:ASP:CG	1:E:22:ARG:HH12	2.20	0.44
1:C:428:ASP:O	1:D:20:LYS:HG2	2.18	0.44
1:E:44:PRO:HB2	1:E:79:ASP:OD2	2.18	0.44
1:B:377:ARG:CZ	1:B:404:HIS:HA	2.47	0.44
1:F:249:THR:OG1	1:F:251:LYS:CE	2.64	0.44
1:A:265:PHE:CD2	1:A:296:ASN:HB2	2.52	0.44
1:B:297:ALA:HA	1:B:298:PRO:C	2.38	0.44
1:D:44:PRO:HB2	1:D:79:ASP:OD2	2.18	0.44
1:B:78:SER:HB2	1:B:81:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ILE:HG21	1:E:218:GLU:HG3	1.98	0.44
1:E:274:ILE:HD13	1:E:274:ILE:HA	1.90	0.44
1:D:94:VAL:HG23	4:D:917:HOH:O	2.17	0.43
1:B:250:GLY:HA2	2:B:800:AGS:O1A	2.18	0.43
1:D:377:ARG:NH2	1:D:404:HIS:HA	2.32	0.43
1:E:302:PHE:CE2	1:E:344:MET:CE	3.01	0.43
2:A:800:AGS:H4'	1:B:360:PHE:CE1	2.54	0.43
1:E:337:GLN:HA	1:E:337:GLN:NE2	2.31	0.43
1:A:28:VAL:HG23	1:A:97:GLY:H	1.83	0.43
1:A:364:ASP:O	1:A:365:ARG:CD	2.65	0.43
1:D:344:MET:HE2	1:D:344:MET:HB3	1.72	0.43
1:E:177:ALA:HB1	1:E:178:PRO:CD	2.48	0.43
1:A:177:ALA:HB1	1:A:178:PRO:CD	2.48	0.43
1:D:297:ALA:HA	1:D:298:PRO:C	2.39	0.43
1:E:299:ALA:O	1:E:341:VAL:HA	2.19	0.43
1:F:265:PHE:CD2	1:F:296:ASN:HB2	2.53	0.43
1:B:249:THR:OG1	1:B:251:LYS:HE2	2.18	0.43
1:C:274:ILE:HD13	1:C:274:ILE:HA	1.89	0.43
1:D:117:LEU:HD13	1:D:187:GLU:O	2.19	0.43
1:D:416:SER:HA	1:E:235:VAL:HG21	2.00	0.43
1:F:297:ALA:HA	1:F:298:PRO:C	2.39	0.43
1:C:424:ARG:O	1:C:427:MET:HB2	2.19	0.43
1:F:271:GLY:O	1:F:275:MET:HG2	2.18	0.43
1:A:85:ASN:OD1	1:A:87:VAL:HB	2.19	0.43
1:B:32:ILE:HG13	1:B:33:ASN:H	1.84	0.43
1:D:78:SER:HB2	1:D:81:LYS:HB2	2.01	0.43
1:C:377:ARG:NH2	1:C:404:HIS:HA	2.33	0.43
1:D:177:ALA:HB1	1:D:178:PRO:CD	2.48	0.43
1:D:40:SER:O	1:D:82:ILE:HG13	2.19	0.42
1:F:177:ALA:HB1	1:F:178:PRO:CD	2.49	0.42
1:F:205:ASP:HA	1:F:383:ILE:HG21	2.01	0.42
1:F:377:ARG:CZ	1:F:404:HIS:HA	2.49	0.42
1:A:78:SER:HB2	1:A:81:LYS:HB2	2.01	0.42
1:A:273:GLU:O	1:A:276:SER:OG	2.35	0.42
1:A:389:LYS:HE2	1:B:232:GLU:O	2.19	0.42
1:C:249:THR:OG1	1:C:251:LYS:CE	2.62	0.42
1:E:117:LEU:HD13	1:E:187:GLU:O	2.19	0.42
1:A:205:ASP:N	1:A:205:ASP:OD1	2.52	0.42
1:C:177:ALA:HB1	1:C:178:PRO:CD	2.48	0.42
1:D:246:PRO:HG3	1:D:371:ILE:HD12	2.02	0.42
1:E:40:SER:O	1:E:82:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:O	1:D:258:VAL:HG23	2.19	0.42
1:F:117:LEU:HD13	1:F:187:GLU:O	2.19	0.42
1:F:347:THR:HG21	1:F:350:PRO:HA	1.99	0.42
1:C:205:ASP:N	1:C:205:ASP:OD1	2.52	0.42
1:C:445:LEU:HD22	1:D:233:ILE:HD12	2.01	0.42
1:D:28:VAL:CG2	4:D:917:HOH:O	2.63	0.42
1:E:78:SER:HB2	1:E:81:LYS:HB2	2.01	0.42
1:B:66:GLU:OE1	1:B:147:ARG:NH1	2.52	0.42
1:B:254:ILE:O	1:B:258:VAL:HG23	2.20	0.42
1:C:284:SER:O	1:C:288:LYS:HB2	2.19	0.42
1:E:205:ASP:OD1	1:E:205:ASP:N	2.53	0.42
1:A:240:GLY:HA2	1:A:343:VAL:O	2.19	0.42
1:A:246:PRO:HG3	1:A:371:ILE:HD12	2.02	0.42
1:C:228:ALA:HA	1:C:231:LYS:HB2	2.02	0.42
1:D:270:ASN:O	1:D:273:GLU:N	2.47	0.42
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.88	0.42
1:A:205:ASP:HA	1:A:383:ILE:HG21	2.01	0.42
1:C:78:SER:HB2	1:C:81:LYS:HB2	2.02	0.42
1:D:434:ASP:O	1:E:226:HIS:HE1	2.02	0.42
1:F:44:PRO:HB2	1:F:79:ASP:OD2	2.18	0.42
1:F:453:ARG:HE	1:F:453:ARG:HB2	1.71	0.42
1:A:250:GLY:HA2	2:A:800:AGS:O1A	2.20	0.42
1:D:244:TYR:OH	1:D:368:ASP:HB2	2.20	0.42
1:E:190:LYS:HB2	1:E:193:ASP:OD2	2.20	0.42
1:E:356:ALA:HA	1:E:359:ARG:HD2	2.02	0.42
1:E:374:ALA:HA	1:E:377:ARG:NH1	2.35	0.42
1:E:434:ASP:O	1:F:226:HIS:CE1	2.73	0.42
1:A:310:ALA:O	1:A:353:ILE:HA	2.20	0.42
1:C:28:VAL:HG23	1:C:97:GLY:H	1.85	0.42
1:C:337:GLN:HA	1:C:337:GLN:NE2	2.32	0.42
1:D:347:THR:HG21	1:D:350:PRO:HA	2.02	0.42
1:E:270:ASN:O	1:E:273:GLU:N	2.49	0.42
1:A:344:MET:HE2	1:A:344:MET:HB3	1.91	0.41
1:F:40:SER:O	1:F:82:ILE:HG13	2.20	0.41
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.88	0.41
1:A:377:ARG:NE	1:A:403:THR:O	2.53	0.41
1:A:427:MET:HE2	1:B:16:ILE:HG13	2.01	0.41
1:B:28:VAL:HG23	1:B:97:GLY:H	1.84	0.41
1:C:206:ILE:C	1:C:206:ILE:HD12	2.41	0.41
1:F:448:THR:O	1:F:451:ASP:HB2	2.20	0.41
1:A:228:ALA:HA	1:A:231:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:OG1	1:A:251:LYS:HE2	2.19	0.41
1:A:252:THR:O	1:A:255:ALA:HB3	2.19	0.41
1:D:89:ARG:HD3	1:D:96:LEU:HG	2.02	0.41
1:A:96:LEU:HD12	1:A:96:LEU:H	1.85	0.41
1:A:270:ASN:O	1:A:271:GLY:C	2.59	0.41
1:B:109:LYS:HD3	1:B:170:PRO:CG	2.51	0.41
1:D:424:ARG:O	1:D:427:MET:HB2	2.20	0.41
1:E:89:ARG:HD3	1:E:96:LEU:HG	2.02	0.41
1:E:347:THR:HG21	1:E:350:PRO:HA	2.02	0.41
1:F:85:ASN:OD1	1:F:87:VAL:HB	2.20	0.41
1:F:89:ARG:HD3	1:F:96:LEU:HG	2.02	0.41
1:F:302:PHE:CD2	1:F:344:MET:HE2	2.55	0.41
1:B:265:PHE:CD2	1:B:296:ASN:HB2	2.54	0.41
1:C:206:ILE:HD11	1:C:213:LEU:HD11	2.02	0.41
1:C:369:ILE:O	1:C:369:ILE:HG22	2.20	0.41
1:D:85:ASN:OD1	1:D:87:VAL:HB	2.20	0.41
1:E:85:ASN:OD1	1:E:87:VAL:HB	2.20	0.41
1:E:228:ALA:HA	1:E:231:LYS:HB2	2.02	0.41
1:F:28:VAL:HG23	1:F:97:GLY:H	1.84	0.41
1:A:89:ARG:HD3	1:A:96:LEU:HG	2.02	0.41
1:A:322:ARG:HH22	1:F:317:HIS:HB2	1.85	0.41
1:C:226:HIS:HB2	1:C:229:LEU:HD12	2.02	0.41
1:F:206:ILE:C	1:F:206:ILE:HD12	2.41	0.41
1:A:206:ILE:HD11	1:A:213:LEU:HD11	2.03	0.41
1:A:432:LEU:HD13	1:B:16:ILE:HD11	2.01	0.41
1:C:354:ASP:HA	1:C:355:PRO:HD2	1.93	0.41
1:D:337:GLN:HA	1:D:337:GLN:NE2	2.34	0.41
1:F:337:GLN:HA	1:F:337:GLN:NE2	2.34	0.41
1:C:89:ARG:HD3	1:C:96:LEU:HG	2.02	0.41
1:D:96:LEU:H	1:D:96:LEU:HD12	1.86	0.41
1:D:190:LYS:HB2	1:D:193:ASP:OD2	2.21	0.41
1:D:205:ASP:OD1	1:D:205:ASP:N	2.53	0.41
1:F:286:LEU:HD23	1:F:286:LEU:HA	1.86	0.41
1:A:117:LEU:HD13	1:A:187:GLU:O	2.21	0.41
1:B:424:ARG:O	1:B:427:MET:HB2	2.21	0.41
1:C:117:LEU:HD13	1:C:187:GLU:O	2.21	0.41
1:D:442:MET:HG3	1:E:232:GLU:HG2	2.02	0.41
1:E:265:PHE:CD2	1:E:296:ASN:HB2	2.56	0.41
1:C:96:LEU:H	1:C:96:LEU:HD12	1.85	0.41
1:D:89:ARG:CG	4:D:917:HOH:O	2.69	0.41
1:E:40:SER:CB	1:E:83:ARG:HB2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLY:HA2	2:E:800:AGS:O1A	2.21	0.41
1:F:360:PHE:CD1	1:F:360:PHE:C	2.94	0.41
1:B:96:LEU:H	1:B:96:LEU:HD12	1.86	0.40
1:C:254:ILE:O	1:C:258:VAL:HG23	2.21	0.40
1:D:228:ALA:HA	1:D:231:LYS:HB2	2.02	0.40
1:E:143:TYR:HA	1:E:176:VAL:O	2.20	0.40
1:A:243:LEU:O	1:A:346:ALA:HA	2.21	0.40
1:C:85:ASN:OD1	1:C:87:VAL:HB	2.20	0.40
1:C:255:ALA:HB2	1:C:302:PHE:CZ	2.56	0.40
1:E:424:ARG:O	1:E:427:MET:HB2	2.20	0.40
1:A:40:SER:O	1:A:82:ILE:HG13	2.21	0.40
1:A:232:GLU:O	1:F:389:LYS:HE2	2.22	0.40
1:A:249:THR:HG22	1:A:407:VAL:HB	2.03	0.40
1:B:85:ASN:OD1	1:B:87:VAL:HB	2.21	0.40
1:A:453:ARG:HE	1:A:453:ARG:HB2	1.71	0.40
1:B:32:ILE:CG2	1:B:83:ARG:NH1	2.76	0.40
1:B:205:ASP:N	1:B:205:ASP:OD1	2.55	0.40
1:B:344:MET:HE2	1:B:344:MET:HB3	1.84	0.40
1:C:244:TYR:OH	1:C:368:ASP:HB2	2.21	0.40
1:C:297:ALA:HA	1:C:298:PRO:C	2.42	0.40
1:E:453:ARG:HE	1:E:453:ARG:HB2	1.72	0.40
1:F:273:GLU:O	1:F:276:SER:OG	2.36	0.40
1:B:228:ALA:HA	1:B:231:LYS:HB2	2.02	0.40
1:D:356:ALA:HA	1:D:359:ARG:HD2	2.04	0.40
1:F:78:SER:HB2	1:F:81:LYS:HB2	2.02	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	449/489 (92%)	426 (95%)	21 (5%)	2 (0%)	34 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	449/489 (92%)	427 (95%)	21 (5%)	1 (0%)	47 69
1	C	449/489 (92%)	425 (95%)	22 (5%)	2 (0%)	34 55
1	D	449/489 (92%)	428 (95%)	19 (4%)	2 (0%)	34 55
1	E	449/489 (92%)	427 (95%)	20 (4%)	2 (0%)	34 55
1	F	449/489 (92%)	429 (96%)	18 (4%)	2 (0%)	34 55
All	All	2694/2934 (92%)	2562 (95%)	121 (4%)	11 (0%)	34 55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	B	128	GLY
1	E	128	GLY
1	C	128	GLY
1	D	128	GLY
1	F	128	GLY
1	A	271	GLY
1	F	271	GLY
1	C	271	GLY
1	D	271	GLY
1	E	271	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	388/419 (93%)	341 (88%)	47 (12%)	5 8
1	B	388/419 (93%)	341 (88%)	47 (12%)	5 8
1	C	388/419 (93%)	343 (88%)	45 (12%)	5 9
1	D	388/419 (93%)	340 (88%)	48 (12%)	4 8
1	E	388/419 (93%)	341 (88%)	47 (12%)	5 8
1	F	388/419 (93%)	342 (88%)	46 (12%)	5 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2328/2514 (93%)	2048 (88%)	280 (12%)	5 8

