Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:59 AM BST

PDB ID	:	6TCA
Title	:	Phosphorylated p38 and MAPKAPK2 complex with inhibitor
Authors	:	Sok, P.; Remenyi, A.
Deposited on	:	2019-11-05
Resolution	:	3.70 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:

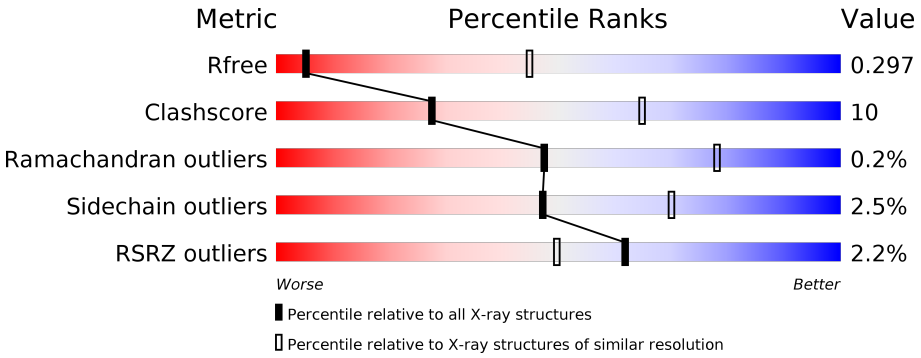
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	371	74% 18% 7%
1	C	371	% 73% 15% 12%
1	E	371	2% 72% 16% 12%
1	G	371	8% 75% 15% 9%
2	B	364	69% 25% 5%
2	D	364	2% 71% 23% 5%

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Mol	Chain	Length	Quality of chain
2	F	364	2% 66% 26% 5%
2	H	364	69% 24% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	39G	H	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21798 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2685	1720	468	479	18			
1	C	326	Total	C	N	O	S	0	0	0
			2623	1668	454	483	18			
1	E	327	Total	C	N	O	S	0	0	0
			2640	1686	452	484	18			
1	G	337	Total	C	N	O	S	0	0	0
			2671	1701	460	492	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	expression tag	UNP P49137
A	40	SER	-	expression tag	UNP P49137
A	401	GLY	-	expression tag	UNP P49137
A	402	SER	-	expression tag	UNP P49137
A	403	ARG	-	expression tag	UNP P49137
A	404	HIS	-	expression tag	UNP P49137
A	405	HIS	-	expression tag	UNP P49137
A	406	HIS	-	expression tag	UNP P49137
A	407	HIS	-	expression tag	UNP P49137
A	408	HIS	-	expression tag	UNP P49137
A	409	HIS	-	expression tag	UNP P49137
C	39	GLY	-	expression tag	UNP P49137
C	40	SER	-	expression tag	UNP P49137
C	401	GLY	-	expression tag	UNP P49137
C	402	SER	-	expression tag	UNP P49137
C	403	ARG	-	expression tag	UNP P49137
C	404	HIS	-	expression tag	UNP P49137
C	405	HIS	-	expression tag	UNP P49137
C	406	HIS	-	expression tag	UNP P49137
C	407	HIS	-	expression tag	UNP P49137
C	408	HIS	-	expression tag	UNP P49137

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Chain	Residue	Modelled	Actual	Comment	Reference
C	409	HIS	-	expression tag	UNP P49137
E	39	GLY	-	expression tag	UNP P49137
E	40	SER	-	expression tag	UNP P49137
E	401	GLY	-	expression tag	UNP P49137
E	402	SER	-	expression tag	UNP P49137
E	403	ARG	-	expression tag	UNP P49137
E	404	HIS	-	expression tag	UNP P49137
E	405	HIS	-	expression tag	UNP P49137
E	406	HIS	-	expression tag	UNP P49137
E	407	HIS	-	expression tag	UNP P49137
E	408	HIS	-	expression tag	UNP P49137
E	409	HIS	-	expression tag	UNP P49137
G	39	GLY	-	expression tag	UNP P49137
G	40	SER	-	expression tag	UNP P49137
G	401	GLY	-	expression tag	UNP P49137
G	402	SER	-	expression tag	UNP P49137
G	403	ARG	-	expression tag	UNP P49137
G	404	HIS	-	expression tag	UNP P49137
G	405	HIS	-	expression tag	UNP P49137
G	406	HIS	-	expression tag	UNP P49137
G	407	HIS	-	expression tag	UNP P49137
G	408	HIS	-	expression tag	UNP P49137
G	409	HIS	-	expression tag	UNP P49137

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	P	S	0	1	0
			2770	1777	470	508	2	13			
2	D	346	Total	C	N	O	P	S	0	0	0
			2760	1767	469	510	2	12			
2	F	344	Total	C	N	O	P	S	0	0	0
			2744	1755	466	511	2	10			
2	H	346	Total	C	N	O	P	S	0	0	0
			2785	1783	478	510	2	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q16539
B	-2	SER	-	expression tag	UNP Q16539
B	-1	ALA	-	expression tag	UNP Q16539

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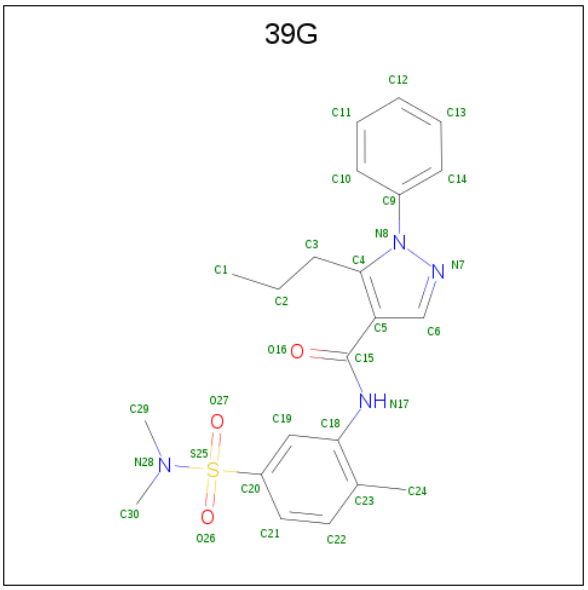
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q16539
D	-3	GLY	-	expression tag	UNP Q16539
D	-2	SER	-	expression tag	UNP Q16539
D	-1	ALA	-	expression tag	UNP Q16539
D	0	SER	-	expression tag	UNP Q16539
F	-3	GLY	-	expression tag	UNP Q16539
F	-2	SER	-	expression tag	UNP Q16539
F	-1	ALA	-	expression tag	UNP Q16539
F	0	SER	-	expression tag	UNP Q16539
H	-3	GLY	-	expression tag	UNP Q16539
H	-2	SER	-	expression tag	UNP Q16539
H	-1	ALA	-	expression tag	UNP Q16539
H	0	SER	-	expression tag	UNP Q16539

