Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2024 – 05:09 am GMT

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 (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:

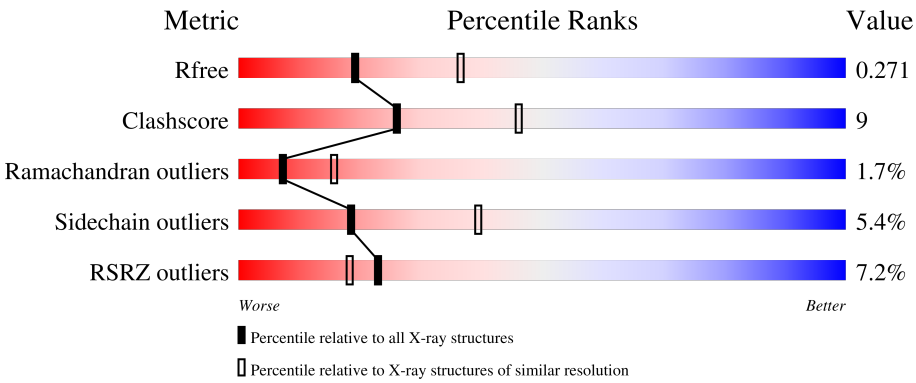
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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 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	504	2%, 62%, 12%, •, 25%
1	B	504	2%, 59%, 14%, •, 25%
1	C	504	5%, 58%, 14%, •, 27%
1	D	504	2%, 63%, 12%, •, 25%
2	E	360	2%, 72%, 22%, •, •

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Mol	Chain	Length	Quality of chain
2	F	360	% 76% 19% 5%
2	G	360	5% 75% 19%
2	H	360	32% 55% 29% 9% 6%

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

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

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

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

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

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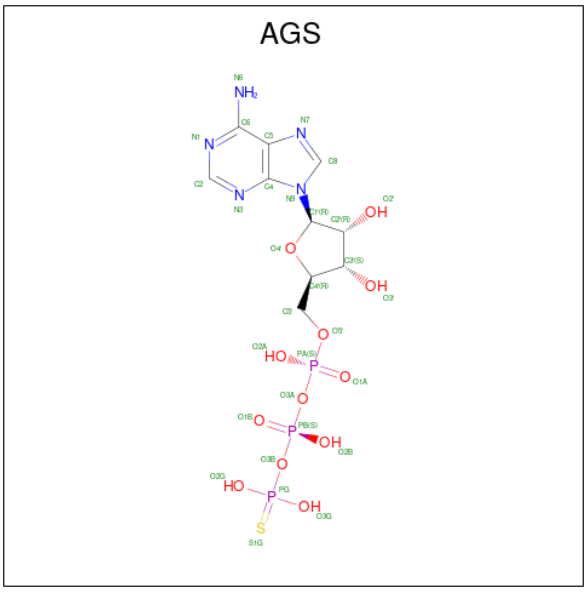
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
3	E	1	1	1	0	0
			Total	Ni		
3	F	1	1	1	0	0

- 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
			Total	C	N	O	P	S		
4	E	1	31	10	5	12	3	1	0	0
			Total	C	N	O	P	S		
4	F	1	31	10	5	12	3	1	0	0
			Total	C	N	O	P	S		
4	G	1	31	10	5	12	3	1	0	0
			Total	C	N	O	P	S		
4	H	1	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
			Total	Mg		
5	E	1	1	1	0	0
			Total	Mg		
5	F	1	1	1	0	0
			Total	Mg		
5	G	2	2	2	0	0

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

- Molecule 6 is water.

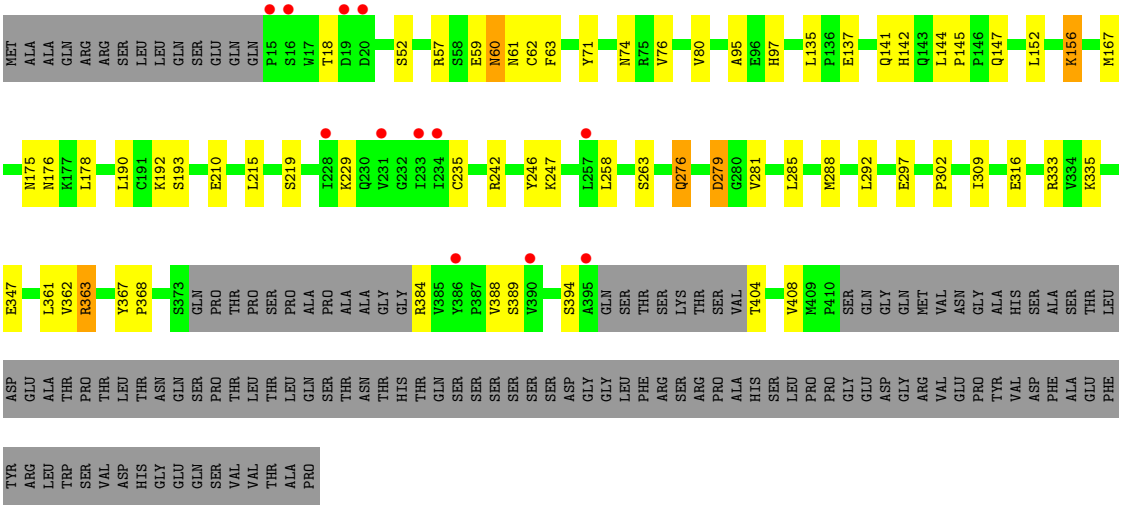
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	9	9	9	0	0
			Total	O		
6	B	5	5	5	0	0
			Total	O		
6	C	3	3	3	0	0
			Total	O		
6	D	3	3	3	0	0
			Total	O		
6	E	9	9	9	0	0
			Total	O		
6	F	10	10	10	0	0
			Total	O		
6	G	3	3	3	0	0

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.

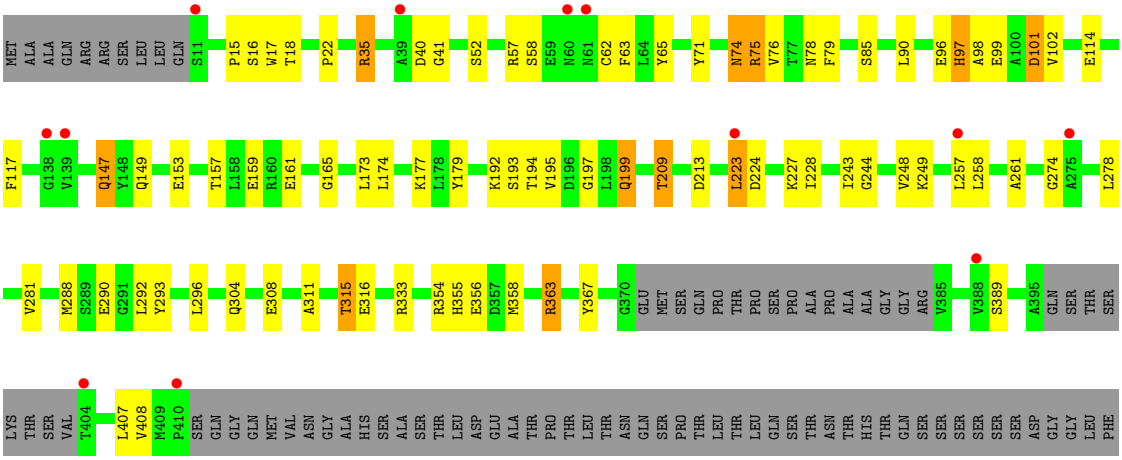
• Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain A:



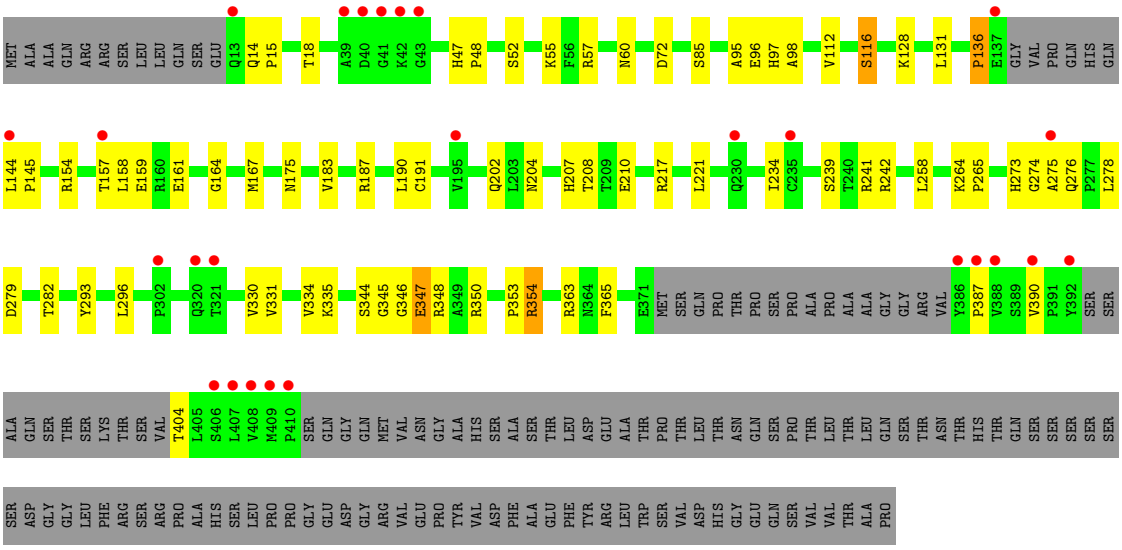
• Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain B:



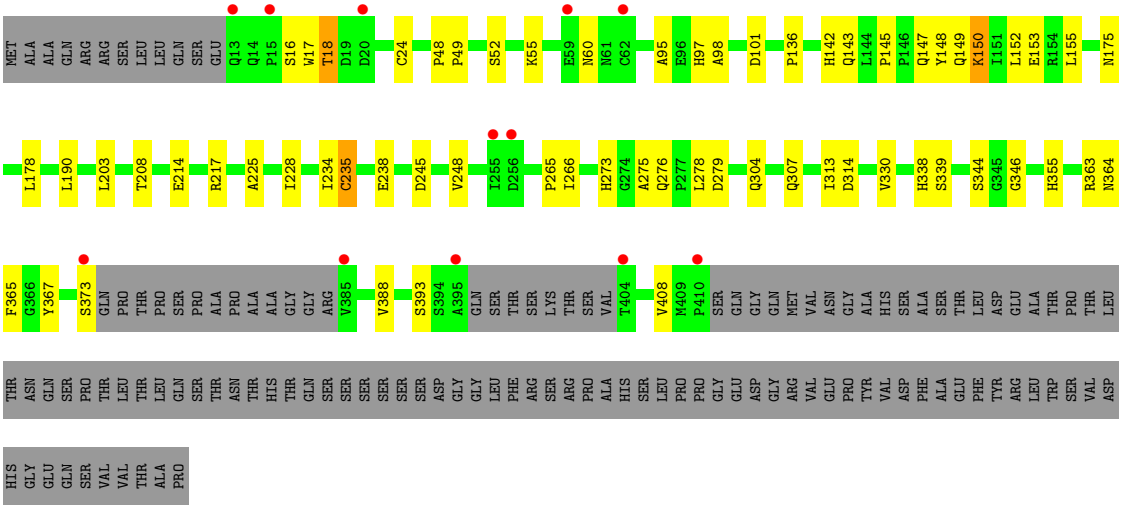
• Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain C:



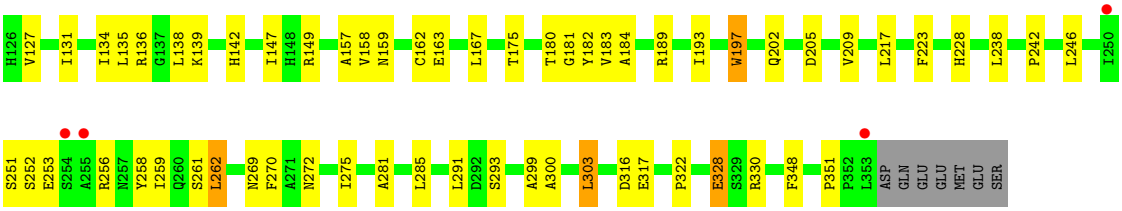
• Molecule 1: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain D:



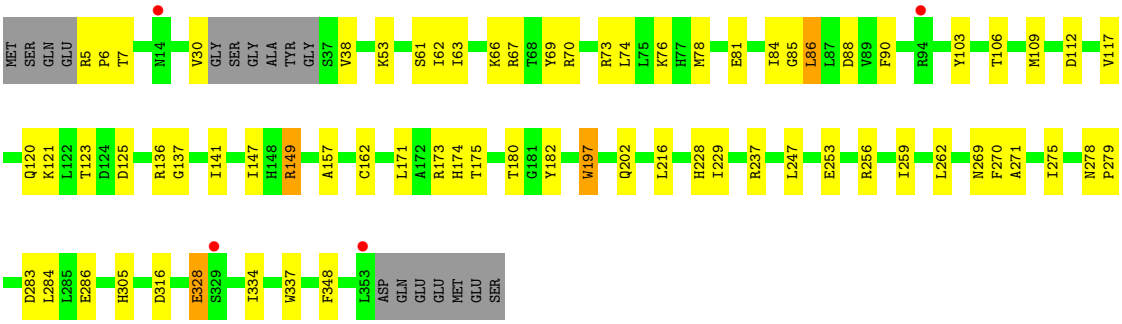
• Molecule 2: Mitogen-activated protein kinase 14

Chain E:



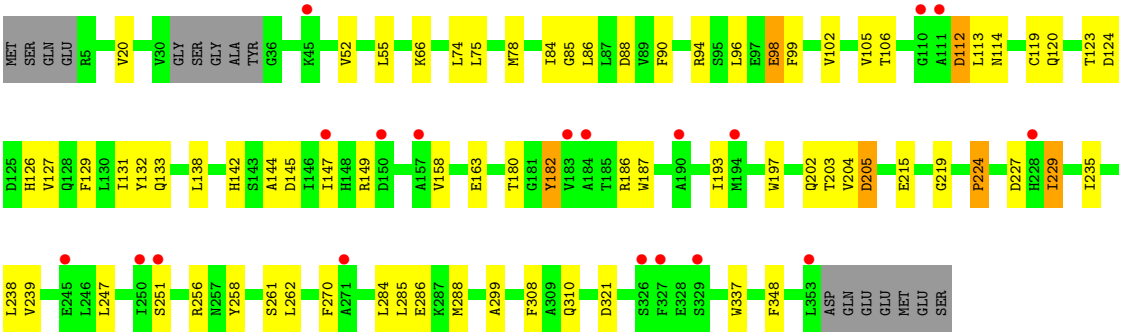
• Molecule 2: Mitogen-activated protein kinase 14

Chain F:



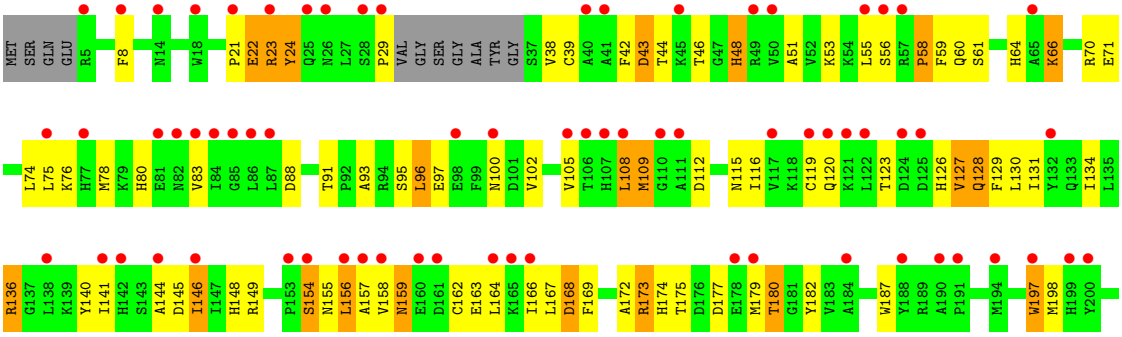
• Molecule 2: Mitogen-activated protein kinase 14

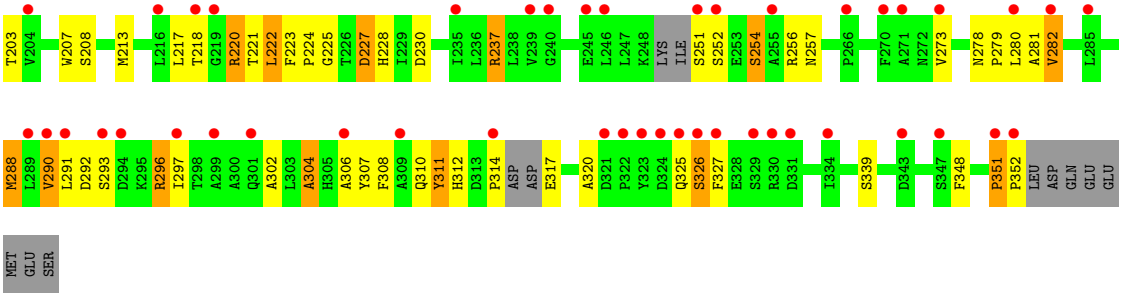
Chain G:



• Molecule 2: Mitogen-activated protein kinase 14

Chain H:




T203 V204 W207 S208 M213 L216 L217 T218 G219 R220 T221 L222 F223 P224 G225 T226 D227 H228 I229 D230 I235 L236 R237 L238 V239 G240 E245 L246 L247 K248 LYS ILE S251 S252 E253 S254 A255 R256 N257 P266 F270 A271 N272 V273 N278 P279 L280 A281 V282 L285
M288 L289 V290 L291 D292 S293 D294 K295 R296 I297 T298 A299 A300 Q301 A302 L303 A304 H305 A306 Y307 F308 A309 Q310 Y311 H312 D313 P314 ASP ASP E317 A320 D321 P322 Y323 D324 Q325 S326 F327 E328 S329 R330 D331 I334 S339 D343 S347 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	16424 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 , 40.2	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, TPO, MG, NI, 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(°)	Ideal(°)
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
1:C:347:GLU:OE1	1:C:350:ARG:NH2	2.26	0.69
2:F:136[B]:ARG:NH2	2:F:316:ASP:O	2.25	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:HH11	1:B:354:ARG:HG2	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:HH11	2:H:220:ARG:HG3	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:43:ASP:HB3	2:H:46:THR:HG22	1.87	0.55
2:H:325:GLN:O	2:H:327:PHE:N	2.40	0.55
1:B:22:PRO:HD2	1:B:57:ARG:O	2.05	0.55
1:A:279:ASP:OD1	1:A:279:ASP:N	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:OD1	2:H:227:ASP:N	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:HD12	2:H:131:ILE:H	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:OE2	2:H:97:GLU:N	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:CG	2:H:136:ARG:HH11	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:HH11	2:H:136:ARG:HG3	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:O	2:H:237:ARG:HD3	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:23:ARG:O	2:H:44:THR:N	2.46	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
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:HD2	1:A:156:LYS:N	2.27	0.48
1:C:207:HIS:CE1	1:C:241:ARG:HD2	2.48	0.48
2:H:95:SER:C	2:H:97:GLU:H	2.17	0.48
2:H:127:VAL:HG21	2:H:217:LEU:CD2	2.43	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:91:THR:HG22	2:H:93:ALA:N	2.28	0.48
2:H:115:ASN:OD1	2:H:116:ILE:N	2.47	0.48
1:C:14:GLN:HG3	2:F:197:TRP:CE2	2.49	0.48
1:C:154:ARG:O	1:C:158:LEU:HD23	2.14	0.48
1:C:234:ILE:O	1:C:242:ARG:NH2	2.43	0.47
1:C:390:VAL:CG2	2:H:123:THR:HA	2.43	0.47
1:D:149:GLN:O	1:D:153:GLU:HG3	2.14	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:HD23	2:G:285:LEU:HA	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:63:PHE:HB2	1:B:173:LEU:HB3	1.98	0.46
1:B:65:TYR:OH	1:B:363:ARG:HD3	2.15	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:16:SER:OG	1:B:18:THR:HG22	2.16	0.45
1:B:147:GLN:H	1:B:147:GLN:CD	2.20	0.45
1:C:167:MET:SD	1:C:167:MET:N	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:HG2	1:B:354:ARG:NH1	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:53:LYS:HZ1	4:E:401:AGS:PB	2.40	0.44
2:E:158:VAL:HA	2:E:163:GLU:O	2.18	0.44
2:H:78:MET:HB2	2:H:78:MET:HE2	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:HIS:HE2	2:H:136:ARG:HG2	1.83	0.44
2:H:156:LEU:HA	2:H:156:LEU:HD23	1.53	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:HD12	2:E:113:LEU:HA	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:HB3	1:C:335:LYS:HE2	1.75	0.43
2:E:147:ILE:HG12	2:E:149:ARG:CG	2.48	0.43
1:A:389:SER:HB3	2:F:121:LYS:HB3	2.00	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
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:HD23	1:B:174:LEU:HA	1.79	0.42
1:C:258:LEU:HD23	1:C:258:LEU:HA	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:70:ARG:O	2:F:74:LEU:HG	2.19	0.42
2:F:171:LEU:HD23	2:F:171:LEU:HA	1.80	0.42
2:G:66:LYS:HD3	2:G:337:TRP:CZ2	2.54	0.42
1:B:278:LEU:HD23	1:B:278:LEU:HA	1.87	0.42
2:E:43:ASP:OD2	2:E:46:THR:OG1	2.25	0.42
2:E:142:HIS:NE2	2:E:205:ASP:OD2	2.37	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:60:ASN:HB3	1:A:62:CYS:SG	2.59	0.42
1:A:285:LEU:HB3	1:A:363:ARG:HB3	2.00	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
1:A:384:ARG:N	2:F:237:ARG:NH2	2.68	0.42
2:F:175:THR:HG21	2:F:202:GLN:CG	2.49	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:85:GLY:O	2:G:106:THR:HG22	2.20	0.42
2:G:235:ILE:O	2:G:239:VAL: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:CD1	2:F:270:PHE:N	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:A:388:VAL:HG12	2:F:275:ILE:O	2.20	0.41
1:C:157:THR:O	1:C:161:GLU:HG3	2.19	0.41
2:E:138:LEU:HD12	2:E:138:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:SER:OG	2:H:96:LEU:N	2.53	0.41
2:H:281:ALA:O	2:H:282:VAL:C	2.56	0.41
1:A:167:MET:SD	1:A:242:ARG:HG2	2.60	0.41
1:B:15:PRO:HB3	2:E:228:HIS:ND1	2.35	0.41
1:B:17:TRP:CE3	1:B:17:TRP:HA	2.55	0.41
1:D:55:LYS:HE3	1:D:55:LYS:HB2	1.95	0.41
1:D:208:THR:CG2	1:D:238:GLU:HG3	2.47	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:24:TYR:HA	2:H:42:PHE:O	2.21	0.41
2:H:127:VAL:HG12	2:H:131:ILE:CD1	2.51	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:HD23	1:B:90:LEU:HA	1.86	0.41
1:C:282:THR:HA	1:C:365:PHE:O	2.21	0.41
2:F:5:ARG:HA	2:F:6:PRO:HD2	1.92	0.41
2:F:90:PHE:CE2	2:F:103:TYR:CG	3.08	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:C:387:PRO:O	2:H:218:THR:HG23	2.21	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:88:ASP:O	2:H:105:VAL:HG12	2.21	0.40
2:H:155:ASN:HD22	2:H:168:ASP:CG	2.25	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:86:LEU:HD23	2:G:86:LEU:HA	1.91	0.40
2:G:215:GLU:O	2:G:219:GLY:N	2.47	0.40
2:G:310:GLN:HG2	2:G:310:GLN:O	2.22	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%)	16	34
1	B	372/504 (74%)	342 (92%)	27 (7%)	3 (1%)	16	34
1	C	359/504 (71%)	336 (94%)	16 (4%)	7 (2%)	6	13
1	D	373/504 (74%)	355 (95%)	12 (3%)	6 (2%)	8	17
2	E	340/360 (94%)	320 (94%)	16 (5%)	4 (1%)	11	24
2	F	338/360 (94%)	323 (96%)	14 (4%)	1 (0%)	37	59
2	G	340/360 (94%)	311 (92%)	26 (8%)	3 (1%)	14	31
2	H	327/360 (91%)	274 (84%)	32 (10%)	21 (6%)	1	1
All	All	2821/3456 (82%)	2608 (92%)	165 (6%)	48 (2%)	7	16

