Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:34 AM BST

PDB ID	:	5NZZ
Title	:	Crystal structure of phosphorylated p38aMAPK in complex with TAB1
Authors	:	Nichols, C.E.; De Nicola, G.F.
Deposited on	:	2017-05-15
Resolution	:	2.60 Å(reported)

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

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

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

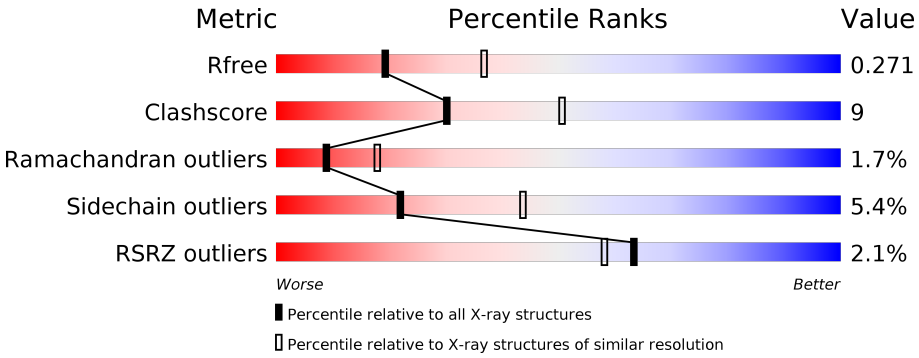
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	504	62% 12% • 25%
1	B	504	% 59% 14% • 25%
1	C	504	2% 58% 14% • 27%
1	D	504	63% 12% • 25%
2	E	360	73% 22% • •
2	F	360	76% 19% • 5%

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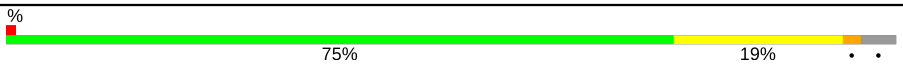
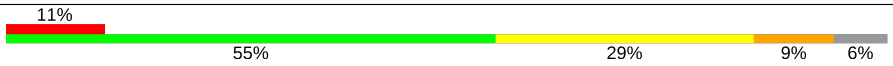
Mol	Chain	Length	Quality of chain
2	G	360	
2	H	360	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22057 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 TGF-beta-activated kinase 1 and MAP3K7-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2850	1790	492	558	10			
1	B	378	Total	C	N	O	S	0	0	0
			2856	1797	494	555	10			
1	C	367	Total	C	N	O	S	0	0	0
			2752	1730	477	535	10			
1	D	379	Total	C	N	O	S	0	0	0
			2843	1784	493	556	10			

- Molecule 2 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	345	Total	C	N	O	P	S	0	1	0
			2743	1754	462	512	2	13			
2	F	343	Total	C	N	O	P	S	0	1	0
			2740	1756	463	506	2	13			
2	G	344	Total	C	N	O	P	S	0	2	0
			2723	1741	459	508	2	13			
2	H	337	Total	C	N	O	P	S	0	0	0
			2372	1501	411	448	2	10			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		

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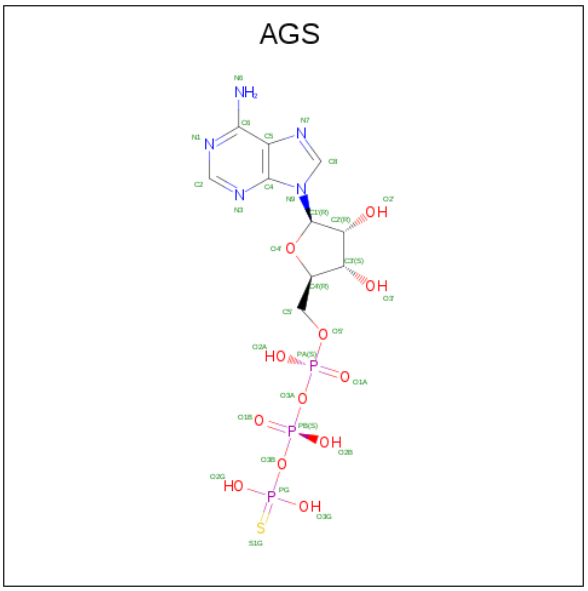
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	F	1	Total Ni 1 1	0	0

- 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	E	1	Total C N O P S 31 10 5 12 3 1	0	0
4	F	1	Total C N O P S 31 10 5 12 3 1	0	0
4	G	1	Total C N O P S 31 10 5 12 3 1	0	0
4	H	1	Total C N O P S 31 10 5 12 3 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total Mg 2 2	0	0
5	G	2	Total Mg 2 2	0	0
5	F	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Mg 1 1	0	0

- Molecule 6 is water.

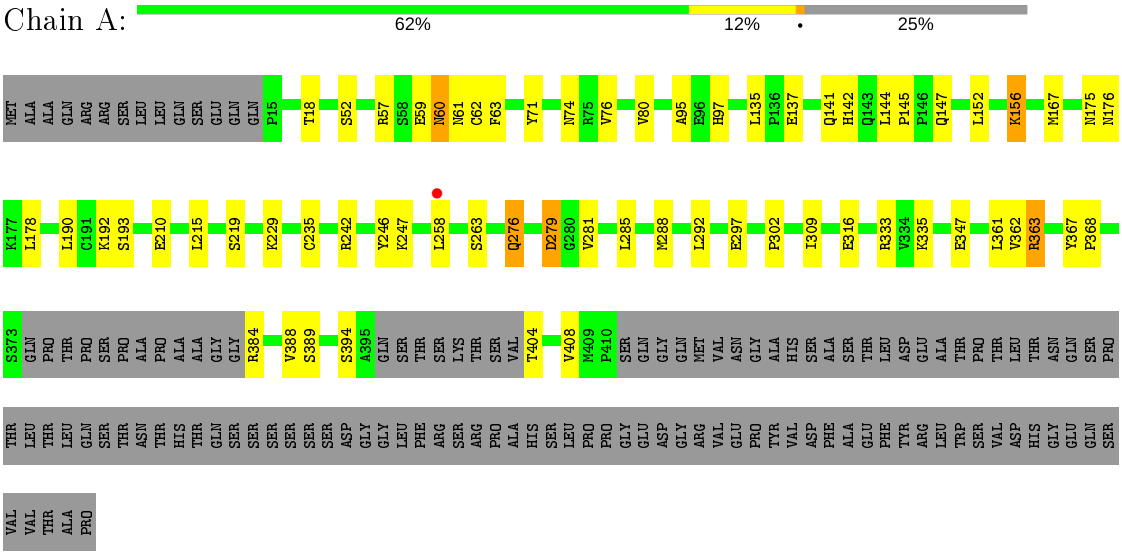
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	B	5	Total O 5 5	0	0
6	C	3	Total O 3 3	0	0
6	D	3	Total O 3 3	0	0
6	E	9	Total O 9 9	0	0
6	F	10	Total O 10 10	0	0
6	G	3	Total O 3 3	0	0

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.

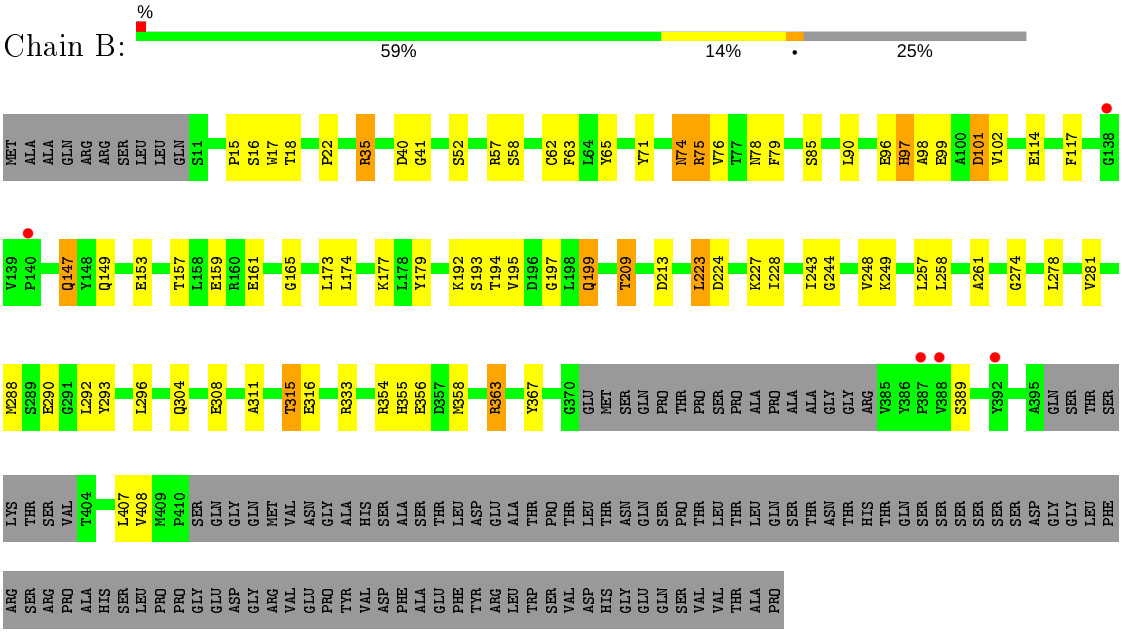
- Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain A:



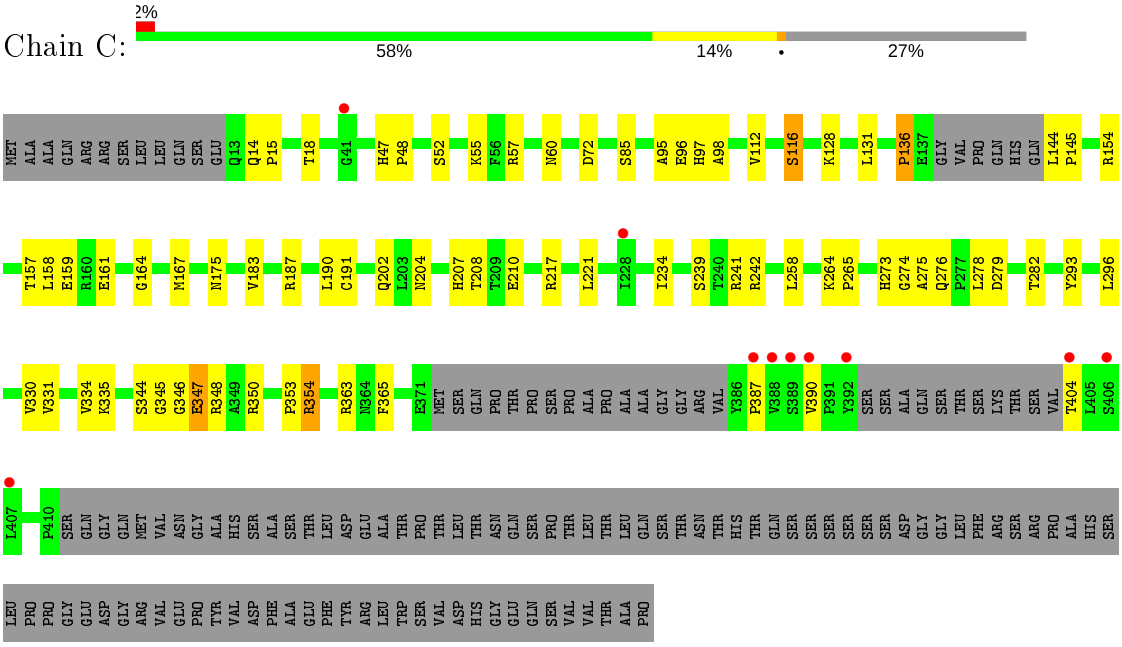
- Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain B:



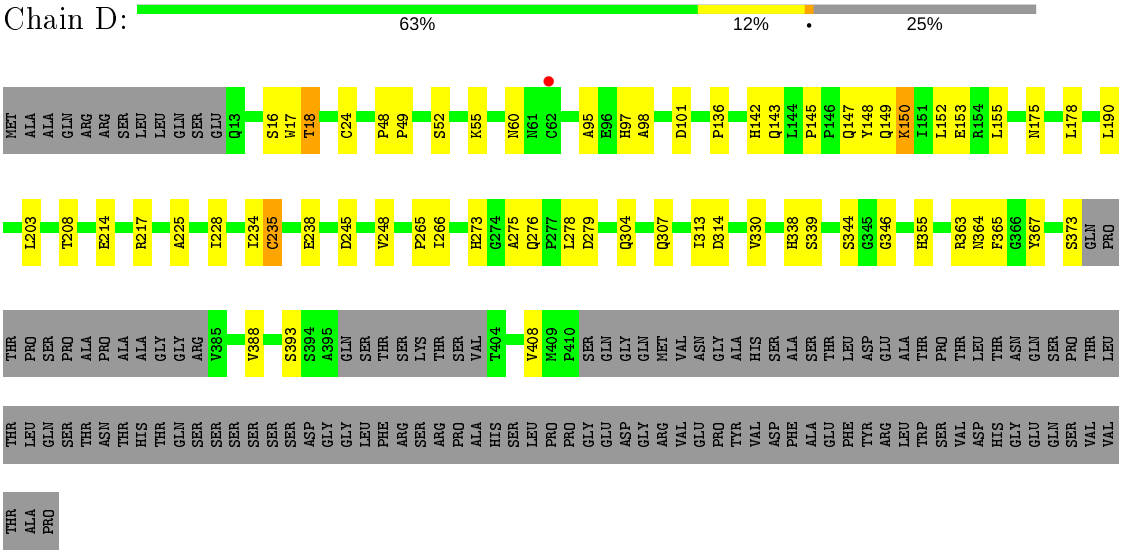
• Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain C:



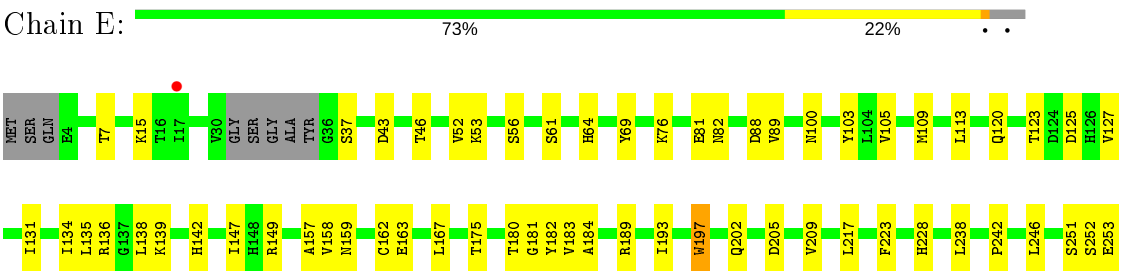
• Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

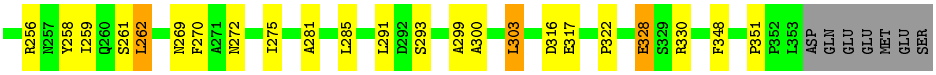
Chain D:



• Molecule 2: Mitogen-activated protein kinase 14

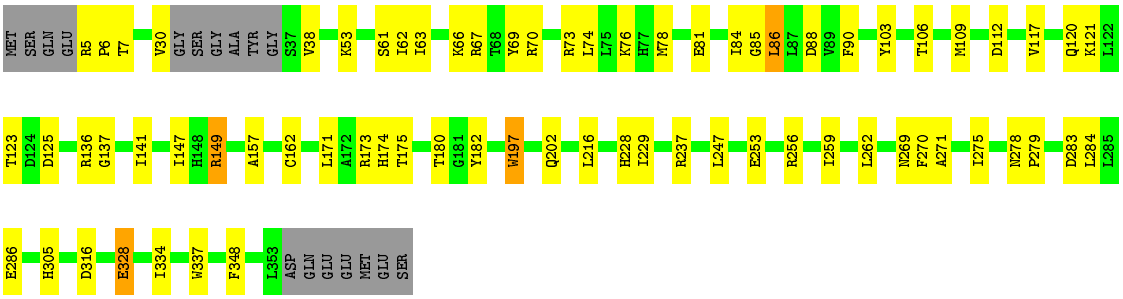
Chain E:





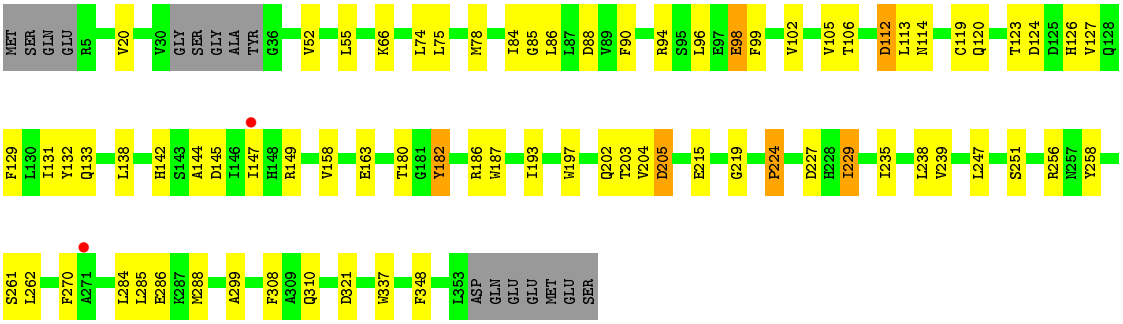
• Molecule 2: Mitogen-activated protein kinase 14

Chain F:



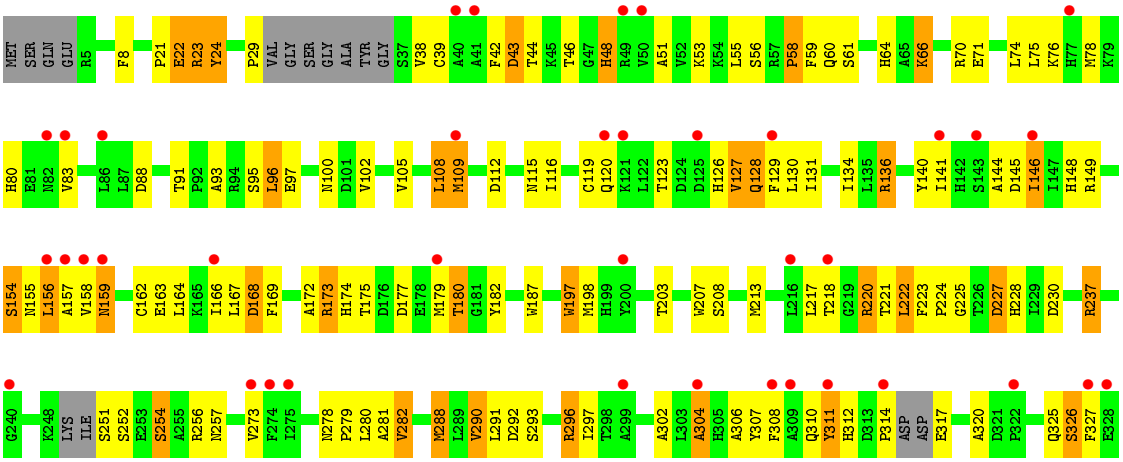
• Molecule 2: Mitogen-activated protein kinase 14

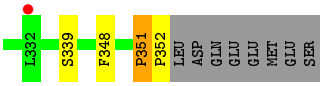
Chain G:



• Molecule 2: Mitogen-activated protein kinase 14

Chain H:




L332
S339
F348
P351
P352
LEU
ASP
GLN
GLU
GLU
MET
GLU
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.88Å 107.63Å 144.20Å 89.26° 76.75° 84.28°	Depositor
Resolution (Å)	140.36 – 2.60 140.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.8 (140.36-2.60) 90.9 (140.36-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.219 , 0.271 0.219 , 0.271	Depositor DCC
R_{free} test set	5465 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22057	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: TPO, NI, MG, AGS, PTR