- Molecule 3 is N-[5-(dimethylsulfamoyl)-2-methylphenyl]-1-phenyl-5-propyl-1H-pyrazole-4-carboxamide (three-letter code: 39G) (formula: $C_{22}H_{26}N_4O_3S$) (labeled as "Ligand of Interest" by author).



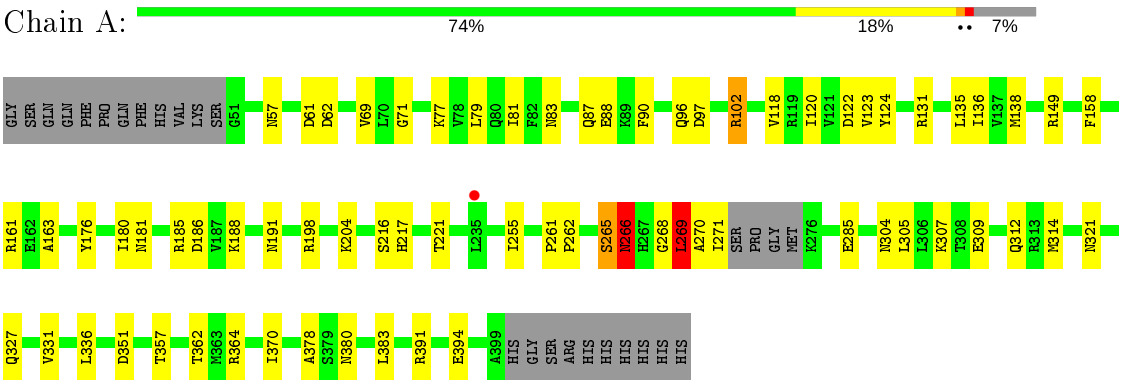
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			30	22	4	3	1		
3	D	1	Total	C	N	O	S	0	0
			30	22	4	3	1		
3	F	1	Total	C	N	O	S	0	0
			30	22	4	3	1		
3	H	1	Total	C	N	O	S	0	0
			30	22	4	3	1		

3 Residue-property plots (i)

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

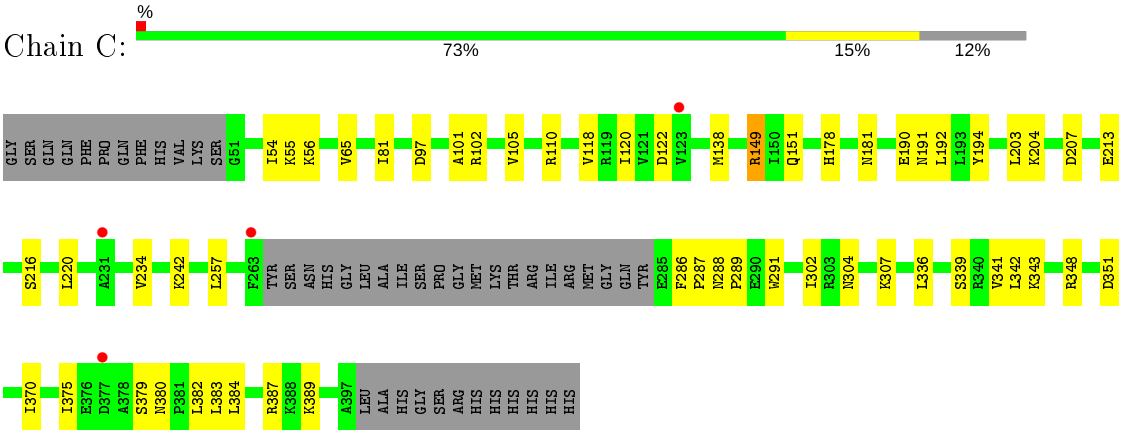
- Molecule 1: MAP kinase-activated protein kinase 2

Chain A:



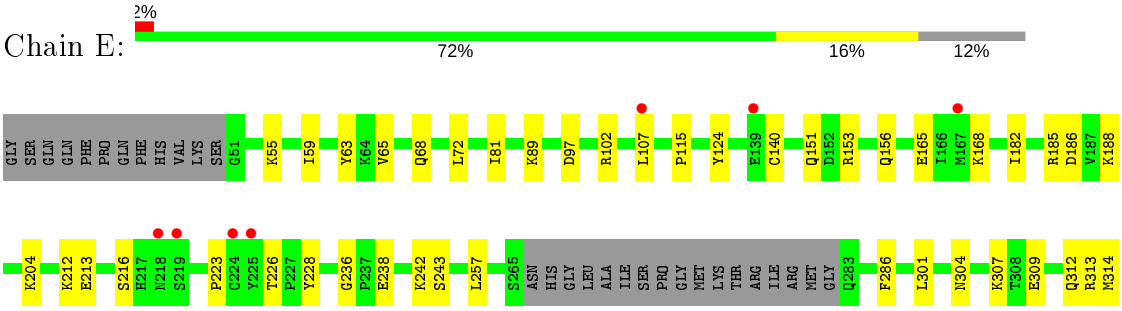
- Molecule 1: MAP kinase-activated protein kinase 2

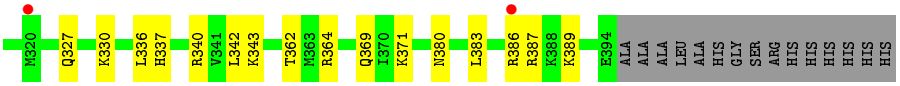
Chain C:



- Molecule 1: MAP kinase-activated protein kinase 2

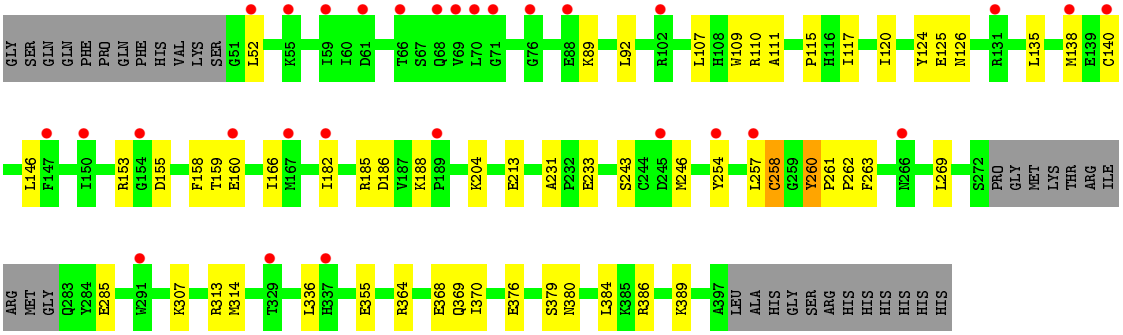
Chain E:





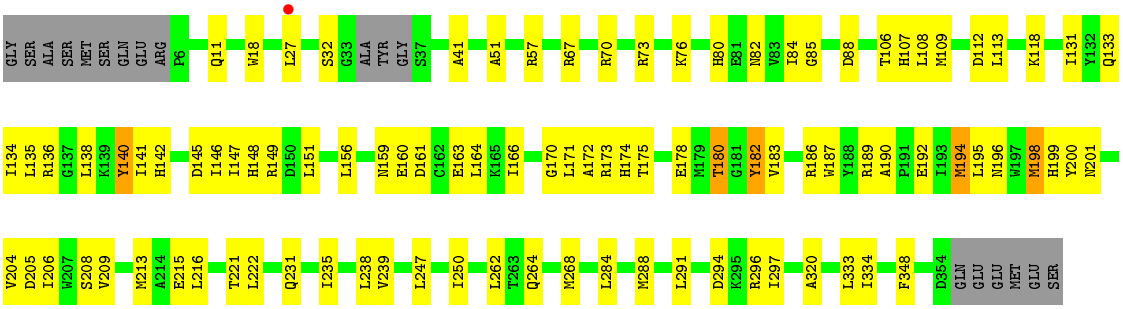
- Molecule 1: MAP kinase-activated protein kinase 2

Chain G:



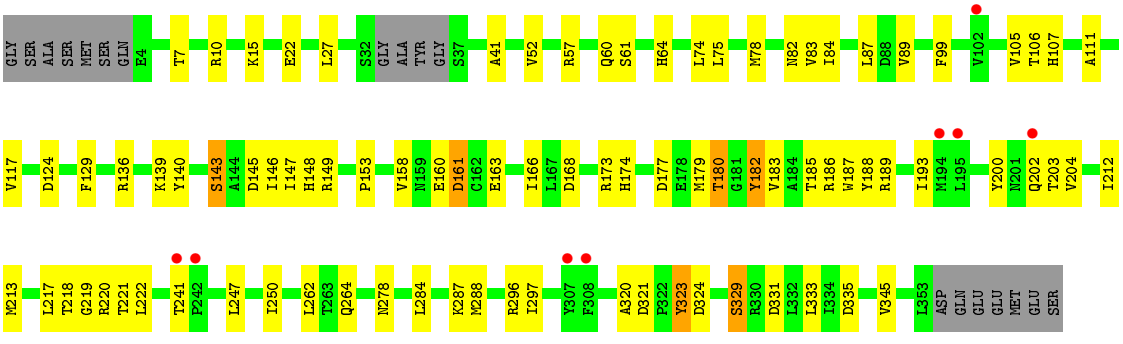
- Molecule 2: Mitogen-activated protein kinase 14

Chain B:



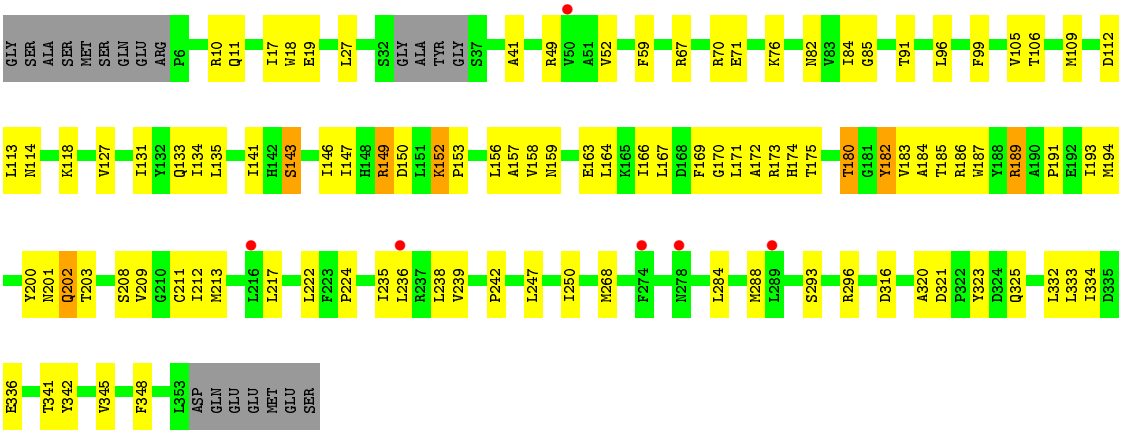
- Molecule 2: Mitogen-activated protein kinase 14

Chain D:



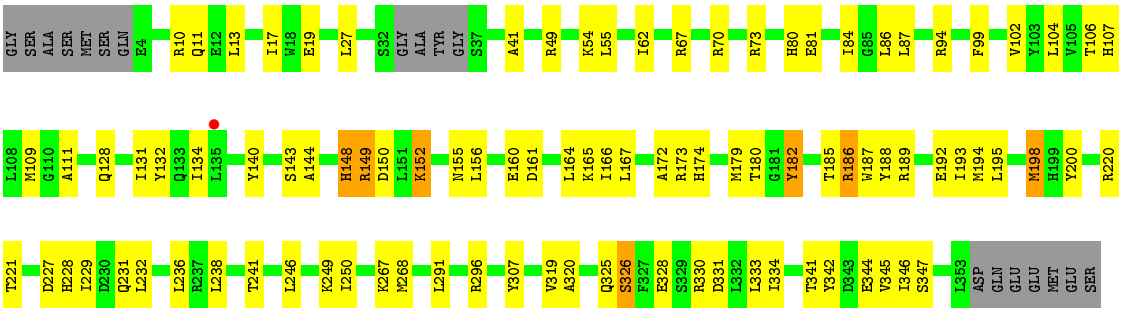
- Molecule 2: Mitogen-activated protein kinase 14

Chain F:



- Molecule 2: Mitogen-activated protein kinase 14

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	279.35Å 69.29Å 221.11Å 90.00° 123.85° 90.00°	Depositor
Resolution (Å)	69.56 – 3.70 69.56 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (69.56-3.70) 98.9 (69.56-3.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.251 , 0.297 0.251 , 0.297	Depositor DCC
R_{free} test set	1995 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å^2)	118.4	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 81.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	21798	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 39G, 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	0.27	0/2738	0.49	2/3705 (0.1%)
1	C	0.23	0/2675	0.41	0/3613
1	E	0.23	0/2695	0.41	0/3640
1	G	0.25	0/2725	0.42	0/3686
2	B	0.24	0/2803	0.45	0/3803
2	D	0.26	0/2792	0.46	0/3790
2	F	0.26	0/2776	0.46	0/3772
2	H	0.25	0/2819	0.45	0/3825
All	All	0.25	0/22023	0.44	2/29834 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	LEU	CA-CB-CG	10.31	139.01	115.30
1	A	269	LEU	CB-CG-CD2	7.55	123.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2685	0	2705	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2623	0	2660	34	0
1	E	2640	0	2669	34	0
1	G	2671	0	2670	38	0
2	B	2770	0	2749	88	0
2	D	2760	0	2725	62	0
2	F	2744	0	2705	81	0
2	H	2785	0	2770	72	0
3	B	30	0	26	0	0
3	D	30	0	26	1	0
3	F	30	0	26	1	0
3	H	30	0	26	2	0
All	All	21798	0	21757	434	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (434) 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:D:173:ARG:HG2	2:D:174:HIS:H	1.39	0.87
2:F:147:ILE:CG1	2:F:175:THR:HG22	2.11	0.81
2:F:147:ILE:HD11	2:F:175:THR:HG22	1.63	0.81
2:H:143:SER:HB2	2:H:319:VAL:HG13	1.64	0.78
1:A:271:ILE:HD11	1:A:285:GLU:HG2	1.66	0.78
2:D:173:ARG:HG2	2:D:174:HIS:N	1.98	0.77
2:H:144:ALA:HB2	2:H:320:ALA:HB3	1.66	0.77
2:B:195:LEU:HD12	2:B:250:ILE:HD12	1.65	0.76
2:F:113:LEU:HD12	2:F:156:LEU:HD12	1.68	0.75
2:H:81:GLU:O	2:H:165:LYS:NZ	2.20	0.74
1:C:54:ILE:O	1:C:54:ILE:HD12	1.88	0.73
2:B:138:LEU:HD23	2:B:141:ILE:HD11	1.71	0.72
1:G:153:ARG:HG3	1:G:155:ASP:H	1.54	0.72
2:F:201:ASN:HD21	2:F:293:SER:HB2	1.55	0.72
1:E:337:HIS:HE1	1:E:340:ARG:HE	1.37	0.72
2:F:147:ILE:CD1	2:F:175:THR:HG22	2.20	0.71
1:A:185:ARG:O	1:A:364:ARG:NH1	2.25	0.70
2:H:333:LEU:HD23	2:H:334:ILE:H	1.57	0.68
2:H:70:ARG:NH1	2:H:172:ALA:O	2.26	0.68
2:H:333:LEU:HD23	2:H:334:ILE:HG12	1.76	0.68
2:D:147:ILE:HG23	2:D:149:ARG:HG2	1.76	0.67
2:B:178:GLU:HA	2:B:198:MET:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASN:HA	1:C:242:LYS:HZ1	1.59	0.67
2:B:70:ARG:HH12	2:B:172:ALA:H	1.42	0.66
2:F:175:THR:HG21	2:F:202:GLN:HG3	1.76	0.66
2:B:135:LEU:HD23	2:B:138:LEU:HD12	1.77	0.66
2:B:186:ARG:HG3	2:B:187:TRP:HD1	1.60	0.66
1:C:341:VAL:O	1:C:348:ARG:NH2	2.28	0.66
2:F:187:TRP:CD1	2:F:224:PRO:HA	2.31	0.66
2:H:143:SER:CB	2:H:319:VAL:HG13	2.24	0.65
1:A:97:ASP:OD2	1:A:102:ARG:NH2	2.29	0.65
2:B:84:ILE:HG13	2:B:106:THR:HG21	1.78	0.65
1:A:364:ARG:NH2	2:B:32:SER:OG	2.29	0.65
1:E:223:PRO:HG2	1:E:226:THR:HG22	1.80	0.64
2:B:27:LEU:HD23	2:B:41:ALA:HB2	1.78	0.64
2:F:70:ARG:HH12	2:F:171:LEU:HA	1.63	0.64
2:B:133:GLN:HB2	2:B:164:LEU:HD21	1.81	0.63
2:D:147:ILE:HD11	2:D:202:GLN:HA	1.81	0.63
1:A:391:ARG:NH1	2:H:331:ASP:OD2	2.31	0.63
2:F:183:VAL:O	2:F:189:ARG:NH1	2.29	0.63
2:F:174:HIS:NE2	2:F:325:GLN:HG3	2.14	0.63
2:D:200:TYR:HB3	2:D:204:VAL:HG21	1.81	0.62
2:B:173:ARG:NH2	2:B:180:TPO:O1P	2.33	0.62
1:E:362:THR:O	2:F:118:LYS:NZ	2.32	0.62
1:G:386:ARG:NH1	2:H:132:TYR:OH	2.32	0.62
2:F:141:ILE:HG23	2:F:146:ILE:HG23	1.81	0.62
2:B:186:ARG:HG3	2:B:187:TRP:CD1	2.35	0.62
2:F:158:VAL:HG23	2:F:164:LEU:HD12	1.79	0.62
1:G:115:PRO:O	1:G:204:LYS:NZ	2.33	0.62
1:A:262:PRO:HB3	1:A:271:ILE:HA	1.81	0.61
2:D:241:THR:HG21	2:D:264:GLN:HA	1.83	0.61
1:A:370:ILE:HG12	2:B:160:GLU:HG3	1.83	0.61
2:B:159:ASN:OD1	2:B:163:GLU:N	2.33	0.61
1:E:115:PRO:O	1:E:204:LYS:NZ	2.34	0.60
2:B:138:LEU:HD22	2:B:142:HIS:HE1	1.64	0.60