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%)	17	36
1	B	300/421 (71%)	280 (93%)	20 (7%)	13	29
1	C	282/421 (67%)	267 (95%)	15 (5%)	19	40
1	D	294/421 (70%)	282 (96%)	12 (4%)	26	51
2	E	285/317 (90%)	273 (96%)	12 (4%)	25	50
2	F	287/317 (90%)	278 (97%)	9 (3%)	35	62
2	G	281/317 (89%)	275 (98%)	6 (2%)	48	73
2	H	189/317 (60%)	160 (85%)	29 (15%)	2	4
All	All	2213/2952 (75%)	2093 (95%)	120 (5%)	18	39

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	H	182	2	15,16,17	1.22	1 (6%)	19,22,24	1.14	2 (10%)
2	PTR	F	182	2	15,16,17	1.45	1 (6%)	19,22,24	0.86	1 (5%)
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	PTR	E	182	2	15,16,17	1.35	1 (6%)	19,22,24	0.65	0
2	TPO	E	180	2	8,10,11	1.66	2 (25%)	10,14,16	0.92	0
2	TPO	G	180	2	8,10,11	1.07	0	10,14,16	1.55	1 (10%)
2	TPO	F	180	2	8,10,11	1.10	0	10,14,16	1.57	3 (30%)

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

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	E	182	PTR	O-C-CA-CB
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	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 oligosaccharides 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	G	500	5	26,33,33	0.88	1 (3%)	26,52,52	0.90	1 (3%)
4	AGS	E	401	5	26,33,33	0.85	1 (3%)	26,52,52	0.88	2 (7%)
4	AGS	H	500	5	26,33,33	0.76	1 (3%)	26,52,52	0.93	2 (7%)
4	AGS	F	401	5	26,33,33	1.00	2 (7%)	26,52,52	0.96	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	G	500	5	-	5/17/38/38	0/3/3/3
4	AGS	E	401	5	-	3/17/38/38	0/3/3/3
4	AGS	H	500	5	-	5/17/38/38	0/3/3/3
4	AGS	F	401	5	-	8/17/38/38	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	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	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	PA-O3A-PB-O1B
4	G	500	AGS	PA-O3A-PB-O1B
4	F	401	AGS	C5'-O5'-PA-O3A
4	E	401	AGS	PB-O3A-PA-O2A
4	F	401	AGS	PB-O3A-PA-O1A
4	H	500	AGS	PB-O3A-PA-O2A
4	F	401	AGS	PG-O3B-PB-O2B
4	G	500	AGS	PG-O3B-PB-O2B
4	E	401	AGS	PA-O3A-PB-O2B
4	E	401	AGS	PB-O3A-PA-O1A
4	F	401	AGS	PA-O3A-PB-O2B
4	G	500	AGS	PB-O3A-PA-O2A
4	H	500	AGS	PA-O3A-PB-O1B
4	H	500	AGS	O4'-C4'-C5'-O5'