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	0.51	0/2900	0.70	1/3938 (0.0%)
1	B	0.47	0/2906	0.69	0/3943
1	C	0.47	0/2799	0.67	0/3803
1	D	0.50	0/2894	0.65	0/3933
2	E	0.47	1/2778 (0.0%)	0.66	0/3783
2	F	0.50	0/2775	0.73	2/3774 (0.1%)
2	G	0.44	0/2757	0.66	2/3757 (0.1%)
2	H	0.43	0/2398	0.69	1/3292 (0.0%)
All	All	0.48	1/22207 (0.0%)	0.68	6/30223 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	223	PHE	C-N	6.63	1.46	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	173	ARG	NE-CZ-NH2	-8.54	116.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	205	ASP	CB-CG-OD1	6.00	123.69	118.30
2	F	149	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	F	67	ARG	NE-CZ-NH2	-5.39	117.61	120.30
2	G	229	ILE	CG1-CB-CG2	-5.30	99.75	111.40
1	A	135	LEU	CA-CB-CG	5.26	127.41	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	GLU	Peptide
1	C	273	HIS	Peptide
1	C	274	GLY	Peptide
1	D	273	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2850	0	2747	30	1
1	B	2856	0	2788	52	0
1	C	2752	0	2643	46	0
1	D	2843	0	2730	30	0
2	E	2743	0	2634	50	0
2	F	2740	0	2661	50	0
2	G	2723	0	2604	46	0
2	H	2372	0	1963	113	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	E	31	0	12	1	0
4	F	31	0	12	1	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	9	0	0	0	0
6	B	5	0	0	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
6	E	9	0	0	0	0
6	F	10	0	0	1	0
6	G	3	0	0	0	0
All	All	22057	0	20818	397	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:290:VAL:HG22	2:H:291:LEU:H	1.35	0.91
1:C:128:LYS:NZ	1:C:159:GLU:OE2	2.05	0.89
2:H:136:ARG:NH1	2:H:317:GLU:HA	1.89	0.88
2:H:220:ARG:HD2	2:H:221:THR:H	1.41	0.86
1:C:344:SER:O	1:C:346:GLY:N	2.14	0.81
1:A:288:MET:HE1	1:A:309:ILE:HD13	1.62	0.81
2:E:253:GLU:OE1	2:E:256:ARG:NH2	2.13	0.81
2:H:22:GLU:O	2:H:24:TYR:N	2.14	0.81
1:D:217:ARG:NH2	1:D:265:PRO:O	2.15	0.80
2:H:155:ASN:ND2	2:H:168:ASP:OD1	2.15	0.79
2:H:46:THR:HG23	2:H:48:HIS:H	1.46	0.78
2:E:136:ARG:NH1	2:E:316:ASP:O	2.17	0.77
2:G:94:ARG:N	2:G:98:GLU:OE2	2.17	0.77
1:D:95:ALA:O	1:D:175:ASN:ND2	2.18	0.77
1:B:75:ARG:NH1	1:B:161:GLU:O	2.18	0.77
2:H:38:VAL:HG12	2:H:53:LYS:HA	1.68	0.76
1:B:224:ASP:OD2	1:B:227:LYS:N	2.12	0.75
1:B:354:ARG:NH2	1:B:356:GLU:OE2	2.20	0.74
2:H:127:VAL:HG11	2:H:217:LEU:HD21	1.69	0.74
1:C:353:PRO:HB2	1:C:354:ARG:HH11	1.54	0.73
1:B:223:LEU:HD11	1:B:261:ALA:HB2	1.70	0.70
2:G:123:THR:HG22	2:G:126:HIS:ND1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:GLU:OE2	2:F:136[A]:ARG:NH2	2.24	0.69
2:G:138:LEU:HD21	2:G:142:HIS:CE1	2.27	0.69
1:B:407:LEU:HD12	2:G:120:GLN:HE22	1.56	0.69
1:D:203:LEU:HD11	1:D:276:GLN:HG3	1.74	0.69
2:E:123:THR:HG22	2:E:125:ASP:H	1.58	0.69
2:F:136[B]:ARG:NH2	2:F:316:ASP:O	2.25	0.69
1:C:347:GLU:OE1	1:C:350:ARG:NH2	2.26	0.69
2:G:52:VAL:HG22	2:G:105:VAL:HG22	1.75	0.68
2:E:109:MET:O	2:E:159:ASN:ND2	2.27	0.68
2:G:193:ILE:HD11	2:G:204:VAL:HG11	1.76	0.67
2:H:74:LEU:HD22	2:H:146:ILE:HD13	1.76	0.67
2:H:304:ALA:HA	2:H:312:HIS:CE1	2.30	0.67
2:H:140:TYR:CE2	2:H:320:ALA:HB2	2.30	0.67
1:C:353:PRO:HB2	1:C:354:ARG:NH1	2.09	0.66
2:H:156:LEU:HD21	2:H:166:ILE:HD13	1.76	0.66
2:H:207:TRP:HD1	2:H:296:ARG:HH22	1.43	0.66
1:B:354:ARG:HG2	1:B:354:ARG:HH11	1.61	0.66
2:H:292:ASP:O	2:H:296:ARG:HD2	1.96	0.66
1:C:347:GLU:C	1:C:350:ARG:HH21	1.99	0.65
1:D:408:VAL:O	2:E:120:GLN:NE2	2.29	0.65
2:F:247:LEU:HG	2:F:256:ARG:HG3	1.78	0.65
1:C:14:GLN:HG2	1:C:15:PRO:HD2	1.78	0.64
2:H:112:ASP:H	2:H:115:ASN:HD21	1.46	0.64
1:C:14:GLN:HG3	2:F:197:TRP:CD2	2.33	0.64
2:H:278:ASN:OD1	2:H:280:LEU:HB2	1.98	0.64
1:B:223:LEU:HD21	1:B:258:LEU:HA	1.79	0.64
2:H:155:ASN:HD22	2:H:168:ASP:CB	2.11	0.64
1:B:99:GLU:HG3	1:B:179:TYR:HE2	1.62	0.63
2:H:278:ASN:O	2:H:281:ALA:N	2.25	0.63
1:D:208:THR:HG22	1:D:238:GLU:HG3	1.81	0.62
2:G:74:LEU:O	2:G:78:MET:HG2	1.98	0.62
1:B:96:GLU:N	1:B:96:GLU:OE1	2.32	0.62
2:F:283:ASP:OD2	2:F:305:HIS:NE2	2.22	0.62
2:F:76:LYS:HE3	2:F:348:PHE:HD1	1.63	0.62
2:H:220:ARG:HD2	2:H:221:THR:N	2.13	0.62
2:H:307:TYR:HD1	2:H:308:PHE:CE1	2.16	0.62
2:H:71:GLU:O	2:H:75:LEU:HD13	2.00	0.61
2:H:123:THR:HG23	2:H:126:HIS:H	1.64	0.61
2:H:290:VAL:HG22	2:H:291:LEU:N	2.12	0.61
1:D:314:ASP:OD1	1:D:367:TYR:OH	2.15	0.61
2:H:66:LYS:O	2:H:70:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:VAL:HG23	2:F:38:VAL:HG23	1.81	0.61
2:H:80:HIS:HB3	2:H:83:VAL:HG22	1.82	0.61
2:H:109:MET:HG2	2:H:157:ALA:HB1	1.81	0.61
1:B:194:THR:HG23	1:B:197:GLY:H	1.66	0.60
2:H:8:PHE:HA	2:H:21:PRO:HA	1.82	0.60
2:H:173:ARG:HH21	2:H:179:MET:HG2	1.66	0.60
2:H:128:GLN:HA	2:H:307:TYR:CE1	2.36	0.60
2:E:281:ALA:O	2:E:285:LEU:HD12	2.02	0.60
2:H:141:ILE:HG23	2:H:146:ILE:HG23	1.83	0.60
1:A:145:PRO:HB2	1:A:147:GLN:OE1	2.02	0.59
2:H:308:PHE:O	2:H:312:HIS:N	2.33	0.59
2:F:38:VAL:HG21	4:F:401:AGS:O4'	2.01	0.59
2:H:123:THR:O	2:H:127:VAL:HG23	2.02	0.59
2:G:229:ILE:HD11	2:G:258:TYR:OH	2.02	0.59
1:C:331:VAL:O	1:C:335:LYS:HG3	2.03	0.59
2:G:227:ASP:OD1	2:G:229:ILE:HG22	2.03	0.59
2:G:147:ILE:HD12	2:G:149:ARG:HD3	1.83	0.58
1:B:304:GLN:O	1:B:308:GLU:HG3	2.02	0.58
2:E:157:ALA:HB2	2:E:167:LEU:HD11	1.84	0.58
2:H:156:LEU:HD13	2:H:164:LEU:HD11	1.84	0.58
2:H:75:LEU:HD11	2:H:169:PHE:HB2	1.86	0.58
1:C:208:THR:HG23	1:C:210:GLU:H	1.67	0.58
2:H:220:ARG:HG3	2:H:220:ARG:HH11	1.69	0.58
2:E:109:MET:HG2	2:E:157:ALA:HB1	1.86	0.58
2:F:253:GLU:OE2	2:F:256:ARG:NH1	2.37	0.58
2:H:136:ARG:HH12	2:H:317:GLU:HA	1.65	0.58
1:C:264:LYS:HE2	2:E:322:PRO:HD3	1.85	0.58
1:B:407:LEU:HD12	2:G:120:GLN:NE2	2.18	0.57
2:H:61:SER:OG	2:H:64:HIS:ND1	2.33	0.57
1:B:58:SER:OG	1:B:62:CYS:HB3	2.04	0.57
1:A:95:ALA:HB1	1:A:175:ASN:ND2	2.19	0.57
2:H:187:TRP:CD1	2:H:224:PRO:HA	2.40	0.57
2:H:74:LEU:HD13	2:H:146:ILE:HD11	1.86	0.57
2:E:258:TYR:O	2:E:261:SER:OG	2.19	0.56
1:B:74:ASN:OD1	1:B:78:ASN:ND2	2.37	0.56
2:H:293:SER:HA	2:H:296:ARG:HD3	1.88	0.56
2:E:69:TYR:HE2	2:E:328:GLU:HG2	1.69	0.56
1:C:390:VAL:HG21	2:H:123:THR:HA	1.89	0.55
2:H:51:ALA:HB2	2:H:108:LEU:HD12	1.89	0.55
2:H:310:GLN:HB3	2:H:311:TYR:CD2	2.41	0.55
2:G:247:LEU:O	2:G:251:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:325:GLN:O	2:H:327:PHE:N	2.40	0.55
2:H:43:ASP:HB3	2:H:46:THR:HG22	1.87	0.55
1:B:22:PRO:HD2	1:B:57:ARG:O	2.05	0.55
1:A:279:ASP:N	1:A:279:ASP:OD1	2.40	0.55
2:H:297:ILE:CG1	2:H:302:ALA:HB2	2.37	0.55
2:E:269:ASN:HB3	2:E:272:ASN:OD1	2.07	0.55
1:C:347:GLU:HB2	2:H:60:GLN:HA	1.88	0.54
1:D:304:GLN:OE1	1:D:307:GLN:NE2	2.40	0.54
2:H:91:THR:HG22	2:H:93:ALA:H	1.72	0.54
1:D:388:VAL:HG12	2:E:275:ILE:O	2.08	0.54
2:G:238:LEU:HD21	2:G:270:PHE:CZ	2.42	0.54
2:H:227:ASP:N	2:H:227:ASP:OD1	2.39	0.54
2:E:52:VAL:HG22	2:E:105:VAL:HG22	1.89	0.54
2:F:73:ARG:NH1	6:F:502:HOH:O	2.40	0.54
2:H:75:LEU:CD1	2:H:169:PHE:HB2	2.38	0.54
2:F:175:THR:HG21	2:F:202:GLN:HG2	1.89	0.53
2:G:258:TYR:CZ	2:G:262:LEU:HD21	2.43	0.53
2:H:131:ILE:H	2:H:131:ILE:HD12	1.73	0.53
2:H:146:ILE:HD11	2:H:172:ALA:HB1	1.91	0.53
2:E:81:GLU:OE1	2:E:136:ARG:NH2	2.42	0.53
2:F:147:ILE:HB	2:F:175:THR:HG22	1.91	0.53
1:C:72:ASP:HB2	1:C:164:GLY:HA2	1.90	0.53
2:H:97:GLU:N	2:H:97:GLU:OE2	2.42	0.53
2:E:147:ILE:HD12	2:E:202:GLN:HA	1.91	0.52
2:E:61:SER:OG	2:E:64:HIS:ND1	2.33	0.52
2:H:76:LYS:HE3	2:H:348:PHE:HD1	1.74	0.52
1:C:208:THR:HG23	1:C:210:GLU:N	2.25	0.52
2:H:136:ARG:HH11	2:H:136:ARG:CG	2.23	0.52
2:G:138:LEU:HD22	2:G:299:ALA:HB2	1.92	0.52
1:D:214:GLU:OE1	1:D:217:ARG:NH1	2.42	0.52
2:F:69:TYR:HE2	2:F:328:GLU:HG2	1.75	0.52
2:H:288:MET:HG3	2:H:297:ILE:HG21	1.90	0.52
2:H:290:VAL:CG2	2:H:291:LEU:H	2.17	0.51
1:C:167:MET:HE2	1:C:239:SER:HB2	1.91	0.51
1:C:347:GLU:CD	1:C:350:ARG:HH22	2.14	0.51
2:H:136:ARG:HG3	2:H:136:ARG:HH11	1.75	0.51
2:E:299:ALA:O	2:E:303:LEU:HD22	2.10	0.51
2:H:155:ASN:HD22	2:H:168:ASP:HB2	1.76	0.51
2:H:203:THR:HG21	2:H:296:ARG:HD3	1.92	0.51
1:A:71:TYR:OH	1:A:242:ARG:HD3	2.10	0.51
2:E:136:ARG:HD2	2:E:317:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:182:PTR:O2P	2:G:186:ARG:NH1	2.41	0.51
1:A:152:LEU:O	1:A:156:LYS:HD2	2.11	0.50
2:G:147:ILE:HG22	2:G:202:GLN:HA	1.93	0.50
1:B:292:LEU:HA	1:B:358:MET:HG2	1.93	0.50
2:G:88:ASP:HA	2:G:348:PHE:CE2	2.47	0.50
1:B:16:SER:O	1:B:17:TRP:HB2	2.11	0.50
2:F:117:VAL:CG2	2:F:216:LEU:HD23	2.42	0.50
1:A:210:GLU:OE2	1:A:229:LYS:NZ	2.43	0.49
1:C:347:GLU:O	1:C:350:ARG:NH2	2.44	0.49
2:G:258:TYR:O	2:G:261:SER:OG	2.22	0.49
1:C:258:LEU:HD22	1:C:265:PRO:HG3	1.94	0.49
1:C:14:GLN:HG2	1:C:15:PRO:CD	2.41	0.49
1:D:178:LEU:HB2	1:D:278:LEU:HD11	1.93	0.49
2:F:109:MET:HG2	2:F:157:ALA:HB1	1.94	0.49
2:G:112:ASP:OD1	2:G:114:ASN:N	2.42	0.49
2:G:129:PHE:O	2:G:133:GLN:HG3	2.11	0.49
1:C:217:ARG:O	1:C:221:LEU:HD13	2.12	0.49
2:E:181:GLY:HA3	2:E:197:TRP:CH2	2.46	0.49
2:G:187:TRP:CD1	2:G:224:PRO:HA	2.47	0.49
2:H:237:ARG:HD3	2:H:237:ARG:O	2.11	0.49
1:D:178:LEU:CB	1:D:278:LEU:HD11	2.43	0.49
2:H:187:TRP:NE1	2:H:224:PRO:HA	2.27	0.49
2:F:66:LYS:HE2	2:F:70:ARG:NH2	2.28	0.49
2:H:127:VAL:O	2:H:129:PHE:N	2.46	0.49
2:H:157:ALA:HB2	2:H:167:LEU:HD11	1.94	0.49
2:H:307:TYR:CD1	2:H:308:PHE:CE1	3.00	0.49
2:H:23:ARG:O	2:H:44:THR:N	2.46	0.49
1:B:76:VAL:HG22	1:B:117:PHE:CZ	2.47	0.48
2:E:259:ILE:O	2:E:262:LEU:HB2	2.13	0.48
1:A:156:LYS:N	1:A:156:LYS:HD2	2.27	0.48
1:C:207:HIS:CE1	1:C:241:ARG:HD2	2.48	0.48
2:H:127:VAL:HG21	2:H:217:LEU:CD2	2.43	0.48
2:H:95:SER:C	2:H:97:GLU:H	2.17	0.48
1:C:112:VAL:O	1:C:116:SER:OG	2.30	0.48
2:E:135:LEU:HD21	2:E:209:VAL:HG11	1.95	0.48
1:A:297:GLU:HG2	1:A:302:PRO:HA	1.95	0.48
1:B:316:GLU:OE2	1:B:333:ARG:NH1	2.47	0.48