2:D:218:THR:HG22	2:D:220:ARG:H	1.66	0.60
1:E:151:GLN:NE2	1:E:342:LEU:O	2.35	0.60
1:A:270:ALA:HB1	2:B:186:ARG:NH2	2.17	0.60
1:E:186:ASP:OD1	1:E:188:LYS:NZ	2.32	0.60
2:H:17:ILE:O	2:H:54:LYS:NZ	2.34	0.60
2:F:149:ARG:HH21	2:F:183:VAL:HG11	1.65	0.60
1:G:111:ALA:HB1	1:G:117:ILE:HD13	1.83	0.60
1:A:265:SER:OG	1:A:266:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ARG:NH1	2:D:180:TPO:O1P	2.33	0.60
2:F:203:THR:HB	2:F:296:ARG:HD2	1.83	0.60
2:B:182:PTR:P	2:B:186:ARG:HH21	2.24	0.59
1:E:243:SER:HB2	1:E:313:ARG:HH11	1.67	0.59
2:H:73:ARG:NH1	2:H:326:SER:OG	2.35	0.59
1:C:291:TRP:HH2	1:C:302:ILE:HD12	1.66	0.59
2:B:149:ARG:NH1	2:B:180:TPO:O2P	2.33	0.59
2:F:84:ILE:HD13	2:F:167:LEU:HB3	1.83	0.59
2:F:70:ARG:NH2	2:F:170:GLY:O	2.36	0.59
2:H:189:ARG:HG3	2:H:193:ILE:HD11	1.85	0.59
2:H:152:LYS:NZ	2:H:185:THR:OG1	2.30	0.59
2:B:80:HIS:HB2	2:B:140:TYR:CD2	2.38	0.59
1:G:120:ILE:HG12	1:G:138:MET:HG2	1.84	0.58
1:G:92:LEU:HD11	1:G:135:LEU:HB3	1.85	0.58
2:H:189:ARG:HH11	2:H:193:ILE:HD11	1.68	0.58
1:A:120:ILE:HD12	1:A:138:MET:HG2	1.85	0.58
1:G:269:LEU:HD13	2:H:194:MET:HG3	1.86	0.58
2:F:131:ILE:HD13	2:F:134:ILE:HD12	1.86	0.58
2:B:134:ILE:O	2:B:138:LEU:N	2.36	0.58
2:D:149:ARG:NH2	2:D:180:TPO:O1P	2.37	0.58
2:H:70:ARG:HH12	2:H:172:ALA:H	1.51	0.57
2:B:51:ALA:HB2	2:B:108:LEU:HD12	1.85	0.57
2:D:173:ARG:HD2	2:D:179:MET:HG3	1.87	0.57
2:F:184:ALA:O	2:F:189:ARG:HD3	2.04	0.57
1:E:65:VAL:HA	1:E:81:ILE:HG22	1.86	0.57
2:D:148:HIS:NE2	2:D:168:ASP:O	2.30	0.57
1:G:261:PRO:HB2	1:G:263:PHE:CE2	2.40	0.57
2:F:166:ILE:HG22	2:F:167:LEU:H	1.70	0.57
2:H:149:ARG:NH2	2:H:200:TYR:OH	2.38	0.57
2:F:143:SER:OG	2:F:320:ALA:N	2.39	0.56
1:G:243:SER:HB2	1:G:313:ARG:HH11	1.69	0.56
2:D:78:MET:HE2	2:D:83:VAL:HG11	1.87	0.56
1:G:380:ASN:O	1:G:384:LEU:N	2.29	0.56
2:B:182:PTR:O1P	2:B:186:ARG:NE	2.36	0.56
1:C:192:LEU:HB3	1:C:203:LEU:HD11	1.87	0.56
2:F:114:ASN:HB2	2:F:153:PRO:HB2	1.86	0.56
1:C:370:ILE:HD13	2:D:160:GLU:HA	1.88	0.56
2:D:57:ARG:HB3	2:D:60:GLN:HG3	1.87	0.56
2:D:61:SER:H	2:D:64:HIS:HB2	1.69	0.56
2:F:187:TRP:HD1	2:F:224:PRO:HA	1.69	0.56
1:A:378:ALA:HB1	2:B:161:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HH11	1:A:364:ARG:HB2	1.70	0.55
2:D:287:LYS:HD3	2:D:297:ILE:HD12	1.88	0.55
2:F:131:ILE:HG13	2:F:213:MET:HG2	1.89	0.55
2:D:193:ILE:HG13	2:D:200:TYR:HE1	1.71	0.55
1:A:181:ASN:HD21	1:A:216:SER:HB3	1.71	0.55
2:D:139:LYS:O	2:D:143:SER:HB3	2.07	0.55
2:D:111:ALA:N	2:D:158:VAL:O	2.38	0.55
2:D:27:LEU:HD23	2:D:41:ALA:HB2	1.89	0.55
1:C:65:VAL:HA	1:C:81:ILE:HG22	1.89	0.55
2:F:27:LEU:HD23	2:F:41:ALA:HB2	1.89	0.55
1:A:186:ASP:O	1:A:191:ASN:ND2	2.40	0.55
2:H:238:LEU:HD12	2:H:268:MET:HE2	1.87	0.55
2:B:192:GLU:N	2:B:192:GLU:OE1	2.40	0.54
1:G:110:ARG:NH2	1:G:213:GLU:OE2	2.40	0.54
2:D:147:ILE:CD1	2:D:202:GLN:HA	2.36	0.54
2:F:143:SER:OG	2:F:320:ALA:O	2.24	0.54
1:E:212:LYS:NZ	1:E:213:GLU:O	2.39	0.54
1:E:304:ASN:OD1	1:E:307:LYS:NZ	2.40	0.54
2:B:82:ASN:OD1	2:B:136:ARG:NH1	2.40	0.54
2:B:204:VAL:O	2:B:208:SER:N	2.40	0.54
2:B:186:ARG:HB2	2:B:231:GLN:HG3	1.88	0.54
2:B:70:ARG:NH2	2:B:170:GLY:O	2.40	0.54
2:D:262:LEU:O	2:D:264:GLN:NE2	2.40	0.53
1:G:52:LEU:HB2	1:G:109:TRP:CG	2.43	0.53
2:B:138:LEU:HD11	2:B:209:VAL:HG21	1.91	0.53
1:C:190:GLU:OE2	2:D:15:LYS:NZ	2.40	0.53
1:C:191:ASN:OD1	1:C:207:ASP:HB3	2.09	0.53
1:E:383:LEU:HD13	1:E:387:ARG:HH22	1.74	0.53
2:B:190:ALA:H	2:B:204:VAL:HG13	1.74	0.53
1:G:186:ASP:OD1	1:G:188:LYS:NZ	2.27	0.53
2:D:82:ASN:OD1	2:D:136:ARG:NH1	2.39	0.53
2:D:124:ASP:OD2	2:D:278:ASN:ND2	2.38	0.53
2:F:141:ILE:O	2:F:146:ILE:HG22	2.09	0.53
2:D:183:VAL:O	2:D:189:ARG:NH2	2.41	0.53
2:F:127:VAL:HG21	2:F:217:LEU:HD23	1.91	0.53
2:H:156:LEU:HD22	2:H:164:LEU:HD21	1.90	0.53
1:A:255:ILE:HD11	1:A:261:PRO:HB3	1.91	0.53
2:F:158:VAL:CG2	2:F:164:LEU:HD12	2.39	0.53
2:H:192:GLU:OE2	2:H:296:ARG:NH1	2.40	0.53
2:B:333:LEU:HD23	2:B:334:ILE:N	2.24	0.53
2:B:138:LEU:HD13	2:B:206:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:SER:N	2:D:161:ASP:OD2	2.42	0.52
1:E:153:ARG:HD3	1:E:156:GLN:HB2	1.90	0.52