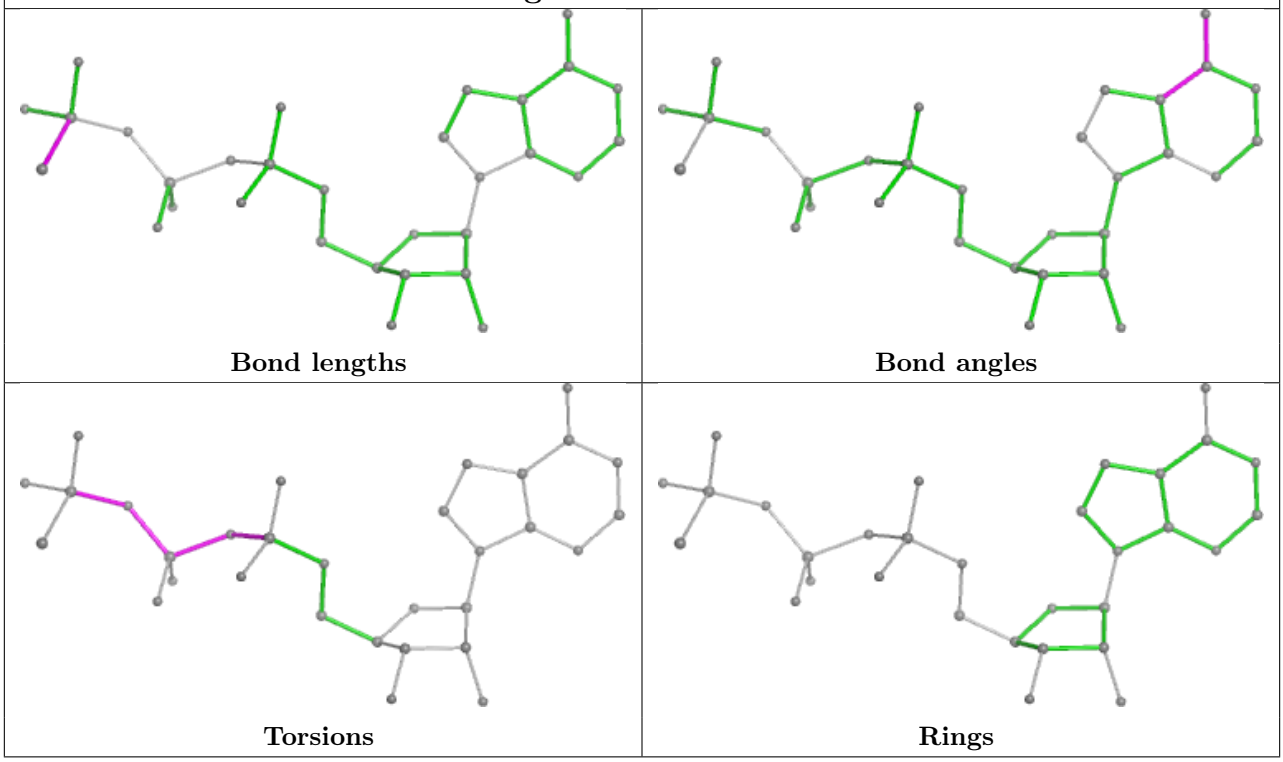
There are no ring outliers.

2 monomers are involved in 2 short contacts:

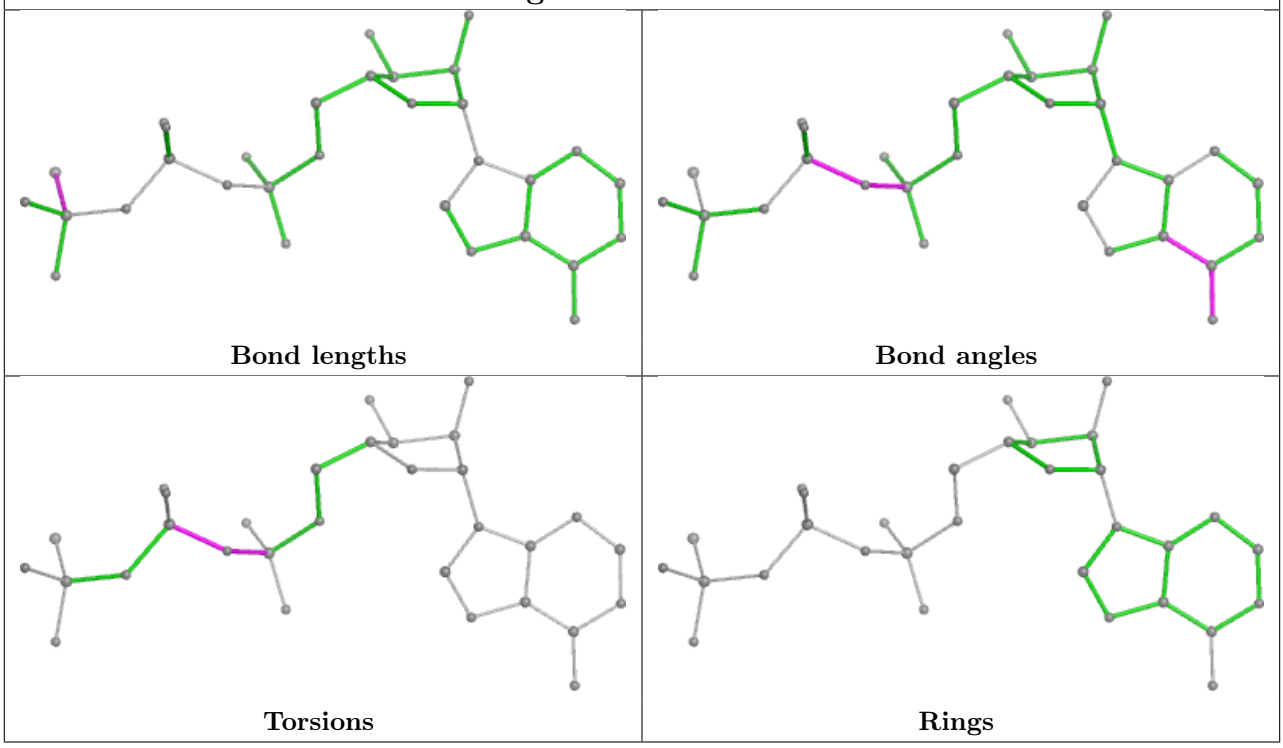
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	AGS	1	0
4	F	401	AGS	1	0