2:G:55:LEU:HD12	2:G:102:VAL:HB	1.96	0.48
2:G:270:PHE:CD2	2:G:286:GLU:HG2	2.48	0.48
2:H:213:MET:O	2:H:217:LEU:HG	2.13	0.48
2:E:147:ILE:HG12	2:E:149:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:HE1	1:A:309:ILE:CD1	2.41	0.48
1:B:114:GLU:OE2	1:B:243:ILE:HA	2.13	0.48
2:E:175:THR:HG21	2:E:202:GLN:HG3	1.96	0.48
2:F:270:PHE:CD1	2:F:286:GLU:HG2	2.49	0.48
2:H:154:SER:OG	2:H:155:ASN:OD1	2.20	0.48
1:B:71:TYR:CZ	1:B:165:GLY:HA3	2.48	0.48
1:C:144:LEU:HG	1:C:145:PRO:HD2	1.96	0.48
1:D:225:ALA:HA	1:D:228:ILE:HG22	1.96	0.48
2:G:147:ILE:HD12	2:G:149:ARG:CD	2.43	0.48
2:H:115:ASN:OD1	2:H:116:ILE:N	2.47	0.48
2:H:91:THR:HG22	2:H:93:ALA:N	2.28	0.48
1:C:154:ARG:O	1:C:158:LEU:HD23	2.14	0.48
1:C:14:GLN:HG3	2:F:197:TRP:CE2	2.49	0.48
1:C:234:ILE:O	1:C:242:ARG:NH2	2.43	0.47
1:D:149:GLN:O	1:D:153:GLU:HG3	2.14	0.47
1:C:390:VAL:CG2	2:H:123:THR:HA	2.43	0.47
2:F:85:GLY:O	2:F:106:THR:HG22	2.14	0.47
1:B:192:LYS:HB3	1:B:199:GLN:HG3	1.96	0.47
2:H:131:ILE:HA	2:H:134:ILE:HD12	1.97	0.47
2:F:78:MET:HE1	2:F:141:ILE:HG23	1.97	0.47
2:G:285:LEU:HA	2:G:285:LEU:HD23	1.77	0.47
1:A:361:LEU:HD23	1:A:362:VAL:N	2.30	0.47
2:H:78:MET:HB3	2:H:83:VAL:HG21	1.97	0.47
1:A:192:LYS:HD3	1:A:281:VAL:HG13	1.97	0.46
1:B:97:HIS:O	1:B:98:ALA:HB3	2.15	0.46
2:F:228:HIS:CE1	2:F:229:ILE:HG13	2.50	0.46
2:G:112:ASP:OD1	2:G:114:ASN:HB3	2.16	0.46
2:G:124:ASP:HA	2:G:127:VAL:HG12	1.96	0.46
1:B:65:TYR:OH	1:B:363:ARG:HD3	2.15	0.46
1:B:63:PHE:HB2	1:B:173:LEU:HB3	1.98	0.46
2:E:242:PRO:HB3	2:E:246:LEU:HD23	1.97	0.46
2:H:254:SER:HA	2:H:257:ASN:HB2	1.97	0.46
1:B:15:PRO:HB3	2:E:228:HIS:CE1	2.51	0.46
1:B:228:ILE:HD13	1:B:257:LEU:HD11	1.97	0.46
1:A:57:ARG:NH2	1:A:61:ASN:OD1	2.49	0.46
2:E:88:ASP:HA	2:E:348:PHE:CE2	2.51	0.46
1:A:367:TYR:HA	1:A:368:PRO:HD3	1.77	0.46
1:D:364:ASN:OD1	1:D:365:PHE:N	2.48	0.46
2:F:76:LYS:HG2	2:F:86:LEU:HD12	1.97	0.46
2:H:149:ARG:NH1	2:H:180:TPO:O1P	2.45	0.46
1:A:57:ARG:HB2	1:A:63:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:O	1:A:80:VAL:HG13	2.16	0.46
1:C:47:HIS:ND1	1:C:48:PRO:O	2.42	0.46
2:F:228:HIS:ND1	2:F:229:ILE:HG13	2.31	0.46
2:H:278:ASN:O	2:H:280:LEU:N	2.49	0.46
1:D:408:VAL:H	2:E:120:GLN:HE22	1.63	0.46
2:H:148:HIS:O	2:H:149:ARG:HB2	2.14	0.46
1:B:153:GLU:O	1:B:157:THR:HG23	2.15	0.45
1:D:16:SER:C	1:D:18:THR:H	2.19	0.45
2:F:284:LEU:HB2	2:F:305:HIS:CE1	2.50	0.45
2:F:269:ASN:ND2	2:F:271:ALA:HB3	2.31	0.45
2:H:74:LEU:HD13	2:H:146:ILE:CD1	2.46	0.45
1:B:65:TYR:CZ	1:B:363:ARG:HD3	2.52	0.45
2:E:242:PRO:HG3	2:E:291:LEU:HD13	1.98	0.45
2:F:66:LYS:HE3	2:F:337:TRP:CZ2	2.52	0.45
1:B:147:GLN:H	1:B:147:GLN:CD	2.20	0.45
1:B:16:SER:OG	1:B:18:THR:HG22	2.16	0.45
1:C:167:MET:N	1:C:167:MET:SD	2.89	0.45
2:E:285:LEU:HD12	2:E:285:LEU:H	1.81	0.45
2:E:89:VAL:HG23	2:E:103:TYR:O	2.17	0.45
2:H:149:ARG:NH2	2:H:180:TPO:O1P	2.47	0.45
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.81	0.45
2:F:259:ILE:HA	2:F:262:LEU:HG	1.99	0.45
2:G:127:VAL:O	2:G:131:ILE:HG12	2.16	0.45
1:B:194:THR:OG1	1:B:195:VAL:N	2.50	0.45
2:H:130:LEU:O	2:H:134:ILE:HG13	2.17	0.45
1:C:278:LEU:HD23	1:C:365:PHE:CE1	2.52	0.45
2:F:123:THR:HG22	2:F:125:ASP:H	1.81	0.45
1:B:173:LEU:HD12	1:B:177:LYS:O	2.17	0.45
1:B:354:ARG:NH1	1:B:354:ARG:HG2	2.30	0.45
1:B:408:VAL:HG12	2:G:120:GLN:OE1	2.17	0.45
2:G:84:ILE:HD11	2:G:106:THR:HB	1.99	0.45
2:H:58:PRO:HB2	2:H:59:PHE:CE2	2.52	0.45
1:B:209:THR:HG21	1:B:228:ILE:O	2.17	0.44
1:D:145:PRO:HB2	1:D:147:GLN:OE1	2.17	0.44
2:H:109:MET:SD	2:H:159:ASN:ND2	2.90	0.44
2:F:81:GLU:CD	2:F:136[A]:ARG:HH22	2.15	0.44
2:H:351:PRO:HA	2:H:352:PRO:HD3	1.84	0.44
1:A:288:MET:CE	1:A:292:LEU:HD23	2.48	0.44
2:E:158:VAL:HA	2:E:163:GLU:O	2.18	0.44
2:E:53:LYS:HZ1	4:E:401:AGS:PB	2.40	0.44
2:H:80:HIS:HE2	2:H:136:ARG:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:LEU:HA	2:H:156:LEU:HD23	1.53	0.44
2:H:78:MET:HB2	2:H:78:MET:HE2	1.70	0.44
2:F:88:ASP:HA	2:F:348:PHE:CE2	2.52	0.44
2:F:66:LYS:HE3	2:F:337:TRP:CH2	2.53	0.44
2:G:284:LEU:O	2:G:288:MET:HG3	2.17	0.44
2:H:51:ALA:O	2:H:105:VAL:HA	2.17	0.44
2:G:144:ALA:O	2:G:145:ASP:HB2	2.18	0.44
1:C:154:ARG:O	1:C:157:THR:HG22	2.17	0.44
2:E:76:LYS:HE3	2:E:348:PHE:HD1	1.82	0.44
2:H:278:ASN:C	2:H:280:LEU:N	2.71	0.44
1:B:149:GLN:O	1:B:153:GLU:HG3	2.18	0.44
1:C:95:ALA:HB1	1:C:175:ASN:ND2	2.32	0.44
1:D:148:TYR:O	1:D:152:LEU:HG	2.17	0.44
2:E:113:LEU:HA	2:E:113:LEU:HD12	1.84	0.44
1:B:79:PHE:CE1	1:B:117:PHE:HB2	2.53	0.43
2:E:147:ILE:HB	2:E:175:THR:HG22	1.99	0.43
2:G:96:LEU:O	2:G:99:PHE:HB3	2.18	0.43
1:B:249:LYS:HA	1:B:249:LYS:HD3	1.85	0.43
2:F:173:ARG:HD3	2:F:174:HIS:O	2.17	0.43
2:H:222:LEU:HD13	2:H:223:PHE:CZ	2.52	0.43
1:C:202:GLN:HG2	1:C:204:ASN:O	2.18	0.43
1:B:102:VAL:HG11	1:B:179:TYR:CG	2.54	0.43
1:C:335:LYS:HE2	1:C:335:LYS:HB3	1.75	0.43
2:E:147:ILE:HG12	2:E:149:ARG:CG	2.48	0.43
1:C:187:ARG:HG3	1:C:293:TYR:CE2	2.53	0.43
1:C:190:LEU:HD12	1:C:191:CYS:H	1.83	0.43
1:A:389:SER:HB3	2:F:121:LYS:HB3	2.00	0.43
2:F:278:ASN:HA	2:F:279:PRO:HD2	1.88	0.43
2:G:20:VAL:HG13	2:G:90:PHE:CZ	2.54	0.43
1:B:114:GLU:OE2	1:B:244:GLY:N	2.39	0.43
2:H:158:VAL:HA	2:H:163:GLU:O	2.19	0.43
2:H:187:TRP:CE2	2:H:224:PRO:HA	2.53	0.43
2:E:82:ASN:ND2	2:E:136:ARG:HB3	2.34	0.43
2:G:138:LEU:HD11	2:G:205:ASP:HB3	2.00	0.43
2:H:70:ARG:NH1	2:H:173:ARG:HD2	2.33	0.43
1:C:154:ARG:CZ	1:C:158:LEU:HD21	2.48	0.43
1:D:48:PRO:HA	1:D:49:PRO:HD3	1.87	0.43
2:H:112:ASP:H	2:H:115:ASN:ND2	2.13	0.43
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.79	0.42
1:C:258:LEU:HA	1:C:258:LEU:HD23	1.85	0.42
2:E:242:PRO:HG3	2:E:291:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:LEU:HD23	2:F:171:LEU:HA	1.80	0.42
2:F:70:ARG:O	2:F:74:LEU:HG	2.19	0.42
2:G:66:LYS:HD3	2:G:337:TRP:CZ2	2.54	0.42
1:B:278:LEU:HA	1:B:278:LEU:HD23	1.87	0.42
2:E:142:HIS:NE2	2:E:205:ASP:OD2	2.37	0.42
2:E:43:ASP:OD2	2:E:46:THR:OG1	2.25	0.42
2:G:158:VAL:HA	2:G:163:GLU:O	2.19	0.42
2:H:140:TYR:CZ	2:H:320:ALA:HB2	2.55	0.42
1:A:408:VAL:HG22	2:F:120:GLN:CD	2.40	0.42
2:H:29:PRO:HA	2:H:39:CYS:HA	2.02	0.42
1:A:285:LEU:HB3	1:A:363:ARG:HB3	2.00	0.42
1:A:60:ASN:HB3	1:A:62:CYS:SG	2.59	0.42
1:B:192:LYS:NZ	1:B:281:VAL:HG22	2.35	0.42
1:B:290:GLU:HA	1:B:293:TYR:CE2	2.54	0.42
2:E:238:LEU:HD11	2:E:270:PHE:CE1	2.55	0.42
1:D:142:HIS:O	1:D:143:GLN:HB2	2.19	0.42
1:D:313:ILE:HG12	1:D:330:VAL:HG21	2.02	0.42
2:E:159:ASN:HD22	2:E:159:ASN:HA	1.67	0.42
2:G:75:LEU:HB3	2:G:86:LEU:HG	2.01	0.42
2:H:225:GLY:HA2	2:H:230:ASP:OD2	2.19	0.42
2:F:175:THR:HG21	2:F:202:GLN:CG	2.49	0.42
1:A:384:ARG:N	2:F:237:ARG:NH2	2.68	0.42
1:A:316:GLU:OE2	1:A:333:ARG:NH1	2.42	0.42
2:E:127:VAL:HG21	2:E:217:LEU:HD23	2.02	0.42
2:G:235:ILE:O	2:G:239:VAL:HG22	2.20	0.42
2:G:85:GLY:O	2:G:106:THR:HG22	2.20	0.42
1:B:288:MET:HE1	1:B:293:TYR:HB3	2.02	0.42
2:E:139:LYS:HD2	2:E:300:ALA:HB2	2.02	0.42
2:F:270:PHE:N	2:F:270:PHE:CD1	2.88	0.42
2:G:132:TYR:HB2	2:G:308:PHE:CD1	2.55	0.42
1:B:35:ARG:HG3	1:B:355:HIS:NE2	2.35	0.42
2:E:37:SER:O	2:E:53:LYS:HA	2.20	0.42
2:F:137:GLY:O	2:F:141:ILE:HG13	2.19	0.42
2:H:173:ARG:NH2	2:H:179:MET:HA	2.35	0.42
1:B:101:ASP:N	1:B:101:ASP:OD1	2.52	0.41
1:B:311:ALA:O	1:B:315:THR:HG23	2.19	0.41
1:C:330:VAL:O	1:C:334:VAL:HG23	2.20	0.41
1:A:178:LEU:HB3	1:A:276:GLN:HB2	2.02	0.41
1:C:157:THR:O	1:C:161:GLU:HG3	2.19	0.41
2:E:138:LEU:HA	2:E:138:LEU:HD12	1.73	0.41
1:A:388:VAL:HG12	2:F:275:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:281:ALA:O	2:H:282:VAL:C	2.56	0.41
2:H:95:SER:OG	2:H:96:LEU:N	2.53	0.41
1:A:167:MET:SD	1:A:242:ARG:HG2	2.60	0.41
1:B:17:TRP:CE3	1:B:17:TRP:HA	2.55	0.41
1:D:208:THR:CG2	1:D:238:GLU:HG3	2.47	0.41
1:D:55:LYS:HE3	1:D:55:LYS:HB2	1.95	0.41
1:B:15:PRO:HB3	2:E:228:HIS:ND1	2.35	0.41
1:D:234:ILE:O	1:D:235:CYS:C	2.59	0.41
2:F:38:VAL:HG12	2:F:53:LYS:HB2	2.03	0.41
2:H:127:VAL:HG12	2:H:131:ILE:CD1	2.51	0.41
2:H:24:TYR:HA	2:H:42:PHE:O	2.21	0.41
2:E:189:ARG:HG3	2:E:193:ILE:HD12	2.02	0.41
2:H:197:TRP:CD1	2:H:198:MET:HG3	2.56	0.41
1:A:246:TYR:CE2	1:A:247:LYS:HE3	2.55	0.41
1:B:90:LEU:HA	1:B:90:LEU:HD23	1.86	0.41
1:C:282:THR:HA	1:C:365:PHE:O	2.21	0.41
2:F:90:PHE:CE2	2:F:103:TYR:CG	3.08	0.41
2:F:5:ARG:HA	2:F:6:PRO:HD2	1.92	0.41
2:H:155:ASN:O	2:H:167:LEU:HB2	2.20	0.41
1:C:144:LEU:HG	1:C:145:PRO:CD	2.50	0.41
2:H:88:ASP:HB3	2:H:105:VAL:CG1	2.50	0.41
2:E:131:ILE:HD13	2:E:134:ILE:HD12	2.03	0.41
2:F:61:SER:HA	2:F:334:ILE:HD11	2.03	0.41
2:F:76:LYS:HE3	2:F:348:PHE:CD1	2.50	0.41
1:A:141:GLN:O	1:A:144:LEU:HB2	2.21	0.40
1:A:215:LEU:HD11	1:A:229:LYS:HD2	2.02	0.40
1:D:136:PRO:HD3	1:D:148:TYR:CE1	2.56	0.40
2:G:270:PHE:CG	2:G:286:GLU:HG2	2.56	0.40
2:H:155:ASN:HD22	2:H:168:ASP:CG	2.25	0.40
1:C:387:PRO:O	2:H:218:THR:HG23	2.21	0.40
2:H:88:ASP:O	2:H:105:VAL:HG12	2.21	0.40
1:A:408:VAL:HG22	2:F:120:GLN:OE1	2.20	0.40
1:C:296:LEU:HA	1:C:296:LEU:HD12	1.87	0.40
1:D:150:LYS:HA	1:D:150:LYS:HD2	1.82	0.40
1:C:136:PRO:HD2	1:C:144:LEU:HD21	2.04	0.40
1:D:248:VAL:HB	1:D:266:ILE:HD12	2.03	0.40
1:D:338:HIS:CE1	1:D:355:HIS:HB3	2.56	0.40
2:F:73:ARG:HH11	2:F:73:ARG:HD2	1.74	0.40
2:H:55:LEU:HD12	2:H:102:VAL:CG2	2.52	0.40
2:H:222:LEU:HD23	2:H:222:LEU:HA	1.81	0.40
1:D:97:HIS:O	1:D:98:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:GLU:OE1	2:F:256:ARG:NH2	2.48	0.40
2:G:215:GLU:O	2:G:219:GLY:N	2.47	0.40
2:G:310:GLN:O	2:G:310:GLN:HG2	2.22	0.40
2:G:86:LEU:HA	2:G:86:LEU:HD23	1.91	0.40
2:H:144:ALA:O	2:H:145:ASP:HB2	2.20	0.40
2:H:312:HIS:NE2	2:H:314:PRO:HB3	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLU:O	1:A:176:ASN:ND2[1_655]	2.18	0.02