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	26	LEU
1	A	32	ILE
1	A	38	VAL
1	A	68	VAL
1	A	70	ILE
1	A	73	SER
1	A	75	ASP
1	A	76	THR
1	A	79	ASP
1	A	80	GLU
1	A	109	LYS
1	A	122	THR
1	A	147	ARG
1	A	168	THR
1	A	171	SER
1	A	173	TYR
1	A	179	ASP
1	A	191	ARG
1	A	197	SER
1	A	198	LEU
1	A	200	GLU
1	A	205	ASP
1	A	206	ILE
1	A	225	ARG
1	A	231	LYS
1	A	281	GLU
1	A	282	SER
1	A	285	ASN
1	A	288	LYS
1	A	309	ILE
1	A	314	GLU
1	A	315	LYS
1	A	337	GLN
1	A	349	ARG
1	A	359	ARG
1	A	365	ARG

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Mol	Chain	Res	Type
1	A	366	GLU
1	A	368	ASP
1	A	375	THR
1	A	384	HIS
1	A	420	LEU
1	A	440	GLU
1	A	444	SER
1	A	445	LEU
1	A	459	SER
1	A	460	ASN
1	B	12	LEU
1	B	26	LEU
1	B	32	ILE
1	B	38	VAL
1	B	68	VAL
1	B	70	ILE
1	B	73	SER
1	B	75	ASP
1	B	76	THR
1	B	79	ASP
1	B	80	GLU
1	B	87	VAL
1	B	109	LYS
1	B	122	THR
1	B	147	ARG
1	B	168	THR
1	B	171	SER
1	B	173	TYR
1	B	179	ASP
1	B	191	ARG
1	B	197	SER
1	B	198	LEU
1	B	200	GLU
1	B	205	ASP
1	B	206	ILE
1	B	225	ARG
1	B	231	LYS
1	B	281	GLU
1	B	282	SER
1	B	288	LYS
1	B	309	ILE
1	B	314	GLU

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Mol	Chain	Res	Type
1	B	315	LYS
1	B	337	GLN
1	B	349	ARG
1	B	359	ARG
1	B	365	ARG
1	B	366	GLU
1	B	368	ASP
1	B	375	THR
1	B	384	HIS
1	B	420	LEU
1	B	440	GLU
1	B	444	SER
1	B	445	LEU
1	B	459	SER
1	B	460	ASN
1	C	12	LEU
1	C	26	LEU
1	C	32	ILE
1	C	38	VAL
1	C	68	VAL
1	C	70	ILE
1	C	73	SER
1	C	75	ASP
1	C	76	THR
1	C	79	ASP
1	C	80	GLU
1	C	109	LYS
1	C	122	THR
1	C	147	ARG
1	C	168	THR
1	C	171	SER
1	C	173	TYR
1	C	191	ARG
1	C	197	SER
1	C	198	LEU
1	C	200	GLU
1	C	205	ASP
1	C	206	ILE
1	C	225	ARG
1	C	231	LYS
1	C	281	GLU
1	C	282	SER

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Mol	Chain	Res	Type
1	C	285	ASN
1	C	288	LYS
1	C	309	ILE
1	C	314	GLU
1	C	315	LYS
1	C	337	GLN
1	C	349	ARG
1	C	359	ARG
1	C	366	GLU
1	C	368	ASP
1	C	375	THR
1	C	384	HIS
1	C	420	LEU
1	C	440	GLU
1	C	444	SER
1	C	445	LEU
1	C	459	SER
1	C	460	ASN
1	D	12	LEU
1	D	26	LEU
1	D	32	ILE
1	D	38	VAL
1	D	68	VAL
1	D	70	ILE
1	D	73	SER
1	D	75	ASP
1	D	76	THR
1	D	79	ASP
1	D	80	GLU
1	D	109	LYS
1	D	122	THR
1	D	147	ARG
1	D	168	THR
1	D	171	SER
1	D	173	TYR
1	D	179	ASP
1	D	191	ARG
1	D	197	SER
1	D	198	LEU
1	D	200	GLU
1	D	205	ASP
1	D	206	ILE