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 G 500



Ligand AGS E 401



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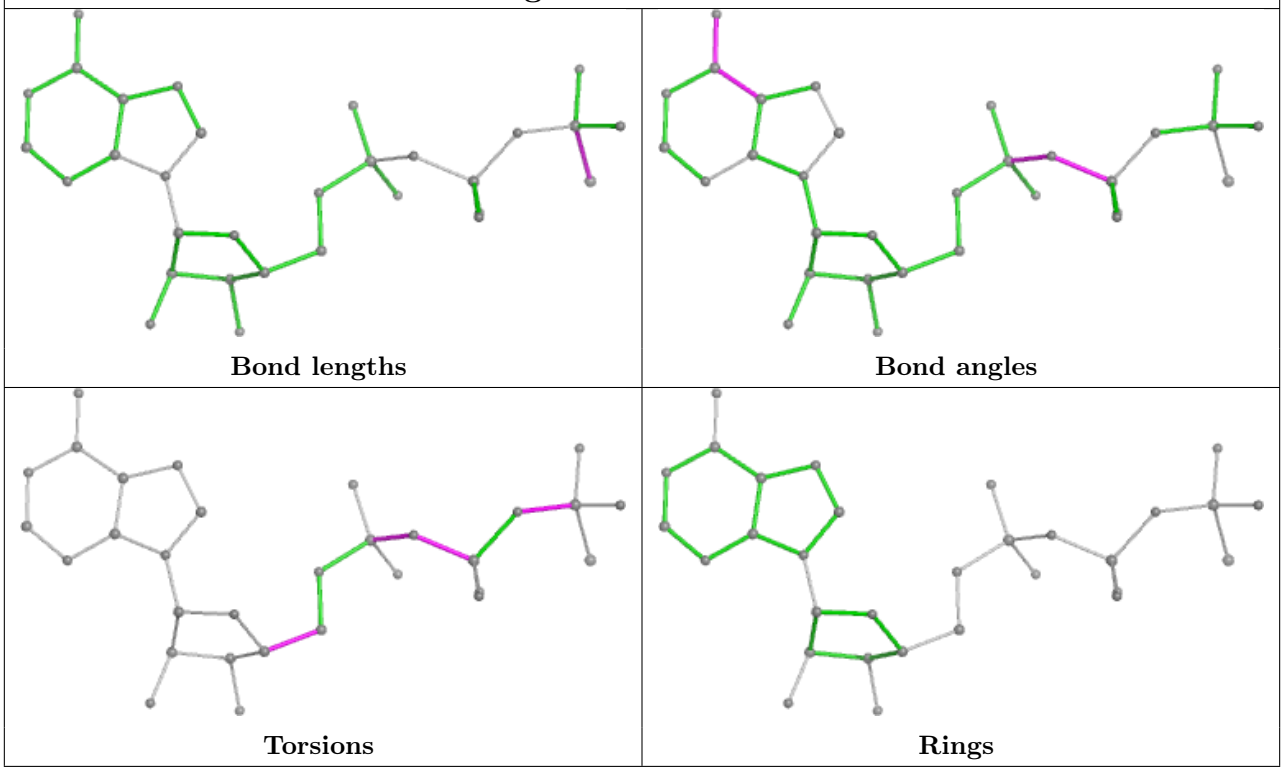

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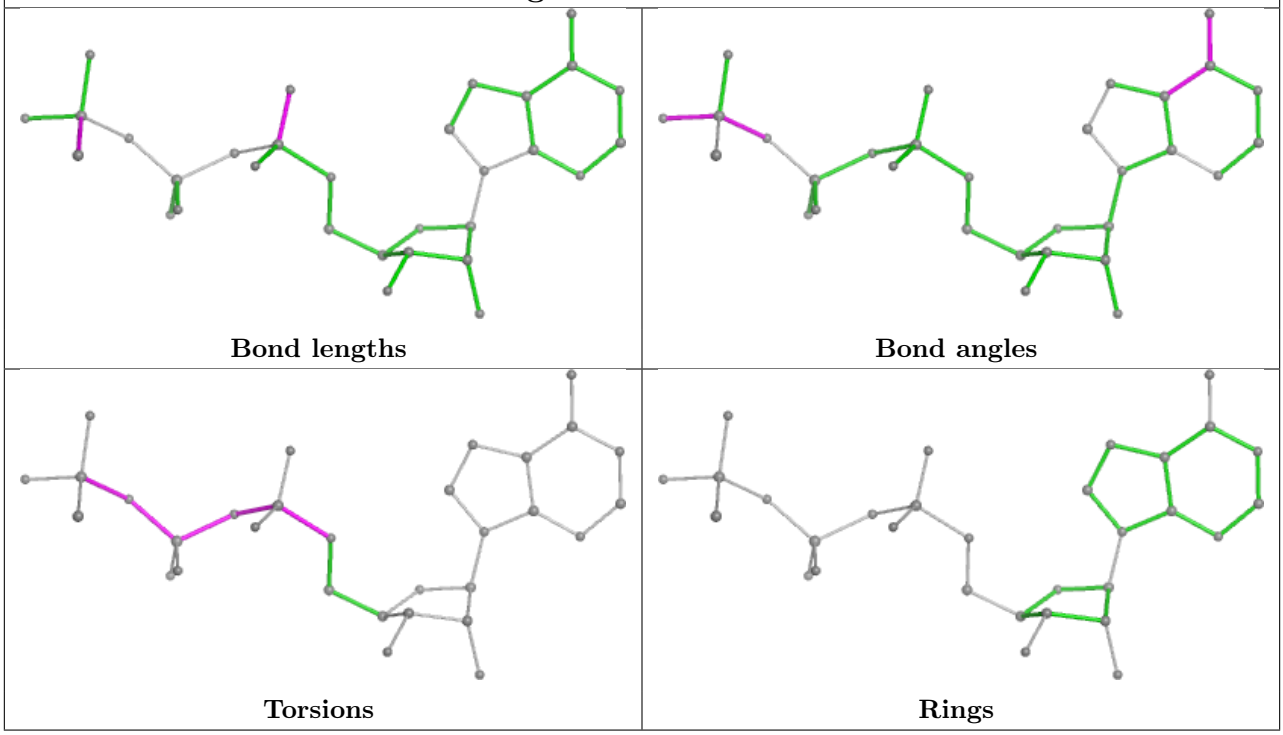