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	372/504 (74%)	347 (93%)	22 (6%)	3 (1%)	19 39
1	B	372/504 (74%)	342 (92%)	27 (7%)	3 (1%)	19 39
1	C	359/504 (71%)	336 (94%)	16 (4%)	7 (2%)	8 15
1	D	373/504 (74%)	355 (95%)	12 (3%)	6 (2%)	9 19
2	E	340/360 (94%)	320 (94%)	16 (5%)	4 (1%)	13 27
2	F	338/360 (94%)	323 (96%)	14 (4%)	1 (0%)	41 64
2	G	340/360 (94%)	311 (92%)	26 (8%)	3 (1%)	17 35
2	H	327/360 (91%)	274 (84%)	32 (10%)	21 (6%)	1 1
All	All	2821/3456 (82%)	2608 (92%)	165 (6%)	48 (2%)	9 18

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	GLU
1	C	60	ASN
1	C	96	GLU
1	C	275	ALA
1	C	345	GLY
1	D	60	ASN
1	D	275	ALA
2	G	119	CYS
2	H	22	GLU
2	H	23	ARG
2	H	162	CYS
2	H	282	VAL
2	H	306	ALA
2	H	326	SER
1	A	60	ASN
1	B	41	GLY
1	B	274	GLY
1	C	347	GLU
1	D	235	CYS
2	H	100	ASN
2	H	127	VAL
2	H	128	GLN
2	H	304	ALA
1	A	258	LEU
1	C	136	PRO
2	E	15	LYS
2	E	197	TRP
2	H	96	LEU
2	H	197	TRP
1	B	40	ASP
2	G	197	TRP
2	H	168	ASP
2	H	256	ARG
2	H	351	PRO
1	C	98	ALA
2	E	100	ASN
2	G	224	PRO
2	H	120	GLN
2	H	273	VAL
1	D	17	TRP
1	D	245	ASP
2	E	184	ALA
2	F	197	TRP

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Mol	Chain	Res	Type
2	H	58	PRO
2	H	119	CYS
2	H	279	PRO
1	D	346	GLY
2	H	290	VAL

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	295/421 (70%)	278 (94%)	17 (6%)	20 40
1	B	300/421 (71%)	280 (93%)	20 (7%)	16 33
1	C	282/421 (67%)	267 (95%)	15 (5%)	22 45
1	D	294/421 (70%)	282 (96%)	12 (4%)	30 56
2	E	285/317 (90%)	273 (96%)	12 (4%)	30 55
2	F	287/317 (90%)	278 (97%)	9 (3%)	40 66
2	G	281/317 (89%)	275 (98%)	6 (2%)	53 77
2	H	189/317 (60%)	160 (85%)	29 (15%)	2 4
All	All	2213/2952 (75%)	2093 (95%)	120 (5%)	22 44

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	52	SER
1	A	74	ASN
1	A	97	HIS
1	A	142	HIS
1	A	156	LYS
1	A	190	LEU
1	A	193	SER
1	A	219	SER
1	A	235	CYS

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Mol	Chain	Res	Type
1	A	263	SER
1	A	276	GLN
1	A	279	ASP
1	A	335	LYS
1	A	363	ARG
1	A	394	SER
1	A	404	THR
1	B	35	ARG
1	B	52	SER
1	B	74	ASN
1	B	75	ARG
1	B	85	SER
1	B	97	HIS
1	B	101	ASP
1	B	147	GLN
1	B	159	GLU
1	B	193	SER
1	B	199	GLN
1	B	209	THR
1	B	213	ASP
1	B	223	LEU
1	B	248	VAL
1	B	296	LEU
1	B	315	THR
1	B	363	ARG
1	B	367	TYR
1	B	389	SER
1	C	18	THR
1	C	52	SER
1	C	55	LYS
1	C	57	ARG
1	C	85	SER
1	C	97	HIS
1	C	116	SER
1	C	131	LEU
1	C	183	VAL
1	C	276	GLN
1	C	279	ASP
1	C	348	ARG
1	C	354	ARG
1	C	363	ARG
1	C	404	THR

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Mol	Chain	Res	Type
1	D	18	THR
1	D	24	CYS
1	D	52	SER
1	D	101	ASP
1	D	150	LYS
1	D	190	LEU
1	D	279	ASP
1	D	339	SER
1	D	344	SER
1	D	363	ARG
1	D	373	SER
1	D	393	SER
2	E	7	THR
2	E	56	SER
2	E	162	CYS
2	E	183	VAL
2	E	251	SER
2	E	252	SER
2	E	262	LEU
2	E	293	SER
2	E	303	LEU
2	E	328	GLU
2	E	330	ARG
2	E	351	PRO
2	F	7	THR
2	F	62	ILE
2	F	63	ILE
2	F	84	ILE
2	F	86	LEU
2	F	112	ASP
2	F	149	ARG
2	F	162	CYS
2	F	328	GLU
2	G	98	GLU
2	G	112	ASP
2	G	113	LEU
2	G	203	THR
2	G	256	ARG
2	G	321	ASP
2	H	24	TYR
2	H	43	ASP
2	H	48	HIS