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Mol	Chain	Res	Type
1	D	225	ARG
1	D	231	LYS
1	D	281	GLU
1	D	282	SER
1	D	285	ASN
1	D	288	LYS
1	D	309	ILE
1	D	314	GLU
1	D	315	LYS
1	D	337	GLN
1	D	349	ARG
1	D	359	ARG
1	D	365	ARG
1	D	366	GLU
1	D	368	ASP
1	D	375	THR
1	D	384	HIS
1	D	420	LEU
1	D	434	ASP
1	D	440	GLU
1	D	444	SER
1	D	445	LEU
1	D	459	SER
1	D	460	ASN
1	E	12	LEU
1	E	26	LEU
1	E	32	ILE
1	E	38	VAL
1	E	68	VAL
1	E	70	ILE
1	E	73	SER
1	E	75	ASP
1	E	76	THR
1	E	79	ASP
1	E	80	GLU
1	E	99	VAL
1	E	109	LYS
1	E	122	THR
1	E	147	ARG
1	E	168	THR
1	E	171	SER
1	E	173	TYR

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Mol	Chain	Res	Type
1	E	179	ASP
1	E	191	ARG
1	E	197	SER
1	E	198	LEU
1	E	200	GLU
1	E	205	ASP
1	E	206	ILE
1	E	225	ARG
1	E	231	LYS
1	E	281	GLU
1	E	282	SER
1	E	285	ASN
1	E	288	LYS
1	E	294	GLU
1	E	309	ILE
1	E	314	GLU
1	E	315	LYS
1	E	337	GLN
1	E	359	ARG
1	E	365	ARG
1	E	366	GLU
1	E	368	ASP
1	E	375	THR
1	E	384	HIS
1	E	420	LEU
1	E	440	GLU
1	E	444	SER
1	E	445	LEU
1	E	459	SER
1	F	12	LEU
1	F	26	LEU
1	F	32	ILE
1	F	38	VAL
1	F	68	VAL
1	F	70	ILE
1	F	73	SER
1	F	75	ASP
1	F	76	THR
1	F	79	ASP
1	F	80	GLU
1	F	109	LYS
1	F	122	THR

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Mol	Chain	Res	Type
1	F	147	ARG
1	F	168	THR
1	F	171	SER
1	F	173	TYR
1	F	191	ARG
1	F	197	SER
1	F	198	LEU
1	F	200	GLU
1	F	205	ASP
1	F	206	ILE
1	F	225	ARG
1	F	231	LYS
1	F	281	GLU
1	F	282	SER
1	F	285	ASN
1	F	288	LYS
1	F	309	ILE
1	F	314	GLU
1	F	315	LYS
1	F	337	GLN
1	F	349	ARG
1	F	359	ARG
1	F	365	ARG
1	F	366	GLU
1	F	368	ASP
1	F	375	THR
1	F	384	HIS
1	F	420	LEU
1	F	440	GLU
1	F	444	SER
1	F	445	LEU
1	F	459	SER
1	F	460	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	215	GLN
1	A	226	HIS
1	A	285	ASN
1	A	337	GLN

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Mol	Chain	Res	Type
1	A	382	GLN
1	A	460	ASN
1	B	91	ASN
1	B	226	HIS
1	B	337	GLN
1	B	382	GLN
1	B	460	ASN
1	C	91	ASN
1	C	285	ASN
1	C	337	GLN
1	C	382	GLN
1	C	460	ASN
1	D	91	ASN
1	D	226	HIS
1	D	285	ASN
1	D	337	GLN
1	D	382	GLN
1	D	460	ASN
1	E	19	GLN
1	E	91	ASN
1	E	226	HIS
1	E	285	ASN
1	E	337	GLN
1	E	382	GLN
1	F	91	ASN
1	F	226	HIS
1	F	285	ASN
1	F	337	GLN
1	F	382	GLN

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 (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	AGS	A	800	3	26,33,33	1.76	3 (11%)	26,52,52	1.53	6 (23%)
2	AGS	E	800	3	26,33,33	1.72	3 (11%)	26,52,52	1.50	6 (23%)
2	AGS	C	800	3	26,33,33	1.76	3 (11%)	26,52,52	1.49	5 (19%)
2	AGS	D	800	3	26,33,33	1.77	3 (11%)	26,52,52	1.49	6 (23%)
2	AGS	B	800	3	26,33,33	1.75	3 (11%)	26,52,52	1.49	6 (23%)
2	AGS	F	800	3	26,33,33	1.93	4 (15%)	26,52,52	1.58	6 (23%)

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
2	AGS	A	800	3	-	3/17/38/38	0/3/3/3
2	AGS	E	800	3	-	4/17/38/38	0/3/3/3
2	AGS	C	800	3	-	3/17/38/38	0/3/3/3
2	AGS	D	800	3	-	3/17/38/38	0/3/3/3
2	AGS	B	800	3	-	3/17/38/38	0/3/3/3
2	AGS	F	800	3	-	3/17/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	800	AGS	PG-S1G	8.30	2.08	1.90
2	D	800	AGS	PG-S1G	7.10	2.06	1.90
2	A	800	AGS	PG-S1G	7.08	2.06	1.90
2	C	800	AGS	PG-S1G	6.84	2.05	1.90
2	B	800	AGS	PG-S1G	6.83	2.05	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	AGS	PG-S1G	6.78	2.05	1.90
2	C	800	AGS	C5-C4	2.86	1.48	1.40
2	E	800	AGS	C5-C4	2.57	1.47	1.40
2	B	800	AGS	C5-C4	2.56	1.47	1.40
2	A	800	AGS	C5-C4	2.51	1.47	1.40
2	D	800	AGS	C5-C4	2.51	1.47	1.40
2	F	800	AGS	C5-C4	2.41	1.47	1.40
2	B	800	AGS	PG-O3G	-2.32	1.47	1.54
2	C	800	AGS	PG-O3G	-2.32	1.47	1.54
2	E	800	AGS	PG-O3G	-2.26	1.47	1.54
2	A	800	AGS	PG-O3G	-2.26	1.47	1.54
2	D	800	AGS	PG-O3G	-2.25	1.47	1.54
2	F	800	AGS	PG-O3G	-2.17	1.47	1.54
2	F	800	AGS	C2-N3	2.01	1.35	1.32

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	800	AGS	N3-C2-N1	-3.67	122.94	128.68
2	D	800	AGS	N3-C2-N1	-3.62	123.01	128.68
2	A	800	AGS	N3-C2-N1	-3.61	123.03	128.68
2	C	800	AGS	N3-C2-N1	-3.55	123.13	128.68
2	E	800	AGS	N3-C2-N1	-3.49	123.22	128.68
2	B	800	AGS	N3-C2-N1	-3.49	123.23	128.68
2	F	800	AGS	PA-O3A-PB	-3.25	121.68	132.83
2	E	800	AGS	PA-O3A-PB	-3.08	122.25	132.83
2	A	800	AGS	PA-O3A-PB	-3.01	122.48	132.83
2	D	800	AGS	PA-O3A-PB	-2.96	122.69	132.83
2	C	800	AGS	PA-O3A-PB	-2.90	122.87	132.83
2	B	800	AGS	PA-O3A-PB	-2.86	123.00	132.83
2	F	800	AGS	O2G-PG-O3B	2.85	114.16	104.64
2	A	800	AGS	C4-C5-N7	-2.58	106.71	109.40
2	E	800	AGS	C4-C5-N7	-2.55	106.74	109.40
2	F	800	AGS	C4-C5-N7	-2.55	106.74	109.40
2	A	800	AGS	C3'-C2'-C1'	2.54	104.80	100.98
2	C	800	AGS	O2G-PG-O3B	2.49	112.95	104.64
2	A	800	AGS	O2G-PG-O3B	2.47	112.89	104.64
2	B	800	AGS	C4-C5-N7	-2.47	106.82	109.40
2	D	800	AGS	O2G-PG-O3B	2.45	112.82	104.64
2	E	800	AGS	O2G-PG-O3B	2.44	112.79	104.64
2	D	800	AGS	C4-C5-N7	-2.44	106.86	109.40
2	B	800	AGS	C3'-C2'-C1'	2.41	104.61	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	800	AGS	C3'-C2'-C1'	2.41	104.61	100.98
2	F	800	AGS	C3'-C2'-C1'	2.41	104.60	100.98
2	B	800	AGS	O2G-PG-O3B	2.39	112.63	104.64
2	C	800	AGS	O3G-PG-O3B	2.38	112.57	104.64
2	A	800	AGS	O3G-PG-O3B	2.30	112.33	104.64
2	D	800	AGS	C3'-C2'-C1'	2.29	104.42	100.98
2	C	800	AGS	C3'-C2'-C1'	2.27	104.40	100.98
2	D	800	AGS	O3G-PG-O3B	2.26	112.19	104.64
2	E	800	AGS	O3G-PG-O3B	2.24	112.11	104.64
2	B	800	AGS	O3G-PG-O3B	2.23	112.07	104.64
2	F	800	AGS	O3G-PG-O3B	2.21	112.02	104.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	AGS	C5'-O5'-PA-O2A
2	B	800	AGS	C5'-O5'-PA-O2A
2	C	800	AGS	C5'-O5'-PA-O2A
2	D	800	AGS	C5'-O5'-PA-O2A
2	E	800	AGS	C5'-O5'-PA-O2A
2	F	800	AGS	C5'-O5'-PA-O2A
2	A	800	AGS	C5'-O5'-PA-O3A
2	B	800	AGS	C5'-O5'-PA-O3A
2	C	800	AGS	C5'-O5'-PA-O3A
2	D	800	AGS	C5'-O5'-PA-O3A
2	E	800	AGS	C5'-O5'-PA-O3A
2	F	800	AGS	C5'-O5'-PA-O3A
2	B	800	AGS	C5'-O5'-PA-O1A
2	C	800	AGS	C5'-O5'-PA-O1A
2	D	800	AGS	C5'-O5'-PA-O1A
2	E	800	AGS	C5'-O5'-PA-O1A
2	E	800	AGS	PA-O3A-PB-O2B
2	A	800	AGS	C5'-O5'-PA-O1A
2	F	800	AGS	C5'-O5'-PA-O1A