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	378/504 (75%)	0.28	12 (3%)	50	45	32, 50, 82, 116	0
1	B	378/504 (75%)	0.28	12 (3%)	50	45	33, 53, 91, 110	0
1	C	367/504 (72%)	0.46	26 (7%)	23	18	32, 54, 98, 139	0
1	D	379/504 (75%)	0.30	12 (3%)	50	45	33, 52, 83, 107	0
2	E	343/360 (95%)	0.33	8 (2%)	61	55	21, 55, 78, 96	1 (0%)
2	F	341/360 (94%)	0.20	4 (1%)	76	72	25, 51, 70, 98	1 (0%)
2	G	342/360 (95%)	0.55	19 (5%)	31	25	22, 62, 85, 101	2 (0%)
2	H	335/360 (93%)	1.71	114 (34%)	1	1	69, 97, 119, 132	0
All	All	2863/3456 (82%)	0.50	207 (7%)	23	18	21, 57, 102, 139	4 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	PRO	7.0
1	C	387	PRO	4.9
2	H	200	TYR	4.8
1	D	62	CYS	4.6
2	H	166	ILE	4.6
2	H	245	GLU	4.6
2	H	330	ARG	4.4
2	G	250	ILE	4.3
1	C	408	VAL	4.2
2	H	49	ARG	4.2
1	B	39	ALA	4.1
2	H	218	THR	4.1
1	C	386	TYR	4.1
1	A	16	SER	4.0
2	H	329	SER	4.0
2	H	157	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	388	VAL	4.0
2	H	199	HIS	3.9
2	H	119	CYS	3.9
2	H	327	PHE	3.9
1	B	61	ASN	3.8
1	A	257	LEU	3.7
2	H	219	GLY	3.6
2	H	107	HIS	3.5
2	H	309	ALA	3.5
2	H	84	ILE	3.5
2	H	289	LEU	3.5
2	H	100	ASN	3.5
1	D	13	GLN	3.5
2	H	125	ASP	3.4
2	H	294	ASP	3.4
1	D	59	GLU	3.4
2	H	273	VAL	3.4
2	H	270	PHE	3.4
1	A	386	TYR	3.3
1	D	15	PRO	3.3
2	H	325	GLN	3.3
2	H	26	ASN	3.3
2	G	329	SER	3.3
2	H	29	PRO	3.3
2	E	250	ILE	3.3
1	B	138	GLY	3.3
1	D	395	ALA	3.2
2	F	353	LEU	3.2
2	H	240	GLY	3.2
1	C	410	PRO	3.2
2	H	352	PRO	3.2
2	H	146	ILE	3.2
2	H	50	VAL	3.2
2	H	41	ALA	3.2
2	H	188	TYR	3.2
2	H	190	ALA	3.1
2	H	75	LEU	3.1
2	H	56	SER	3.1
2	G	327	PHE	3.1
2	E	353	LEU	3.1
1	D	255	ILE	3.0
2	H	331	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	G	111	ALA	3.0
2	G	157	ALA	3.0
2	H	299	ALA	3.0
2	H	301	GLN	3.0
2	H	110	GLY	3.0
1	B	404	THR	3.0
2	H	334	ILE	3.0
1	D	385	VAL	3.0
2	H	321	ASP	2.9
1	C	407	LEU	2.9
1	B	11	SER	2.9
2	H	142	HIS	2.9
2	H	87	LEU	2.9
1	C	42	LYS	2.9
1	B	388	VAL	2.9
2	G	183	VAL	2.9
2	H	322	PRO	2.9
2	H	179	MET	2.8
1	C	137	GLU	2.8
2	F	14	ASN	2.8
2	H	120	GLN	2.8
1	A	19	ASP	2.8
2	H	285	LEU	2.8
2	H	194	MET	2.8
2	H	83	VAL	2.7
2	H	117	VAL	2.7
1	C	157	THR	2.7
2	G	184	ALA	2.7
2	H	106	THR	2.7
2	H	197	TRP	2.7
2	H	77	HIS	2.7
2	H	351	PRO	2.7
1	B	275	ALA	2.6
2	H	40	ALA	2.6
2	H	141	ILE	2.6
1	C	41	GLY	2.6
2	H	252	SER	2.6
1	A	231	VAL	2.6
2	H	314	PRO	2.6
2	F	94	ARG	2.6
2	H	55	LEU	2.6
1	C	13	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	2.6
1	C	406	SER	2.5
2	G	251	SER	2.5
2	H	326	SER	2.5
2	H	323	TYR	2.5
2	G	271	ALA	2.5
2	H	111	ALA	2.5
2	H	347	SER	2.5
2	H	156	LEU	2.5
2	H	25	GLN	2.5
1	C	409	MET	2.5
1	D	256	ASP	2.5
2	H	271	ALA	2.5
2	H	343	ASP	2.5
2	H	191	PRO	2.4
2	H	204	VAL	2.4
2	E	14	ASN	2.4
2	H	290	VAL	2.4
2	G	147	ILE	2.4
2	H	161	ASP	2.4
2	H	178	GLU	2.4
2	H	291	LEU	2.4
2	H	266	PRO	2.4
1	C	230	GLN	2.4
2	H	158	VAL	2.4
2	H	85	GLY	2.4
2	H	98	GLU	2.4
1	D	410	PRO	2.4
2	G	326	SER	2.4
2	H	235	ILE	2.4
1	B	60	ASN	2.4
2	H	81	GLU	2.3
2	H	280	LEU	2.3
2	H	45	LYS	2.3
2	G	190	ALA	2.3
2	H	132	TYR	2.3
1	C	40	ASP	2.3
1	C	195	VAL	2.3
2	F	329	SER	2.3
1	C	43	GLY	2.3
1	C	235	CYS	2.3
1	B	139	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	282	VAL	2.3
2	H	28	SER	2.3
2	H	5	ARG	2.3
2	H	57	ARG	2.3
2	G	110	GLY	2.3
1	B	410	PRO	2.2
1	A	390	VAL	2.2
2	H	184	ALA	2.2
2	H	306	ALA	2.2
2	H	121	LYS	2.2
2	E	13	LEU	2.2
1	C	321	THR	2.2
2	H	14	ASN	2.2
2	H	82	ASN	2.2
1	B	257	LEU	2.2
1	C	144	LEU	2.2
2	G	353	LEU	2.2
2	H	216	LEU	2.2
2	H	293	SER	2.2
1	C	320	GLN	2.2
2	E	17	ILE	2.2
2	G	45	LYS	2.2
2	H	165	LYS	2.2
1	B	223	LEU	2.2
2	H	108	LEU	2.2
2	H	122	LEU	2.2
2	H	18	TRP	2.2
1	C	302	PRO	2.2
1	C	392	TYR	2.2
2	G	150	ASP	2.2
2	H	8	PHE	2.2
2	H	239	VAL	2.2
2	H	86	LEU	2.2
2	G	228	HIS	2.1
1	A	20	ASP	2.1
2	H	324	ASP	2.1
2	H	105	VAL	2.1
2	G	245	GLU	2.1
2	G	194	MET	2.1
2	H	124	ASP	2.1
2	H	297	ILE	2.1
2	H	138	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	246	LEU	2.1
1	C	275	ALA	2.1
2	E	255	ALA	2.1
2	H	65	ALA	2.1
2	H	153	PRO	2.1
1	A	233	ILE	2.1
1	D	20	ASP	2.1
2	H	144	ALA	2.1
2	H	160	GLU	2.1
1	D	404	THR	2.1
1	A	228	ILE	2.1
2	H	164	LEU	2.1
1	C	39	ALA	2.1
2	H	255	ALA	2.1
2	H	21	PRO	2.0
2	E	16	THR	2.0
2	E	254	SER	2.0
2	H	154	SER	2.0
2	H	251	SER	2.0
1	C	390	VAL	2.0
1	D	373	SER	2.0
2	H	23	ARG	2.0
1	A	395	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PTR	F	182	16/17	0.87	0.12	42,51,66,69	0
2	PTR	G	182	16/17	0.87	0.12	52,65,80,84	0
2	PTR	H	182	16/17	0.87	0.17	78,82,93,94	0
2	TPO	H	180	11/12	0.91	0.14	69,85,93,95	0
2	PTR	E	182	16/17	0.93	0.10	51,59,71,73	0
2	TPO	F	180	11/12	0.94	0.08	23,40,42,46	0
2	TPO	G	180	11/12	0.96	0.07	37,46,49,51	0
2	TPO	E	180	11/12	0.98	0.06	24,39,44,51	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

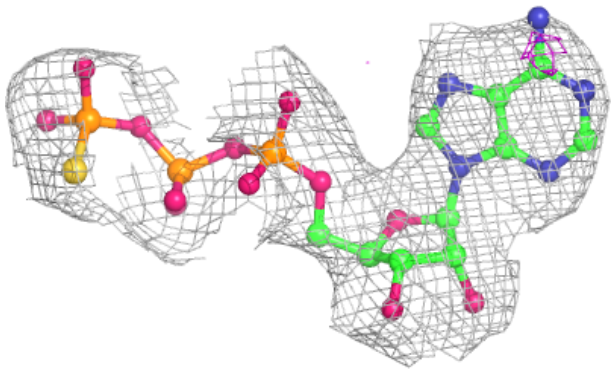
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