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Mol	Chain	Res	Type
2	H	56	SER
2	H	66	LYS
2	H	108	LEU
2	H	109	MET
2	H	136	ARG
2	H	146	ILE
2	H	154	SER
2	H	156	LEU
2	H	159	ASN
2	H	174	HIS
2	H	175	THR
2	H	177	ASP
2	H	208	SER
2	H	220	ARG
2	H	222	LEU
2	H	227	ASP
2	H	228	HIS
2	H	237	ARG
2	H	251	SER
2	H	252	SER
2	H	254	SER
2	H	288	MET
2	H	296	ARG
2	H	311	TYR
2	H	326	SER
2	H	339	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	176	ASN
1	D	304	GLN
1	D	307	GLN
2	E	120	GLN
2	E	159	ASN
2	F	100	ASN
2	G	142	HIS
2	H	159	ASN
2	H	312	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PTR	G	182	2	15,16,17	1.32	1 (6%)	19,22,24	0.67	0
2	TPO	H	180	2	8,10,11	1.35	2 (25%)	10,14,16	1.64	2 (20%)
2	TPO	G	180	2	8,10,11	1.07	0	10,14,16	1.55	1 (10%)
2	PTR	F	182	2	15,16,17	1.45	1 (6%)	19,22,24	0.86	1 (5%)
2	TPO	F	180	2	8,10,11	1.10	0	10,14,16	1.57	3 (30%)
2	TPO	E	180	2	8,10,11	1.66	2 (25%)	10,14,16	0.92	0
2	PTR	H	182	2	15,16,17	1.22	1 (6%)	19,22,24	1.14	2 (10%)
2	PTR	E	182	2	15,16,17	1.35	1 (6%)	19,22,24	0.65	0

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	PTR	G	182	2	-	2/10/11/13	0/1/1/1
2	TPO	H	180	2	-	1/9/11/13	-
2	TPO	G	180	2	-	1/9/11/13	-
2	PTR	F	182	2	-	0/10/11/13	0/1/1/1
2	TPO	F	180	2	-	0/9/11/13	-
2	TPO	E	180	2	-	0/9/11/13	-
2	PTR	H	182	2	-	2/10/11/13	0/1/1/1
2	PTR	E	182	2	-	1/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	182	PTR	OH-CZ	-4.86	1.29	1.40
2	G	182	PTR	OH-CZ	-4.84	1.29	1.40
2	E	182	PTR	OH-CZ	-4.37	1.30	1.40
2	H	182	PTR	OH-CZ	-3.69	1.32	1.40
2	E	180	TPO	P-O1P	3.10	1.60	1.50
2	H	180	TPO	P-O1P	2.44	1.58	1.50
2	H	180	TPO	P-O3P	-2.17	1.46	1.54
2	E	180	TPO	P-O2P	-2.10	1.46	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	180	TPO	P-OG1-CB	-3.89	111.44	123.21
2	G	180	TPO	P-OG1-CB	-3.49	112.67	123.21
2	H	182	PTR	CB-CA-C	-3.22	105.43	111.47
2	F	180	TPO	O2P-P-O1P	-2.51	100.84	110.68
2	H	180	TPO	O3P-P-O1P	-2.34	101.50	110.68
2	F	180	TPO	P-OG1-CB	-2.29	116.30	123.21
2	H	182	PTR	O2P-P-OH	2.17	112.03	105.24
2	F	182	PTR	CB-CA-C	-2.15	107.44	111.47
2	F	180	TPO	CG2-CB-CA	-2.15	108.93	113.16

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	182	PTR	CZ-OH-P-O1P
2	H	180	TPO	O-C-CA-CB
2	H	182	PTR	C-CA-CB-CG
2	E	182	PTR	O-C-CA-CB
2	H	182	PTR	N-CA-CB-CG
2	G	182	PTR	CZ-OH-P-O3P
2	G	180	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	182	PTR	1	0
2	H	180	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 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	H	500	5	26,33,33	0.76	1 (3%)	26,52,52	0.93	2 (7%)
4	AGS	G	500	5	26,33,33	0.88	1 (3%)	26,52,52	0.90	1 (3%)
4	AGS	F	401	5	26,33,33	1.00	2 (7%)	26,52,52	0.96	2 (7%)
4	AGS	E	401	5	26,33,33	0.85	1 (3%)	26,52,52	0.88	2 (7%)

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	H	500	5	-	5/17/38/38	0/3/3/3
4	AGS	G	500	5	-	5/17/38/38	0/3/3/3
4	AGS	F	401	5	-	8/17/38/38	0/3/3/3
4	AGS	E	401	5	-	3/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	AGS	PA-O2A	-2.78	1.42	1.55
4	G	500	AGS	PG-S1G	2.61	1.96	1.90
4	H	500	AGS	PG-S1G	2.61	1.96	1.90
4	E	401	AGS	PG-S1G	2.59	1.96	1.90
4	F	401	AGS	PG-S1G	2.57	1.96	1.90

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	401	AGS	O3G-PG-O3B	3.08	114.94	104.64
4	H	500	AGS	PA-O3A-PB	-2.97	122.62	132.83
4	G	500	AGS	C5-C6-N6	2.42	124.03	120.35
4	F	401	AGS	C5-C6-N6	2.35	123.92	120.35
4	E	401	AGS	PA-O3A-PB	-2.22	125.21	132.83
4	H	500	AGS	C5-C6-N6	2.04	123.45	120.35
4	E	401	AGS	C5-C6-N6	2.02	123.42	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	500	AGS	PB-O3B-PG-O2G
4	G	500	AGS	PB-O3B-PG-O3G
4	H	500	AGS	PB-O3B-PG-O2G
4	H	500	AGS	PB-O3B-PG-O3G
4	F	401	AGS	PB-O3B-PG-O2G
4	F	401	AGS	PB-O3B-PG-O3G
4	F	401	AGS	C5'-O5'-PA-O1A
4	G	500	AGS	PA-O3A-PB-O1B
4	F	401	AGS	PA-O3A-PB-O1B
4	F	401	AGS	C5'-O5'-PA-O3A
4	H	500	AGS	PB-O3A-PA-O2A
4	F	401	AGS	PB-O3A-PA-O1A
4	E	401	AGS	PB-O3A-PA-O2A
4	G	500	AGS	PG-O3B-PB-O2B
4	F	401	AGS	PG-O3B-PB-O2B
4	E	401	AGS	PA-O3A-PB-O2B
4	G	500	AGS	PB-O3A-PA-O2A
4	H	500	AGS	PA-O3A-PB-O1B
4	F	401	AGS	PA-O3A-PB-O2B
4	E	401	AGS	PB-O3A-PA-O1A
4	H	500	AGS	O4'-C4'-C5'-O5'

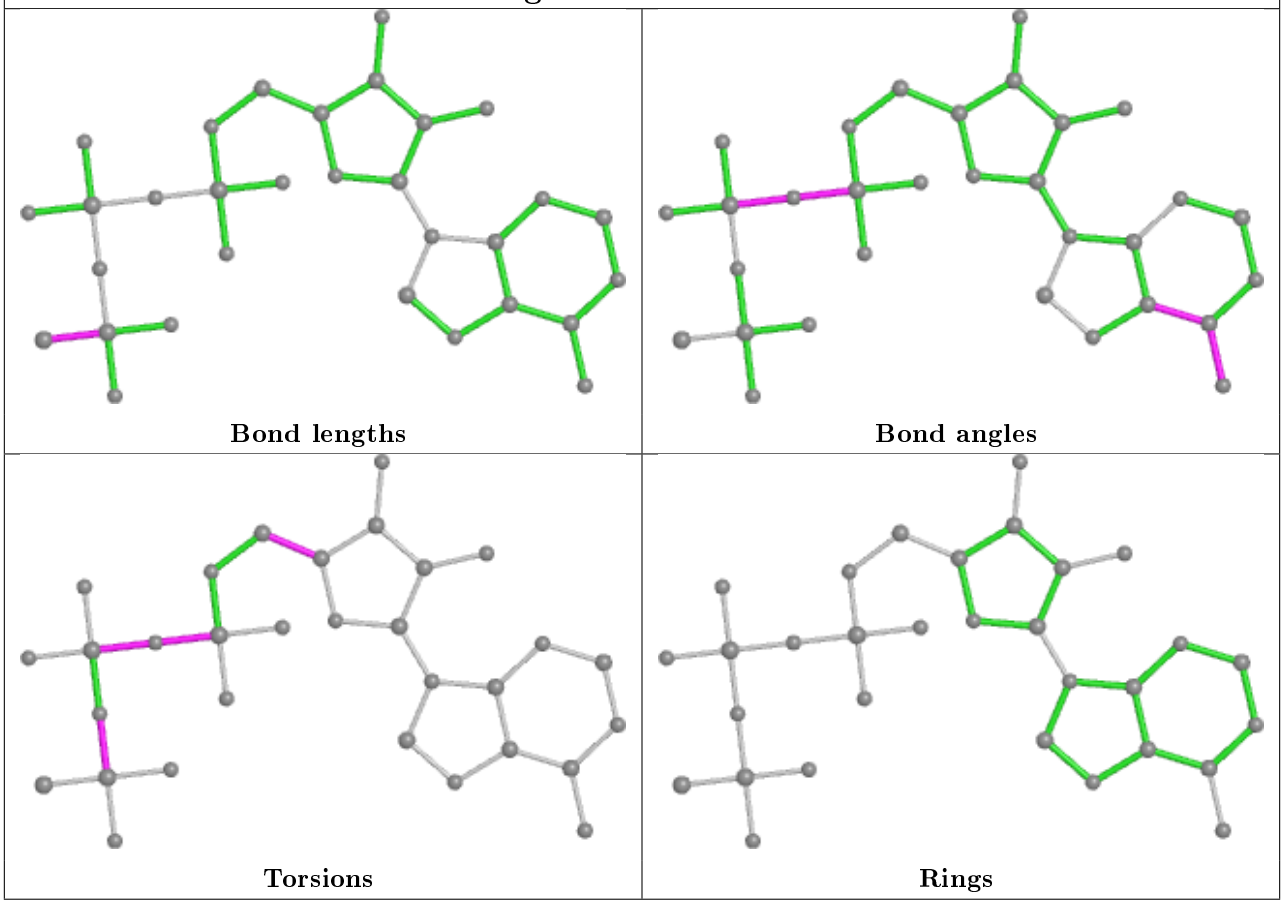
There are no ring outliers.