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	AGS	6	0

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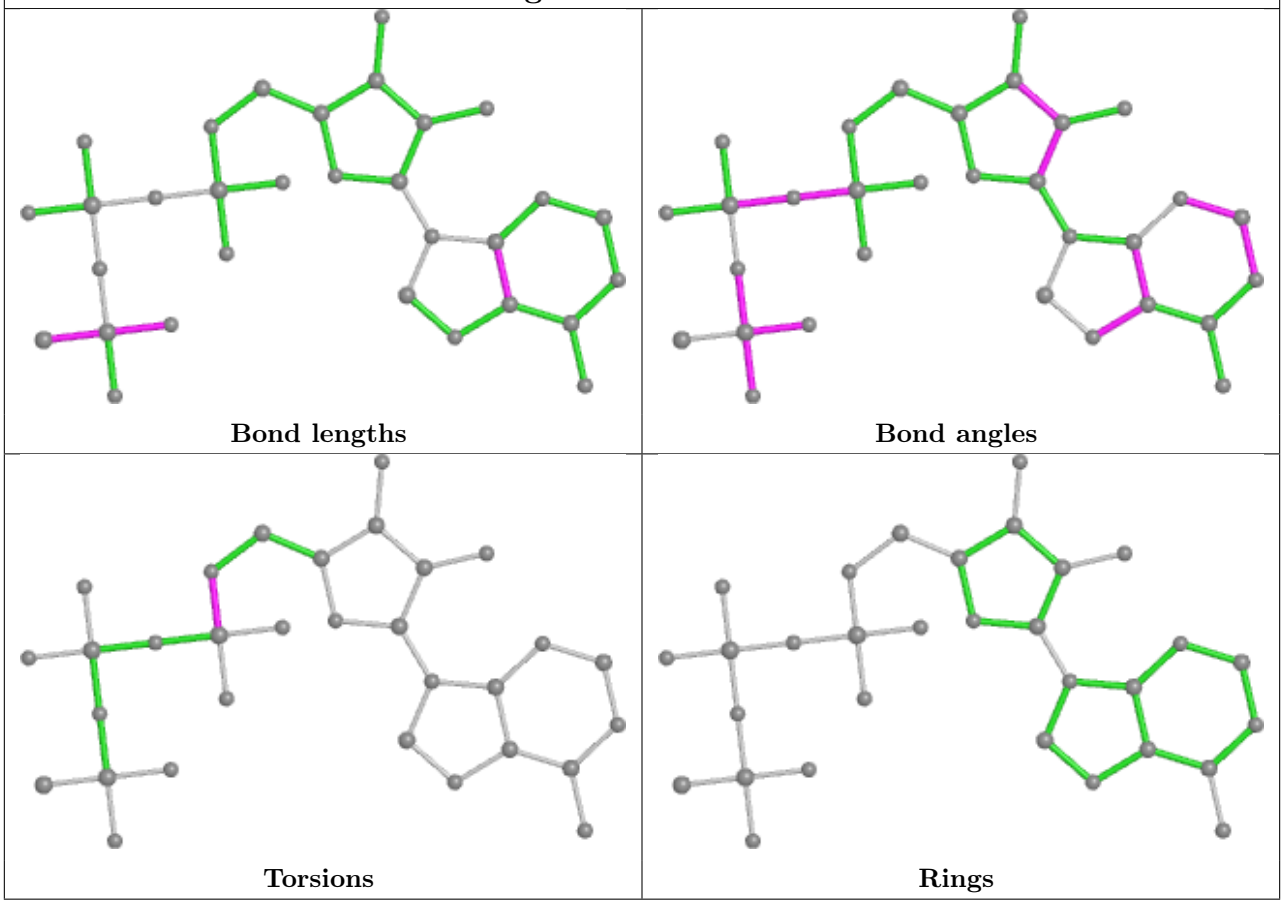
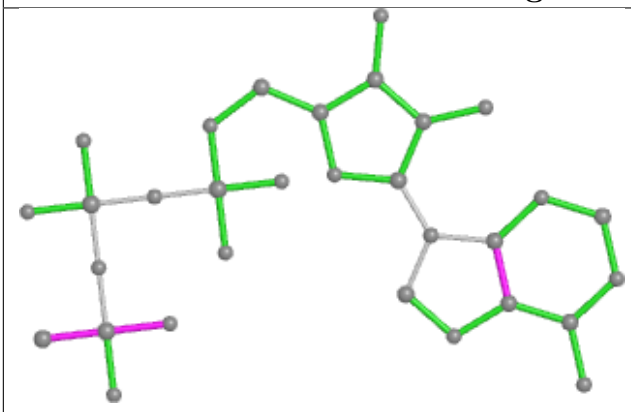
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	800	AGS	5	0
2	C	800	AGS	4	0
2	D	800	AGS	4	0
2	B	800	AGS	5	0
2	F	800	AGS	6	0