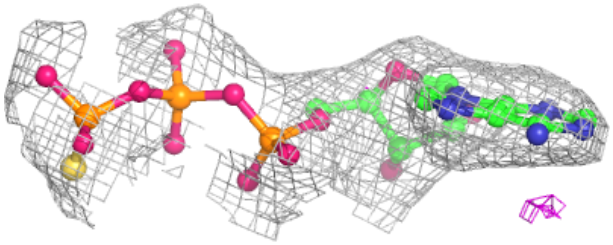
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	G	502	1/1	0.82	0.11	68,68,68,68	0
5	MG	H	502	1/1	0.88	0.13	82,82,82,82	0
4	AGS	H	500	31/31	0.90	0.10	75,90,102,114	0
5	MG	E	402	1/1	0.91	0.15	45,45,45,45	0
4	AGS	G	500	31/31	0.91	0.10	38,55,67,79	0
3	NI	A	601	1/1	0.91	0.13	84,84,84,84	0
5	MG	H	501	1/1	0.92	0.09	90,90,90,90	0
3	NI	E	403	1/1	0.92	0.08	87,87,87,87	0
5	MG	G	501	1/1	0.93	0.09	49,49,49,49	0
3	NI	C	601	1/1	0.94	0.08	97,97,97,97	0
3	NI	D	601	1/1	0.94	0.09	98,98,98,98	0
4	AGS	F	401	31/31	0.95	0.08	32,45,66,87	0
4	AGS	E	401	31/31	0.95	0.08	26,44,64,77	0
3	NI	F	403	1/1	0.96	0.06	97,97,97,97	0
3	NI	B	601	1/1	0.97	0.07	86,86,86,86	1
5	MG	F	402	1/1	0.97	0.08	45,45,45,45	0

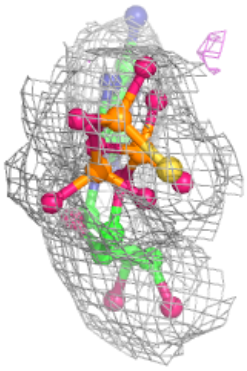
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

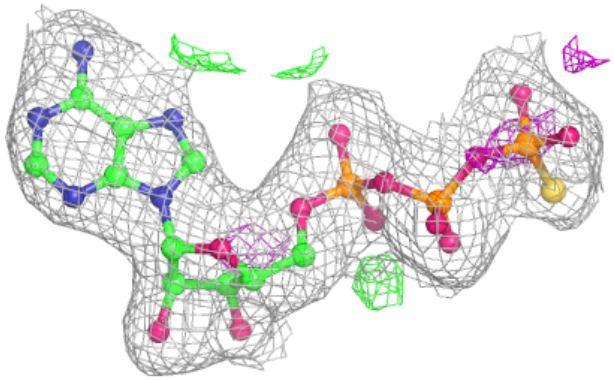


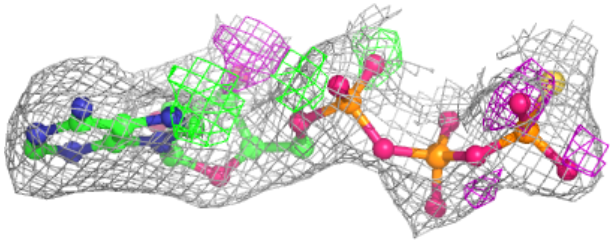


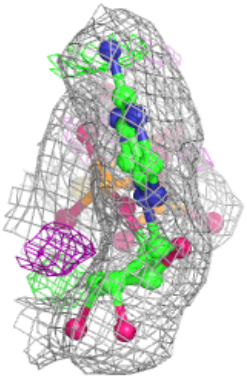


Electron density around AGS G 500:

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

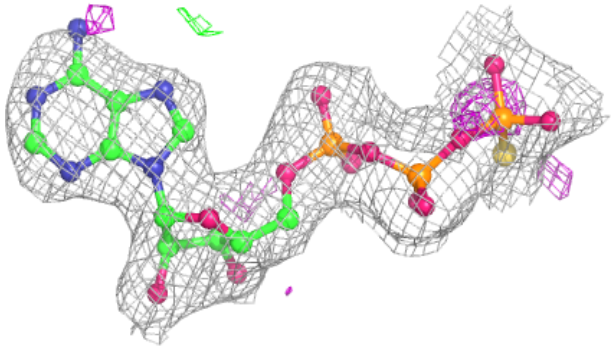


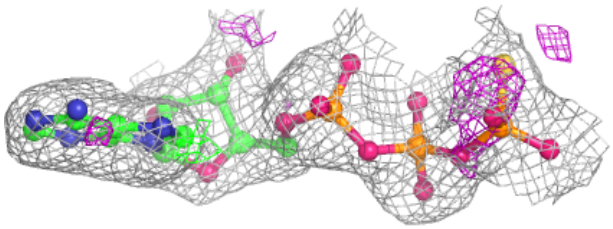


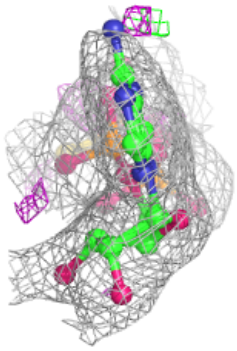


Electron density around AGS F 401:

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

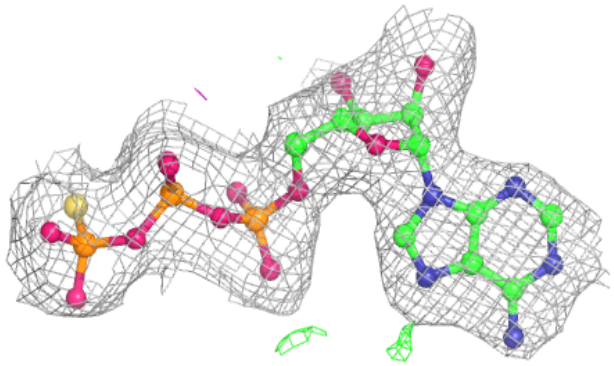


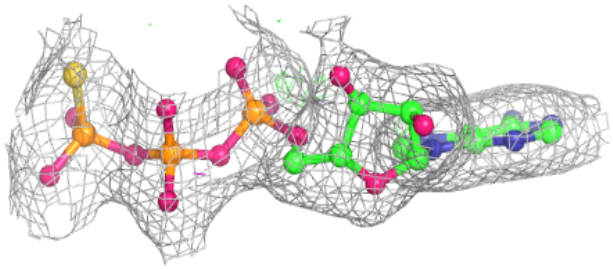


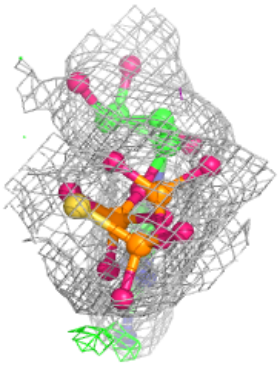


Electron density around AGS E 401:

$2mF_o$-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 (i)

There are no such residues in this entry.