1:G:261:PRO:HB2	1:G:263:PHE:HE2	1.73	0.52
2:D:203:THR:HB	2:D:296:ARG:HD2	1.90	0.52
1:G:52:LEU:HB2	1:G:109:TRP:CD2	2.44	0.52
1:G:146:LEU:HD11	1:G:166:ILE:HD13	1.92	0.52
1:A:268:GLY:O	1:A:269:LEU:CD2	2.57	0.52
2:F:149:ARG:HH22	2:F:180:TPO:HB	1.73	0.52
2:F:67:ARG:HG3	2:F:70:ARG:HH21	1.75	0.52
2:B:201:ASN:O	2:B:201:ASN:ND2	2.42	0.52
2:B:88:ASP:HA	2:B:348:PHE:HE2	1.74	0.52
2:D:188:TYR:CD1	2:D:188:TYR:N	2.76	0.52
2:D:329:SER:O	2:D:329:SER:OG	2.28	0.52
2:F:76:LYS:HE3	2:F:348:PHE:HD1	1.74	0.51
1:G:258:CYS:SG	1:G:260:TYR:HB2	2.49	0.51
2:D:333:LEU:HD23	2:D:335:ASP:H	1.74	0.51
2:D:153:PRO:HD3	2:D:212:ILE:HG12	1.93	0.51
1:E:151:GLN:O	1:E:343:LYS:NZ	2.33	0.51
1:E:72:LEU:HD21	2:F:17:ILE:HG23	1.92	0.51
2:D:173:ARG:CG	2:D:174:HIS:H	2.17	0.51
2:H:326:SER:HB2	2:H:328:GLU:HG3	1.93	0.51
2:H:27:LEU:HD23	2:H:41:ALA:HB2	1.92	0.51
1:E:304:ASN:HB3	1:E:314:MET:HB2	1.93	0.51
2:F:113:LEU:HD12	2:F:156:LEU:CD1	2.41	0.51
2:F:321:ASP:OD1	2:F:321:ASP:N	2.34	0.51
1:G:269:LEU:HD11	2:H:194:MET:O	2.11	0.51
2:B:113:LEU:HD11	2:B:156:LEU:HD12	1.92	0.50
2:F:191:PRO:HG3	2:F:235:ILE:HD13	1.92	0.50
1:G:263:PHE:CE1	1:G:355:GLU:HG2	2.46	0.50
2:H:152:LYS:HE2	2:H:155:ASN:ND2	2.26	0.50
2:H:84:ILE:HB	2:H:166:ILE:O	2.11	0.50
2:D:247:LEU:HD23	2:D:250:ILE:HD12	1.92	0.50
1:G:159:THR:OG1	1:G:160:GLU:N	2.45	0.50
1:A:118:VAL:HA	1:A:204:LYS:HD3	1.94	0.50
2:D:193:ILE:HG13	2:D:200:TYR:CE1	2.47	0.50
2:H:185:THR:HG23	2:H:186:ARG:HH11	1.75	0.50
2:H:140:TYR:CZ	2:H:320:ALA:HB2	2.47	0.50
2:D:84:ILE:HG13	2:D:106:THR:HG21	1.93	0.50
2:F:182:PTR:C	2:F:182:PTR:HD2	2.41	0.50
1:A:188:LYS:HZ2	1:A:357:THR:HG23	1.77	0.49
2:D:185:THR:O	2:D:189:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:ARG:O	1:G:364:ARG:NH1	2.36	0.49
1:A:304:ASN:OD1	1:A:307:LYS:NZ	2.43	0.49
1:E:380:ASN:OD1	1:E:383:LEU:N	2.43	0.49
2:H:236:LEU:HD22	2:H:241:THR:HA	1.95	0.49
2:B:182:PTR:O3P	2:B:186:ARG:NH2	2.39	0.49
1:C:380:ASN:OD1	1:C:383:LEU:N	2.40	0.49
1:E:89:LYS:HE2	1:E:140:CYS:SG	2.53	0.49
2:F:71:GLU:OE2	2:F:170:GLY:HA2	2.13	0.49
2:B:186:ARG:HA	2:B:189:ARG:HG2	1.94	0.49
2:D:74:LEU:O	2:D:78:MET:HG2	2.13	0.49
2:F:211:CYS:HA	2:F:222:LEU:HD12	1.95	0.49
2:H:180:TPO:P	2:H:180:TPO:H	2.35	0.49
2:B:85:GLY:O	2:B:106:THR:HG23	2.13	0.48
2:F:146:ILE:HD11	2:F:172:ALA:HB1	1.93	0.48
2:B:238:LEU:HA	2:B:268:MET:HE2	1.94	0.48
1:C:120:ILE:HG12	1:C:138:MET:HG2	1.95	0.48
1:C:288:ASN:N	1:C:289:PRO:HD2	2.29	0.48
2:B:67:ARG:HG3	2:B:70:ARG:HH21	1.78	0.48
2:B:149:ARG:NE	2:B:183:VAL:HG21	2.28	0.48
1:A:123:VAL:HG12	1:A:136:ILE:HG12	1.95	0.48
2:F:149:ARG:NH2	2:F:180:TPO:HB	2.28	0.48
1:G:124:TYR:N	1:G:135:LEU:O	2.46	0.48
2:B:147:ILE:HD11	2:B:175:THR:HG22	1.95	0.48
2:D:146:ILE:HA	2:D:173:ARG:O	2.13	0.48
1:A:271:ILE:CD1	1:A:285:GLU:HG2	2.42	0.48
2:B:80:HIS:CD2	2:B:140:TYR:HD2	2.30	0.48
1:E:185:ARG:O	1:E:364:ARG:NH1	2.39	0.48
2:B:149:ARG:HE	2:B:183:VAL:HG21	1.79	0.48
1:G:369:GLN:HG2	3:H:401:39G:H10	1.95	0.48
2:H:182:PTR:O	2:H:182:PTR:HD1	2.14	0.48
1:G:125:GLU:O	1:G:126:ASN:ND2	2.47	0.48
1:G:257:LEU:HD23	1:G:336:LEU:HD21	1.96	0.48
1:C:351:ASP:OD1	2:D:57:ARG:NH2	2.46	0.47
2:D:149:ARG:HH21	2:D:173:ARG:HD2	1.79	0.47
2:H:187:TRP:CE3	2:H:221:THR:HG21	2.49	0.47
2:B:333:LEU:HD23	2:B:334:ILE:H	1.79	0.47
1:E:369:GLN:HG2	3:F:401:39G:H10	1.96	0.47
2:F:112:ASP:HA	2:F:156:LEU:O	2.14	0.47
2:F:82:ASN:O	2:F:166:ILE:HD12	2.14	0.47
1:A:83:ASN:O	1:A:87:GLN:N	2.47	0.47
2:B:247:LEU:HD23	2:B:250:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:HD13	1:E:182:ILE:HG23	1.96	0.47
1:C:382:LEU:HD12	2:D:129:PHE:HE1	1.79	0.47
1:E:307:LYS:O	1:E:313:ARG:NH2	2.48	0.47
1:E:309:GLU:HG3	1:E:312:GLN:H	1.80	0.47
1:C:97:ASP:OD2	1:C:102:ARG:NH2	2.48	0.47
2:D:149:ARG:NH2	2:D:173:ARG:HH11	2.13	0.47
1:G:307:LYS:O	1:G:313:ARG:NH2	2.48	0.47
2:B:209:VAL:O	2:B:213:MET:N	2.34	0.47
2:B:113:LEU:HD22	2:B:216:LEU:HD21	1.97	0.46
2:D:321:ASP:OD1	2:D:321:ASP:N	2.46	0.46
2:F:208:SER:O	2:F:212:ILE:HG13	2.15	0.46
2:F:194:MET:O	2:F:250:ILE:HG23	2.14	0.46