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

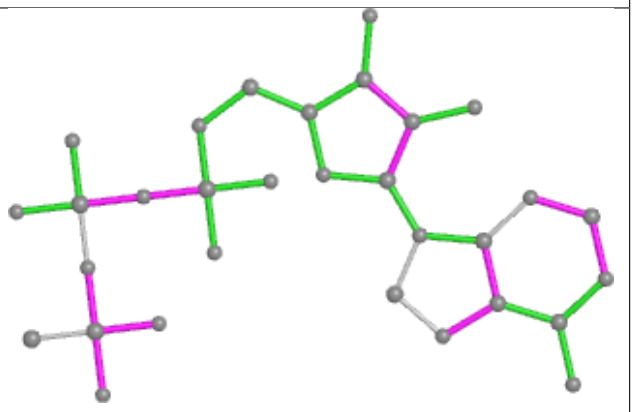
Ligand AGS A 800



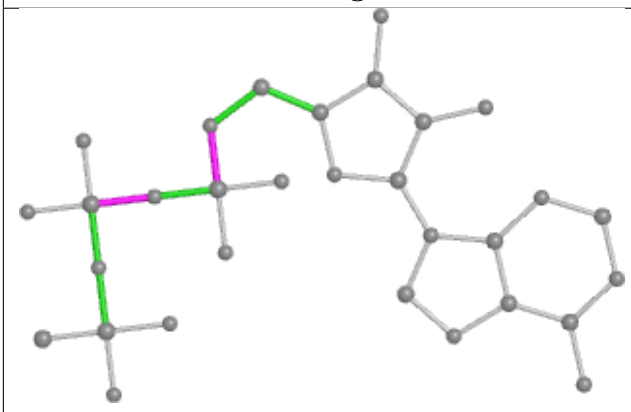
Ligand AGS E 800



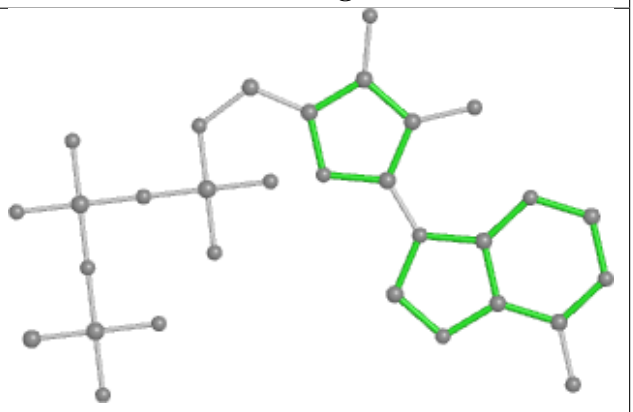
Bond lengths



Bond angles

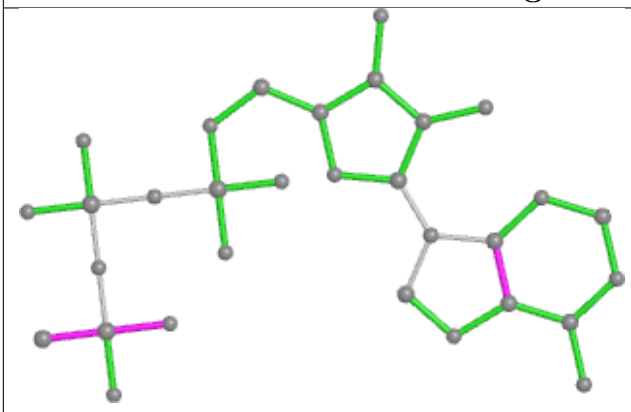


Torsions

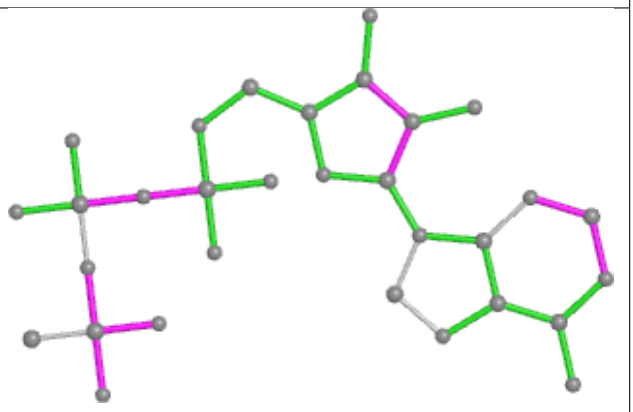


Rings

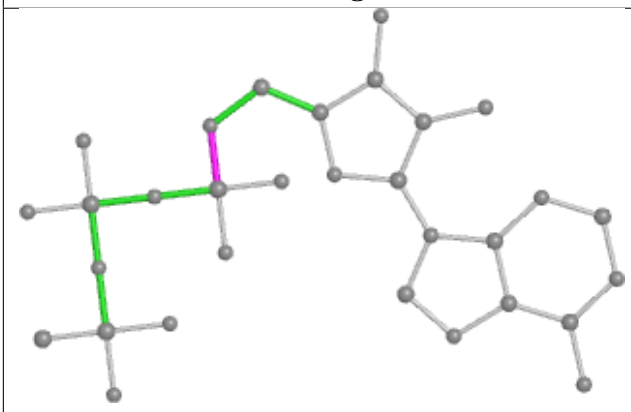
Ligand AGS C 800



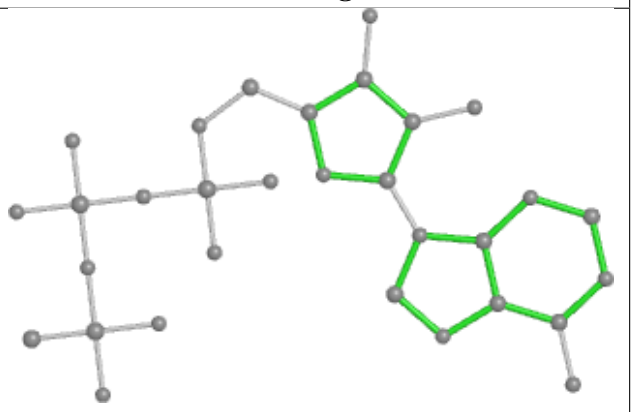
Bond lengths



Bond angles

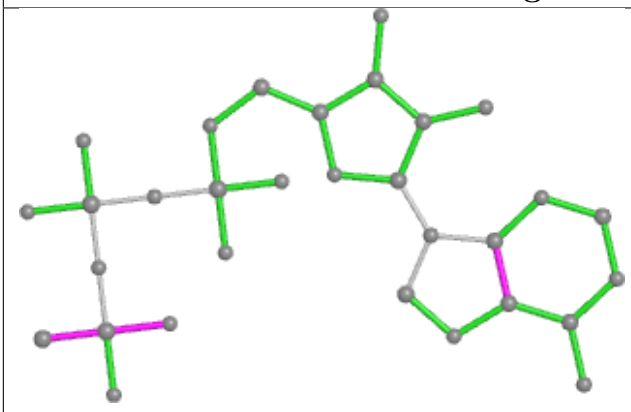


Torsions

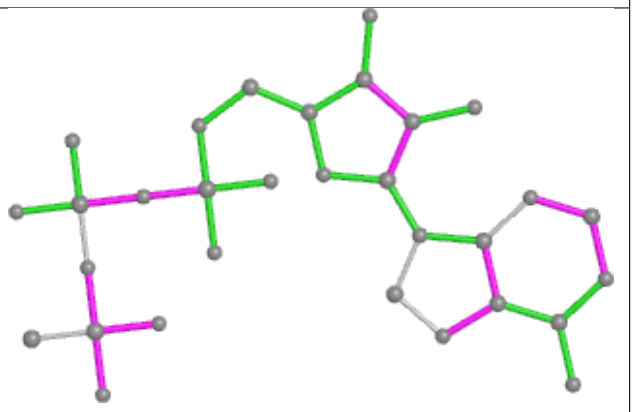


Rings

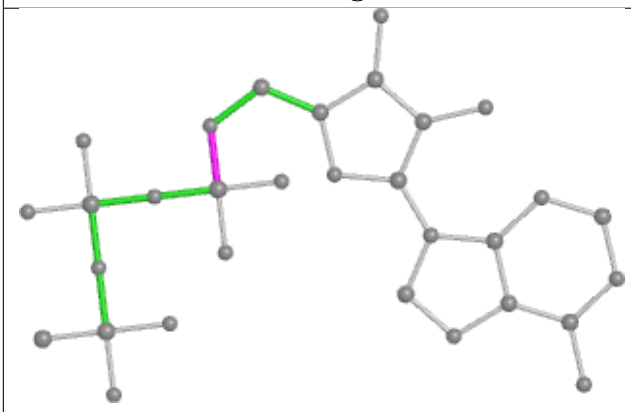
Ligand AGS D 800



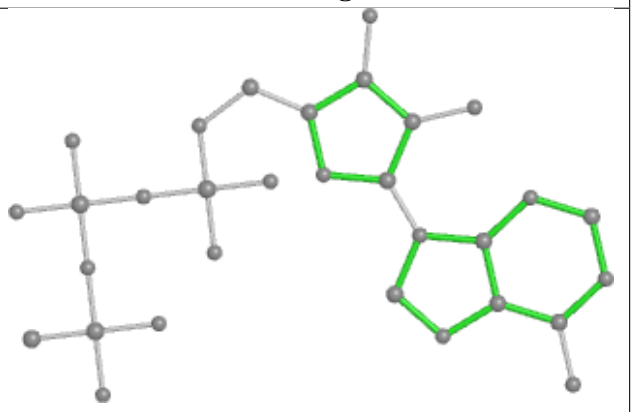
Bond lengths



Bond angles

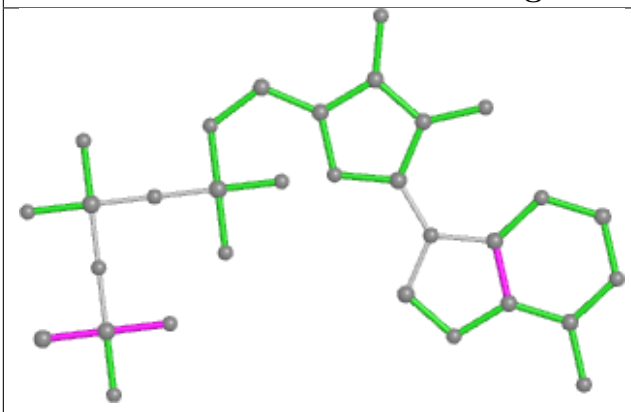


Torsions

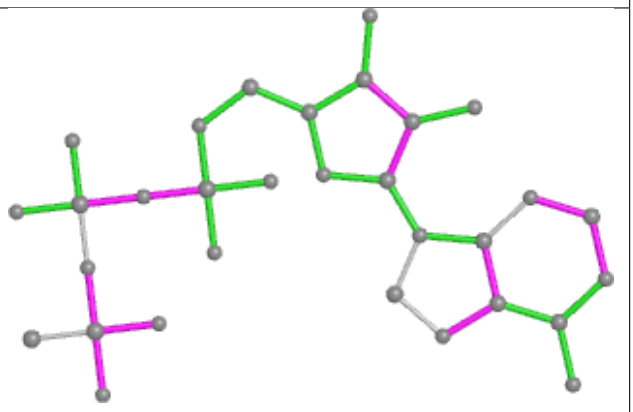


Rings

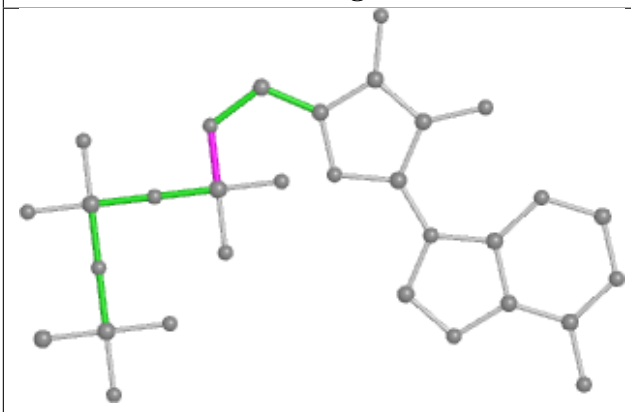
Ligand AGS B 800



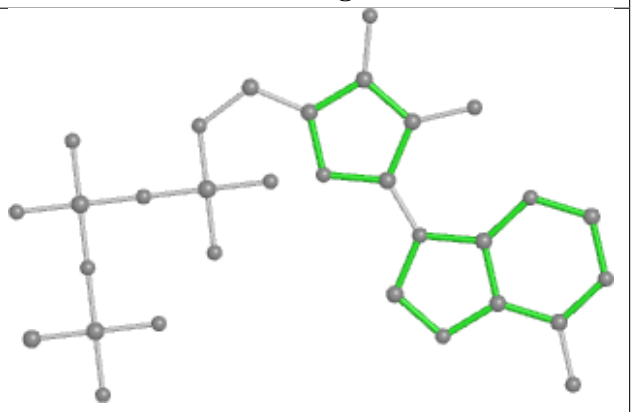
Bond lengths



Bond angles

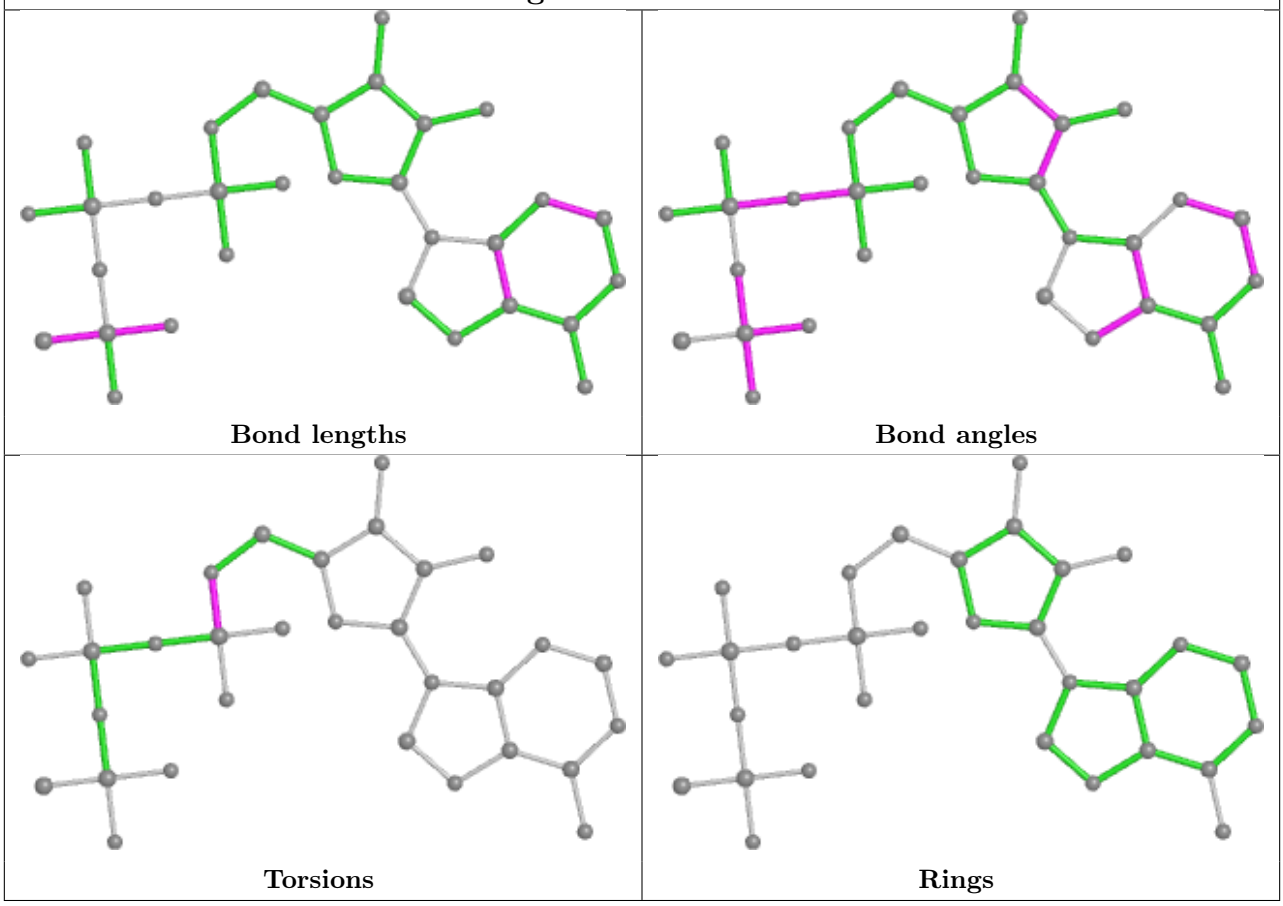


Torsions



Rings

Ligand AGS F 800



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	451/489 (92%)	0.32	17 (3%) 40 34	47, 81, 123, 137	0
1	B	451/489 (92%)	0.32	11 (2%) 59 53	47, 77, 110, 129	0
1	C	451/489 (92%)	0.43	33 (7%) 15 11	43, 89, 130, 150	0
1	D	451/489 (92%)	0.52	38 (8%) 11 7	45, 95, 144, 163	0
1	E	451/489 (92%)	0.83	56 (12%) 4 2	52, 93, 156, 173	0
1	F	451/489 (92%)	0.48	30 (6%) 17 13	37, 89, 132, 152	0
All	All	2706/2934 (92%)	0.48	185 (6%) 17 13	37, 86, 136, 173	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	41	LEU	7.8
1	E	173	TYR	7.2
1	E	437	ILE	6.7
1	E	69	CYS	6.7
1	E	72	LEU	6.5
1	E	51	LEU	6.5
1	D	41	LEU	5.9
1	B	314	GLU	5.5
1	F	72	LEU	5.3
1	E	32	ILE	5.0
1	E	114	ILE	4.9
1	E	52	PHE	4.8
1	A	72	LEU	4.8
1	E	143	TYR	4.8
1	E	429	LEU	4.7
1	D	462	SER	4.7
1	A	158	MET	4.6
1	F	158	MET	4.5
1	D	128	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	182	ILE	4.5
1	E	71	VAL	4.5
1	E	128	GLY	4.5
1	E	442	MET	4.5
1	D	135	LEU	4.4
1	B	158	MET	4.3
1	D	20	LYS	4.2
1	A	437	ILE	4.2
1	E	439	ALA	4.2
1	F	182	ILE	4.2
1	E	75	ASP	3.9
1	F	139	PHE	3.9
1	C	72	LEU	3.9
1	F	32	ILE	3.9
1	F	114	ILE	3.9
1	C	161	VAL	3.8
1	E	198	LEU	3.8
1	E	104	PRO	3.8
1	E	141	GLU	3.8
1	D	113	ARG	3.7
1	E	146	ILE	3.7
1	E	57	VAL	3.6
1	C	182	ILE	3.6
1	E	38	VAL	3.6
1	E	183	HIS	3.6
1	E	113	ARG	3.6
1	F	68	VAL	3.5
1	E	77	CYS	3.5
1	D	72	LEU	3.5