2 monomers are involved in 2 short contacts:

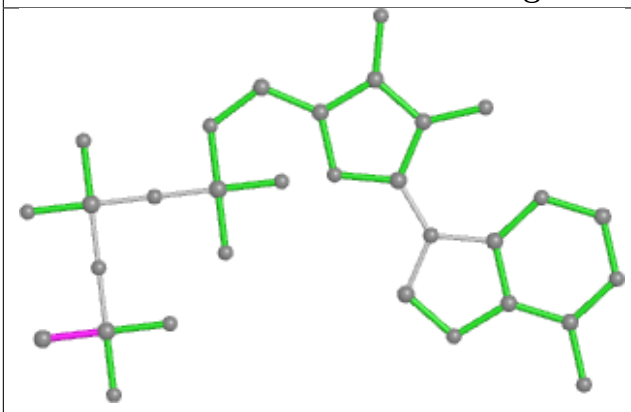
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	AGS	1	0
4	E	401	AGS	1	0

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

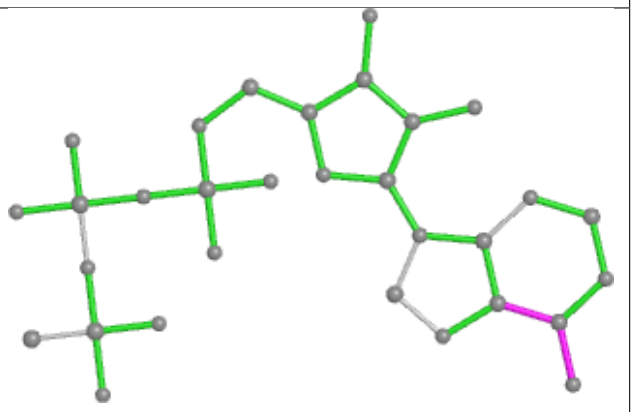
Ligand AGS H 500



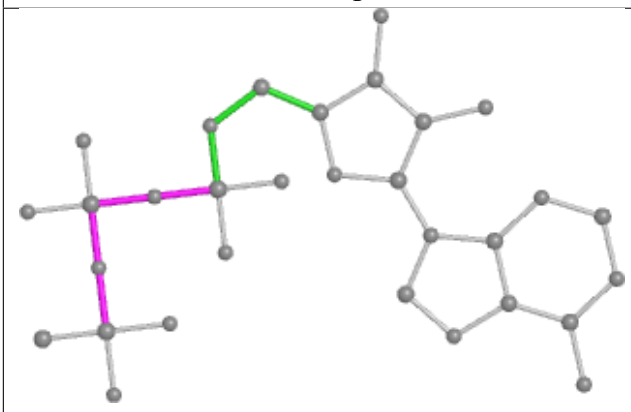
Ligand AGS G 500



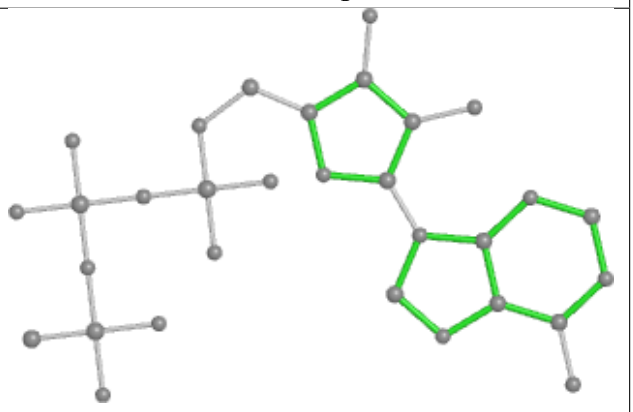
Bond lengths



Bond angles

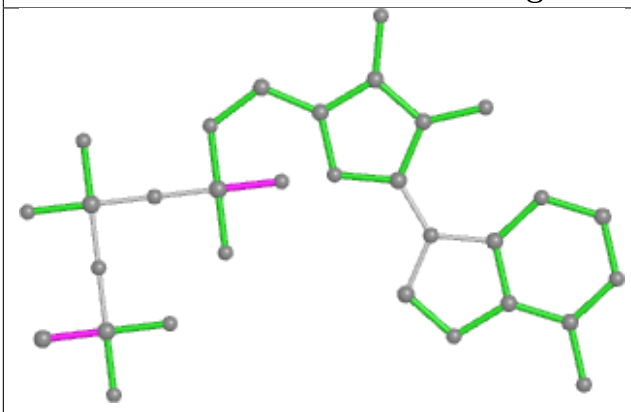


Torsions

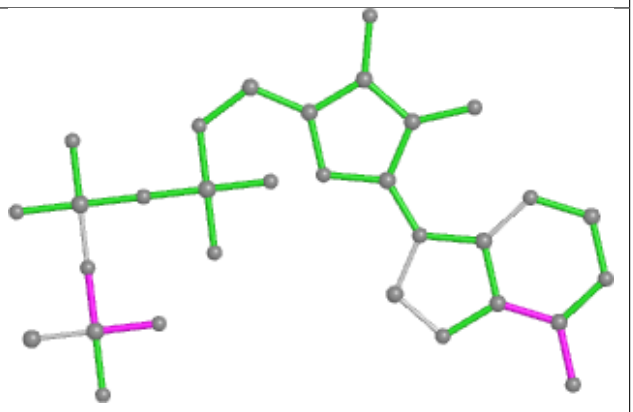


Rings

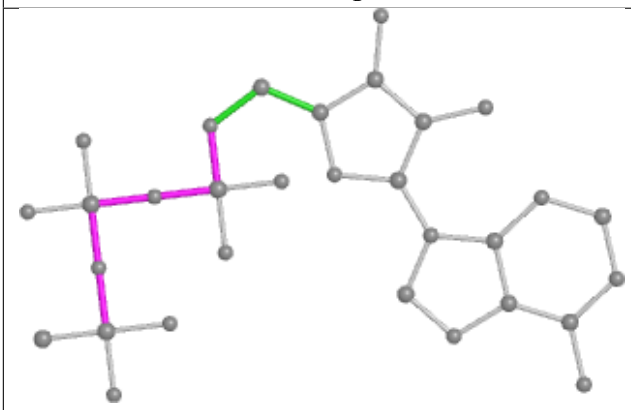
Ligand AGS F 401



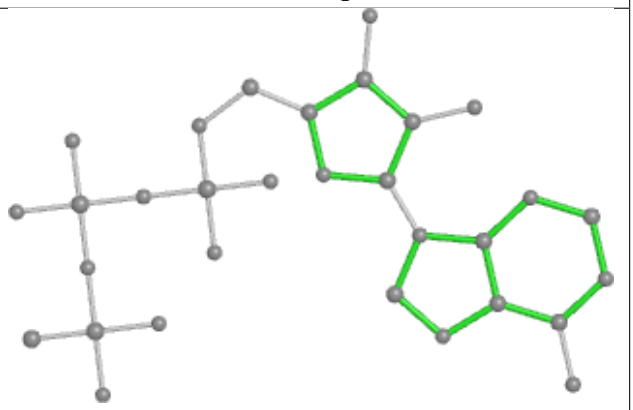
Bond lengths



Bond angles

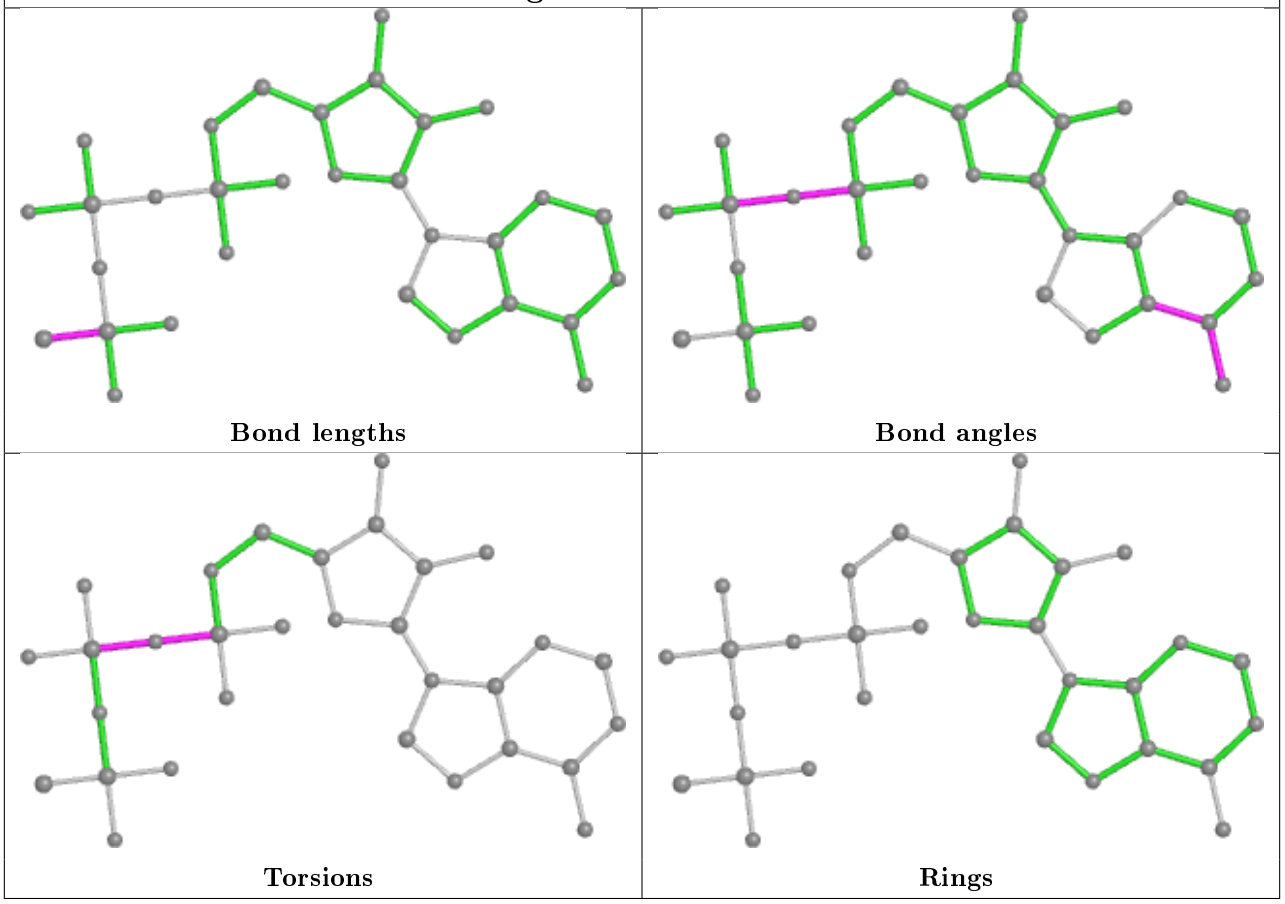


Torsions



Rings

Ligand AGS E 401



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	378/504 (75%)	-0.24	1 (0%) 94 93	32, 50, 82, 116	0
1	B	378/504 (75%)	-0.23	5 (1%) 77 73	33, 53, 91, 110	0
1	C	367/504 (72%)	-0.11	10 (2%) 54 48	32, 55, 98, 139	0
1	D	379/504 (75%)	-0.28	1 (0%) 94 93	33, 52, 83, 107	0
2	E	343/360 (95%)	-0.29	1 (0%) 94 93	35, 55, 78, 96	0
2	F	341/360 (94%)	-0.26	0 100 100	32, 51, 70, 98	0
2	G	342/360 (95%)	-0.18	2 (0%) 89 88	42, 62, 85, 101	0
2	H	335/360 (93%)	0.51	39 (11%) 4 3	69, 97, 119, 132	0
All	All	2863/3456 (82%)	-0.14	59 (2%) 63 58	32, 57, 102, 139	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	388	VAL	9.0
2	H	309	ALA	6.8
2	H	166	ILE	4.4
2	H	304	ALA	4.1
1	B	388	VAL	4.1
2	H	125	ASP	3.9
1	C	387	PRO	3.7
2	H	308	PHE	3.7
2	H	146	ILE	3.6
2	H	40	ALA	3.5
1	C	389	SER	3.3
1	B	138	GLY	3.2
2	H	322	PRO	3.1
2	H	121	LYS	3.1
2	H	86	LEU	3.0
1	B	140	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	328	GLU	2.9
2	H	141	ILE	2.9
2	H	200	TYR	2.9
2	H	327	PHE	2.9
1	A	258	LEU	2.8
2	H	83	VAL	2.8
2	H	143	SER	2.8
2	H	82	ASN	2.8
1	C	390	VAL	2.8
2	H	109	MET	2.7
2	H	41	ALA	2.7
2	H	332	LEU	2.7
2	H	156	LEU	2.7
2	H	218	THR	2.7
2	H	179	MET	2.6
2	H	129	PHE	2.6
2	H	274	PHE	2.6
2	H	120	GLN	2.6
2	H	157	ALA	2.6
1	D	62	CYS	2.5
2	H	158	VAL	2.4
2	H	273	VAL	2.4
2	H	77	HIS	2.4
2	H	240	GLY	2.4
1	B	392	TYR	2.3
2	E	17	ILE	2.3
2	G	271	ALA	2.3
2	H	50	VAL	2.3
1	C	41	GLY	2.3
2	H	216	LEU	2.3
1	C	404	THR	2.2
2	H	275	ILE	2.2
2	H	49	ARG	2.2
2	H	314	PRO	2.2
1	B	387	PRO	2.2
1	C	392	TYR	2.1
2	H	299	ALA	2.1
1	C	406	SER	2.1
2	H	311	TYR	2.1
1	C	228	ILE	2.0
1	C	407	LEU	2.0
2	G	147	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	159	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	PTR	H	182	16/17	0.89	0.18	78,82,93,94	0
2	PTR	G	182	16/17	0.90	0.14	52,65,80,84	0
2	TPO	H	180	11/12	0.93	0.14	69,85,93,95	0
2	PTR	F	182	16/17	0.94	0.13	42,51,66,69	0
2	PTR	E	182	16/17	0.95	0.14	51,59,71,73	0
2	TPO	G	180	11/12	0.98	0.13	37,46,49,51	0
2	TPO	F	180	11/12	0.98	0.13	23,40,42,46	0
2	TPO	E	180	11/12	0.99	0.14	24,39,44,51	0