1	A	155	ARG	3.5
1	A	128	GLY	3.5
1	D	26	LEU	3.5
1	D	153	LEU	3.4
1	C	130	LEU	3.4
1	D	58	LEU	3.4
1	F	338	ARG	3.4
1	F	38	VAL	3.4
1	E	70	ILE	3.3
1	C	133	VAL	3.3
1	A	51	LEU	3.3
1	B	157	GLY	3.3
1	B	462	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	39	VAL	3.3
1	C	338	ARG	3.3
1	E	432	LEU	3.2
1	E	139	PHE	3.2
1	F	152	PHE	3.2
1	D	112	LYS	3.2
1	C	317	HIS	3.2
1	F	113	ARG	3.2
1	F	111	GLY	3.2
1	F	173	TYR	3.1
1	C	51	LEU	3.1
1	C	26	LEU	3.1
1	D	437	ILE	3.1
1	D	182	ILE	3.1
1	F	175	ILE	3.1
1	E	84	MET	3.1
1	A	445	LEU	3.0
1	E	105	CYS	3.0
1	D	163	PHE	3.0
1	F	71	VAL	3.0
1	C	135	LEU	3.0
1	E	158	MET	3.0
1	F	70	ILE	3.0
1	E	229	LEU	2.9
1	F	227	PRO	2.9
1	C	141	GLU	2.9
1	B	441	VAL	2.9
1	B	283	GLU	2.9
1	F	337	GLN	2.8
1	C	163	PHE	2.8
1	B	51	LEU	2.8
1	C	71	VAL	2.8
1	D	173	TYR	2.8
1	E	156	GLY	2.8
1	C	452	PHE	2.8
1	D	92	LEU	2.8
1	C	17	LEU	2.8
1	E	181	VAL	2.8
1	E	58	LEU	2.7
1	E	59	LEU	2.7
1	F	184	CYS	2.7
1	F	51	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	THR	2.7
1	D	127	THR	2.7
1	E	153	LEU	2.7
1	E	314	GLU	2.7
1	E	462	SER	2.7
1	D	17	LEU	2.7
1	C	110	TYR	2.6
1	D	445	LEU	2.6
1	E	317	HIS	2.6
1	A	135	LEU	2.6
1	D	51	LEU	2.6
1	E	102	ILE	2.6
1	C	56	THR	2.5
1	D	152	PHE	2.5
1	F	427	MET	2.5
1	D	146	ILE	2.5
1	C	445	LEU	2.5
1	E	67	ALA	2.5
1	F	136	LYS	2.5
1	D	52	PHE	2.5
1	B	155	ARG	2.5
1	C	461	PRO	2.5
1	B	437	ILE	2.5
1	E	174	CYS	2.5
1	C	179	ASP	2.5
1	C	92	LEU	2.4
1	E	68	VAL	2.4
1	F	360	PHE	2.4
1	A	41	LEU	2.4
1	C	49	LEU	2.4
1	F	57	VAL	2.4
1	C	113	ARG	2.4
1	C	70	ILE	2.4
1	E	176	VAL	2.4
1	E	92	LEU	2.3
1	D	452	PHE	2.3
1	C	198	LEU	2.3
1	C	175	ILE	2.3
1	C	201	VAL	2.3
1	D	38	VAL	2.3
1	E	108	VAL	2.3
1	D	183	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	172	PRO	2.3
1	A	241	ILE	2.3
1	C	41	LEU	2.3
1	F	102	ILE	2.3
1	A	19	GLN	2.3
1	C	337	GLN	2.3
1	D	110	TYR	2.3
1	D	141	GLU	2.3
1	F	135	LEU	2.3
1	E	175	ILE	2.3
1	A	130	LEU	2.2
1	B	156	GLY	2.2
1	C	229	LEU	2.2
1	F	224	LEU	2.2
1	D	71	VAL	2.2
1	C	181	VAL	2.2
1	D	187	GLU	2.2
1	D	233	ILE	2.2
1	D	139	PHE	2.2
1	E	53	ARG	2.1
1	E	140	LEU	2.1
1	D	328	LEU	2.1
1	A	26	LEU	2.1
1	A	183	HIS	2.1
1	E	430	ILE	2.1
1	E	445	LEU	2.1
1	F	146	ILE	2.1
1	A	184	CYS	2.1
1	D	158	MET	2.1
1	F	123	VAL	2.1
1	D	140	LEU	2.0
1	D	241	ILE	2.0
1	E	452	PHE	2.0
1	C	140	LEU	2.0
1	A	32	ILE	2.0
1	B	337	GLN	2.0
1	D	23	PRO	2.0
1	C	388	MET	2.0
1	F	153	LEU	2.0
1	D	161	VAL	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)

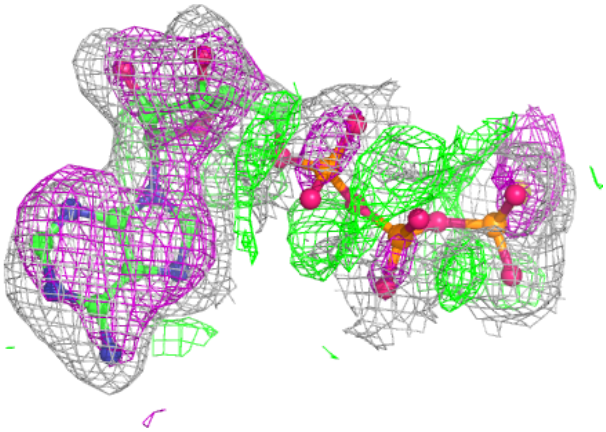
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

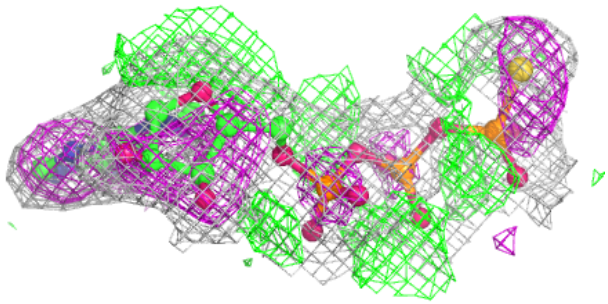
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AGS	A	800	31/31	0.95	0.18	24,27,29,29	0
3	MG	F	801	1/1	0.95	0.21	4,4,4,4	0
2	AGS	E	800	31/31	0.96	0.19	39,40,42,43	0
2	AGS	F	800	31/31	0.96	0.19	12,12,13,14	0
3	MG	C	801	1/1	0.96	0.18	13,13,13,13	0
3	MG	D	801	1/1	0.96	0.21	24,24,24,24	0
2	AGS	B	800	31/31	0.96	0.17	28,29,30,30	0
2	AGS	D	800	31/31	0.97	0.17	34,43,45,46	0
2	AGS	C	800	31/31	0.97	0.17	25,31,36,37	0
3	MG	E	801	1/1	0.98	0.19	19,19,19,19	0
3	MG	A	801	1/1	0.98	0.17	12,12,12,12	0
3	MG	B	801	1/1	0.99	0.19	14,14,14,14	0

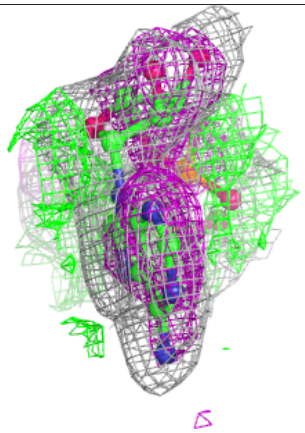
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS A 800:

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

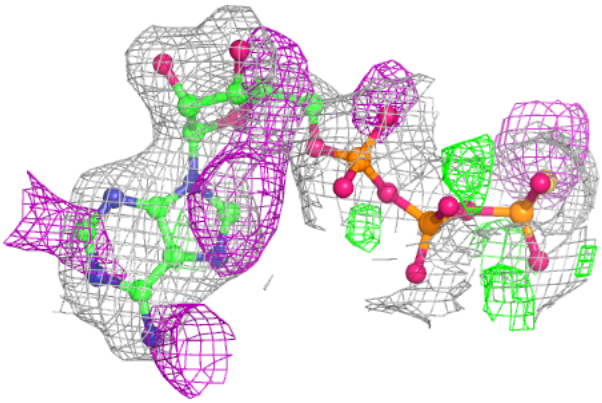


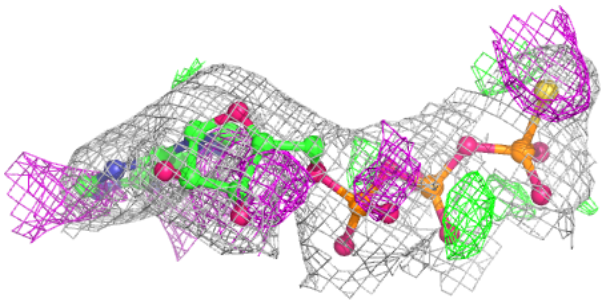


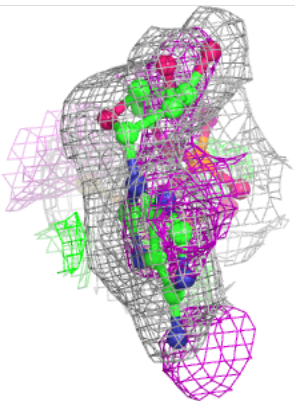


Electron density around AGS E 800:

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

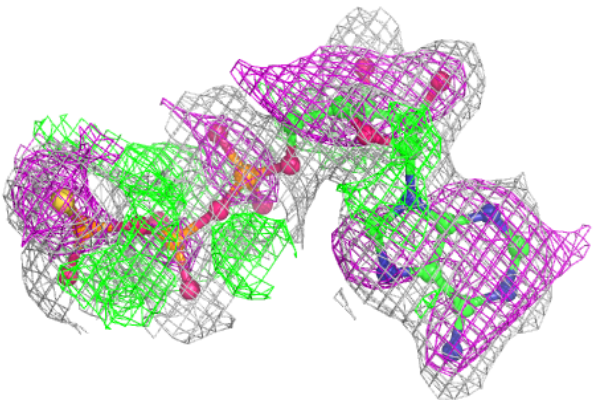


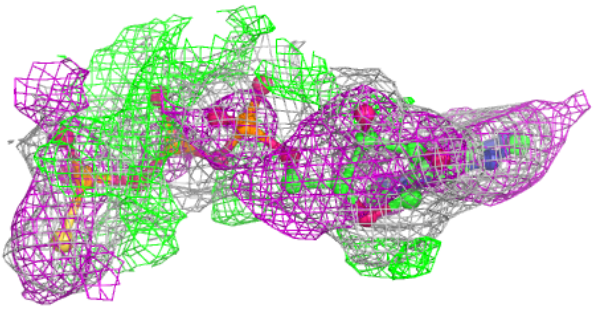


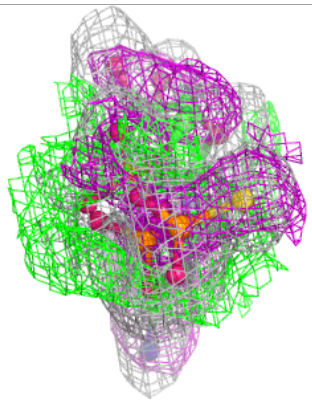


Electron density around AGS F 800:

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

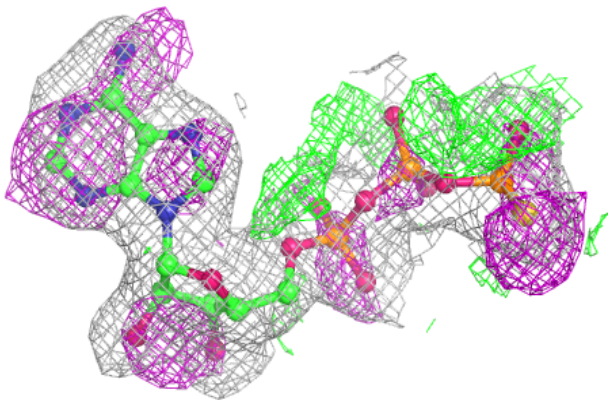


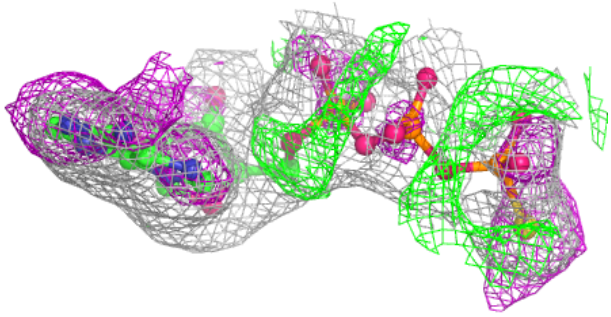


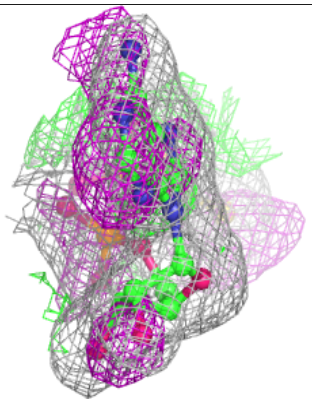


Electron density around AGS B 800:

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

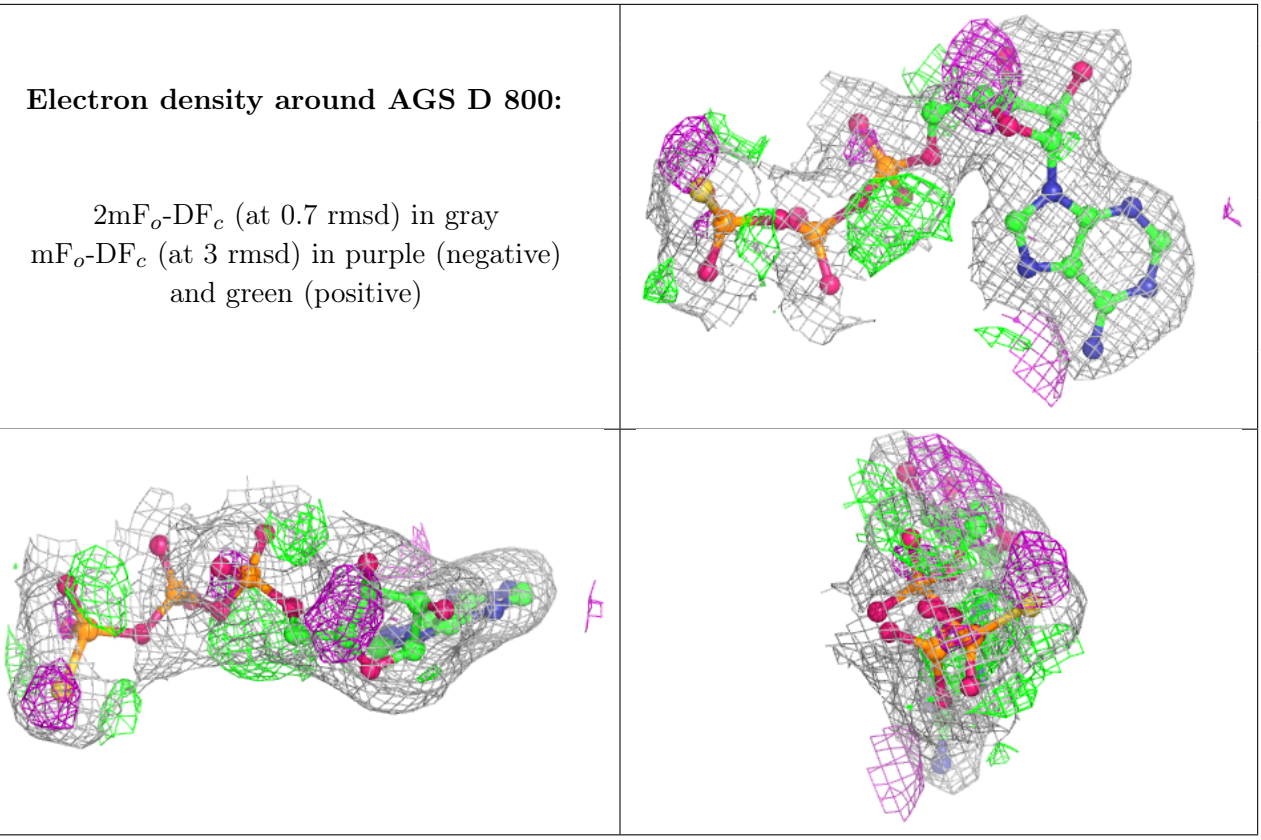






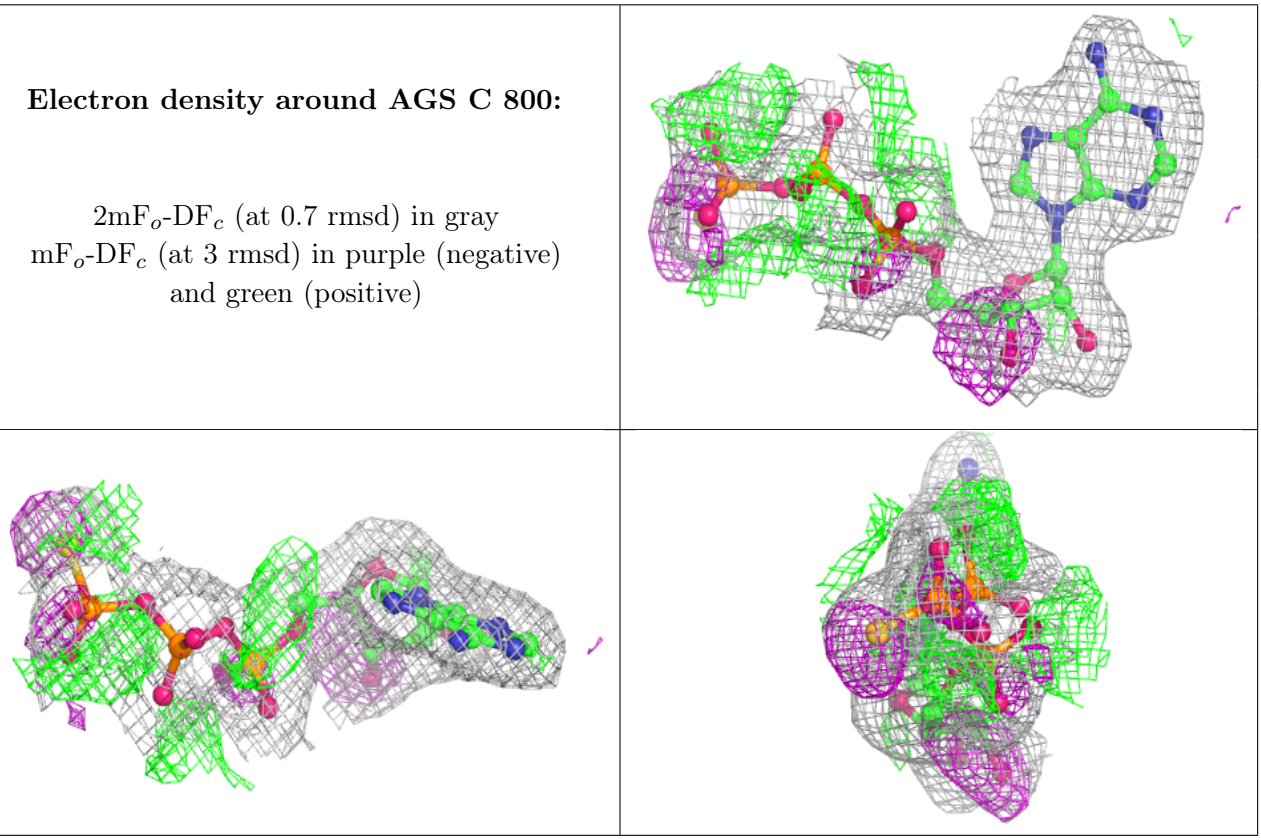
Electron density around AGS D 800:

$2mF_o$-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 C 800:

$2mF_o$-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.