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	G	501	1/1	0.78	0.11	49,49,49,49	0
3	NI	A	601	1/1	0.92	0.19	84,84,84,84	0
5	MG	H	502	1/1	0.92	0.12	82,82,82,82	0
5	MG	F	402	1/1	0.93	0.18	45,45,45,45	0
4	AGS	H	500	31/31	0.93	0.16	75,90,102,114	0
4	AGS	G	500	31/31	0.94	0.15	38,55,67,79	0
3	NI	E	403	1/1	0.94	0.11	87,87,87,87	0
3	NI	D	601	1/1	0.95	0.14	98,98,98,98	0
3	NI	B	601	1/1	0.95	0.15	86,86,86,86	1

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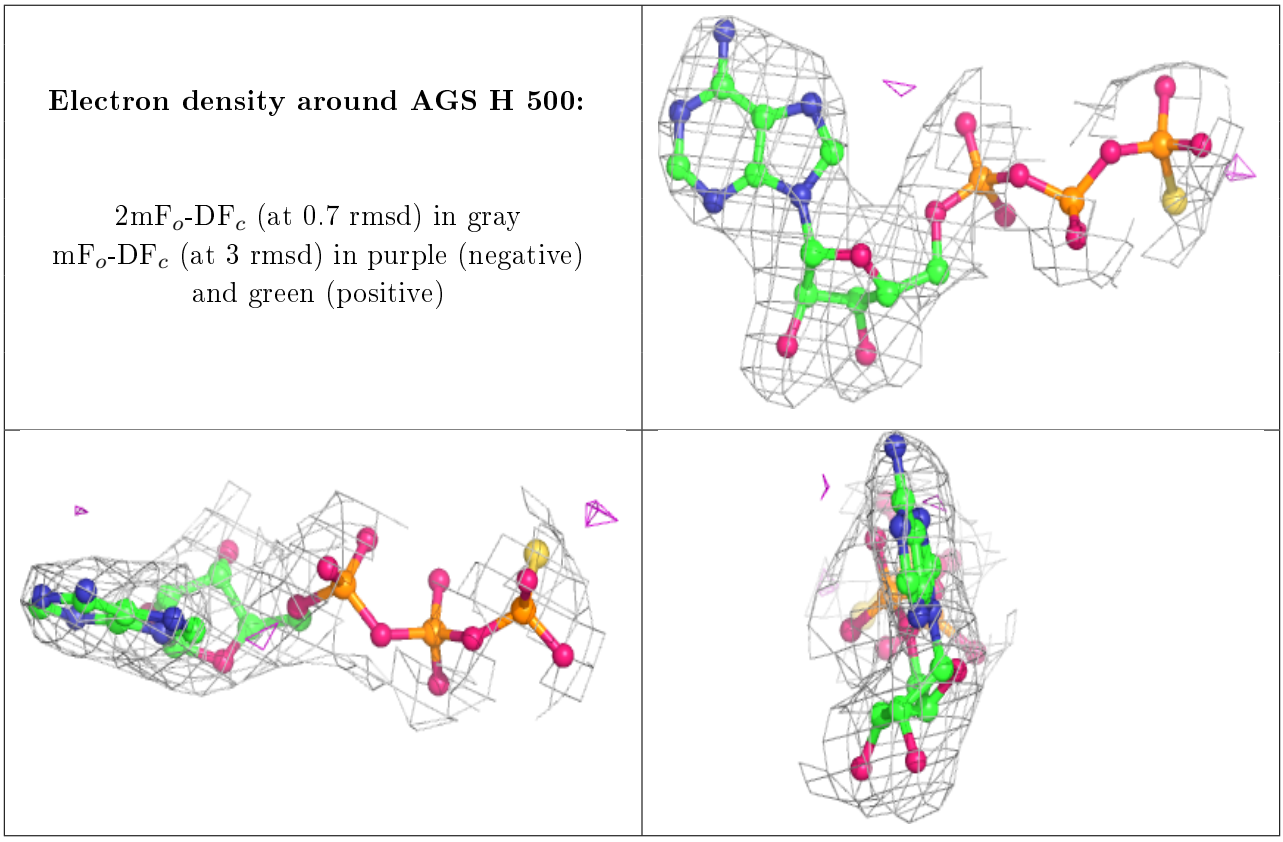
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	E	402	1/1	0.96	0.25	45,45,45,45	0
3	NI	C	601	1/1	0.96	0.14	97,97,97,97	0
5	MG	G	502	1/1	0.97	0.16	68,68,68,68	0
3	NI	F	403	1/1	0.97	0.06	97,97,97,97	0
4	AGS	F	401	31/31	0.97	0.15	32,45,66,87	0
4	AGS	E	401	31/31	0.97	0.13	26,44,64,77	0
5	MG	H	501	1/1	0.98	0.10	90,90,90,90	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.

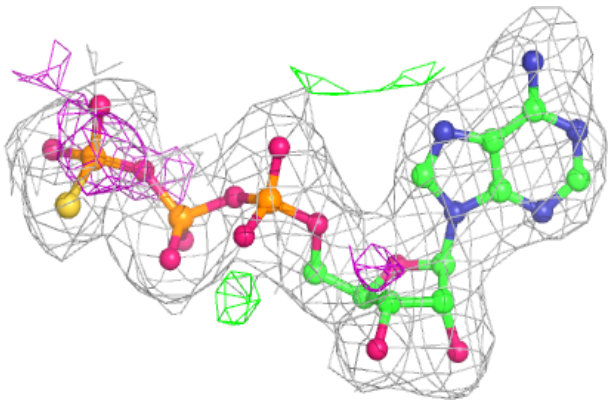
Electron density around AGS H 500:

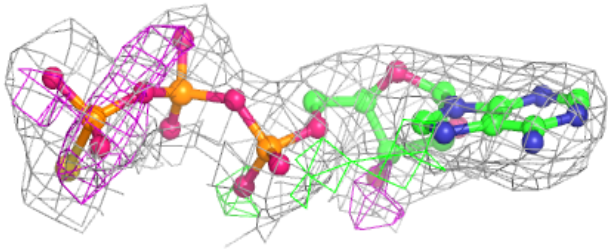
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around AGS G 500:

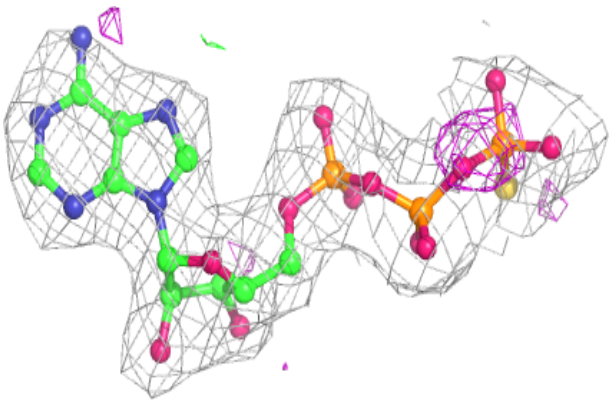
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

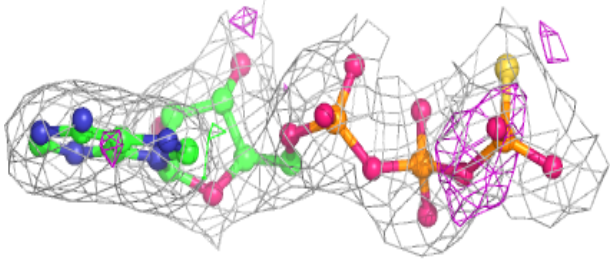


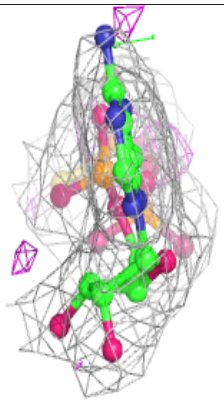


Electron density around AGS F 401:

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

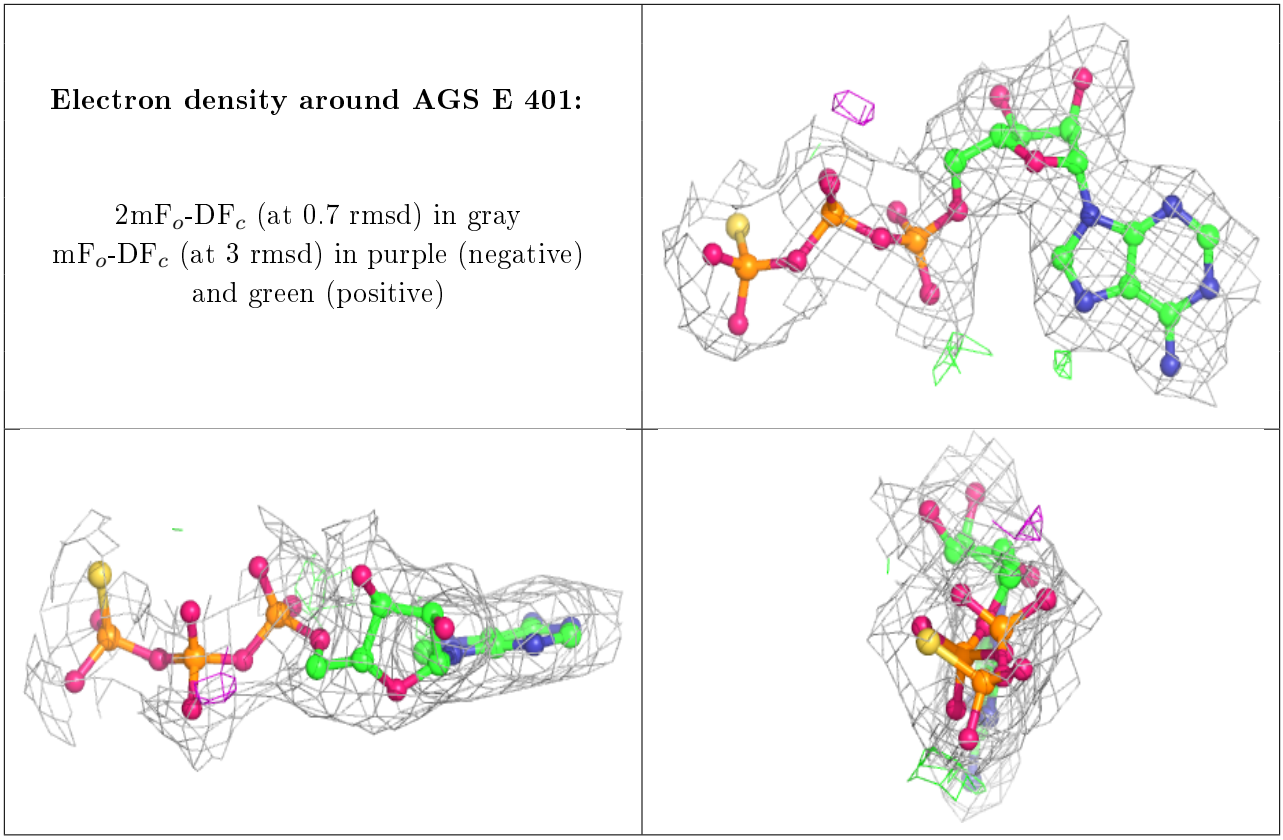






Electron density around AGS E 401:

$2mF_o$-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

There are no such residues in this entry.