1:A:69:VAL:HG22	1:A:71:GLY:H	1.80	0.46
2:F:193:ILE:HD12	2:F:194:MET:N	2.31	0.46
2:H:84:ILE:HG13	2:H:106:THR:HG21	1.96	0.46
2:H:10:ARG:HG2	2:H:19:GLU:HG2	1.98	0.46
1:A:185:ARG:NH1	1:A:364:ARG:HB2	2.31	0.46
2:B:215:GLU:OE2	2:B:221:THR:HA	2.16	0.46
2:H:73:ARG:NE	2:H:344:GLU:OE1	2.41	0.46
1:A:181:ASN:ND2	1:A:216:SER:HB3	2.30	0.46
2:D:7:THR:OG1	2:D:22:GLU:OE1	2.33	0.46
2:F:10:ARG:HG2	2:F:19:GLU:HB3	1.98	0.46
2:B:106:THR:HG22	2:B:107:HIS:H	1.81	0.46
2:B:140:TYR:CE1	2:B:320:ALA:HB2	2.51	0.46
1:C:178:HIS:HA	1:C:242:LYS:HE2	1.97	0.46
2:D:158:VAL:HA	2:D:163:GLU:O	2.16	0.46
1:A:96:GLN:OE1	1:A:131:ARG:NH1	2.49	0.46
2:F:143:SER:CB	2:F:320:ALA:H	2.29	0.46
2:F:159:ASN:OD1	2:F:163:GLU:N	2.49	0.46
2:F:147:ILE:HG22	2:F:149:ARG:HG3	1.98	0.46
1:A:221:THR:HG23	1:A:221:THR:O	2.16	0.46
1:A:266:ASN:ND2	1:A:266:ASN:O	2.46	0.46
2:B:82:ASN:ND2	2:B:133:GLN:OE1	2.49	0.46
1:C:257:LEU:O	1:C:336:LEU:HD21	2.16	0.45
1:E:165:GLU:HA	1:E:168:LYS:HB3	1.97	0.45
2:F:135:LEU:HD21	2:F:209:VAL:HG11	1.97	0.45
2:H:182:PTR:O1P	2:H:186:ARG:HD3	2.16	0.45
1:A:96:GLN:HE22	1:A:131:ARG:HH11	1.65	0.45
2:F:70:ARG:NH1	2:F:171:LEU:HA	2.29	0.45
2:F:96:LEU:HD13	2:F:342:TYR:HB2	1.99	0.45
1:A:158:PHE:HD2	1:A:336:LEU:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:150:ASP:O	2:F:152:LYS:HG2	2.17	0.45
2:H:333:LEU:HD23	2:H:334:ILE:N	2.29	0.45
2:F:186:ARG:HG3	2:F:187:TRP:N	2.31	0.45
2:F:238:LEU:HA	2:F:268:MET:HE2	1.98	0.45
2:H:195:LEU:HD21	2:H:232:LEU:HD21	1.98	0.45
2:B:145:ASP:O	2:B:174:HIS:HA	2.16	0.45
2:D:84:ILE:HB	2:D:166:ILE:O	2.17	0.45
2:H:62:ILE:HG13	2:H:334:ILE:HD13	1.98	0.45
2:B:109:MET:O	2:B:159:ASN:HA	2.16	0.45
2:F:91:THR:HG22	2:F:345:VAL:HG11	1.98	0.45
2:H:182:PTR:C	2:H:182:PTR:HD1	2.46	0.45
1:A:81:ILE:HG23	1:A:90:PHE:HB2	1.98	0.45
2:B:131:ILE:HA	2:B:134:ILE:HD12	1.98	0.45
2:B:192:GLU:OE2	2:B:296:ARG:NH2	2.39	0.45
2:B:199:HIS:O	2:B:200:TYR:CG	2.70	0.45
2:D:323:TYR:CD2	2:D:323:TYR:O	2.70	0.45
1:C:234:VAL:HG21	1:E:68:GLN:HB2	1.99	0.45
1:G:254:TYR:CD1	1:G:262:PRO:HD3	2.52	0.45
1:A:380:ASN:OD1	1:A:383:LEU:N	2.45	0.45
1:C:151:GLN:HE22	1:C:342:LEU:HB3	1.81	0.45
2:H:140:TYR:CE2	2:H:320:ALA:HB2	2.52	0.45
1:A:370:ILE:HD13	2:B:160:GLU:HA	1.99	0.44
1:C:149:ARG:HG3	1:C:194:TYR:CD2	2.51	0.44
1:G:370:ILE:HG13	1:G:370:ILE:H	1.63	0.44
1:C:118:VAL:HA	1:C:204:LYS:HD3	1.99	0.44
1:C:110:ARG:NH2	1:C:213:GLU:OE2	2.48	0.44
1:G:233:GLU:OE1	2:H:220:ARG:NE	2.44	0.44
2:B:112:ASP:OD1	2:B:112:ASP:N	2.49	0.44
1:E:59:ILE:HG12	1:E:63:TYR:HB2	1.99	0.44
1:A:309:GLU:HG3	1:A:312:GLN:H	1.82	0.44
2:H:246:LEU:HD12	2:H:249:LYS:HD3	2.00	0.44
1:A:351:ASP:OD1	2:B:57:ARG:NH2	2.38	0.44
2:B:82:ASN:ND2	2:B:133:GLN:HB3	2.33	0.44
1:A:394:GLU:OE2	2:H:62:ILE:N	2.29	0.44
2:H:179:MET:O	2:H:198:MET:HG3	2.17	0.44
2:B:140:TYR:CD1	2:B:320:ALA:HB2	2.52	0.44
2:B:88:ASP:HA	2:B:348:PHE:CE2	2.51	0.44
1:E:236:GLY:O	1:E:238:GLU:N	2.51	0.44
1:E:243:SER:HB2	1:E:313:ARG:NH1	2.32	0.44
1:G:370:ILE:HD13	2:H:160:GLU:HA	1.98	0.44
2:B:149:ARG:NH2	2:B:200:TYR:OH	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:LYS:HE2	1:E:371:LYS:HB3	1.75	0.44
1:A:362:THR:O	2:B:118:LYS:NZ	2.51	0.43
1:C:257:LEU:HA	1:C:336:LEU:HD11	1.99	0.43
2:H:150:ASP:OD1	2:H:155:ASN:ND2	2.51	0.43
1:G:231:ALA:O	2:H:220:ARG:NH1	2.51	0.43
1:C:375:ILE:HD13	1:C:375:ILE:HA	1.89	0.43
2:F:284:LEU:O	2:F:288:MET:HG3	2.18	0.43
2:H:55:LEU:HD12	2:H:102:VAL:HB	2.00	0.43
2:D:140:TYR:CZ	2:D:320:ALA:HB2	2.54	0.43
2:F:52:VAL:HG22	2:F:105:VAL:HG22	2.01	0.43
2:H:187:TRP:CD1	2:H:187:TRP:N	2.86	0.43
2:H:227:ASP:OD1	2:H:229:ILE:HG13	2.19	0.43
1:A:370:ILE:H	1:A:370:ILE:HG13	1.64	0.43
2:D:149:ARG:HH22	2:D:173:ARG:HH11	1.67	0.43
2:F:147:ILE:HG12	2:F:175:THR:HG22	1.95	0.43
2:H:341:THR:O	2:H:345:VAL:HG23	2.18	0.43
2:B:196:ASN:HB3	2:B:199:HIS:CB	2.49	0.43
2:D:145:ASP:O	2:D:174:HIS:HA	2.19	0.43
2:F:70:ARG:HH12	2:F:171:LEU:CA	2.31	0.43
2:H:246:LEU:HD21	2:H:291:LEU:HD12	2.00	0.43
1:A:271:ILE:HD13	1:A:271:ILE:HG21	1.66	0.43
1:C:384:LEU:HA	1:C:387:ARG:HB2	2.01	0.43
2:F:332:LEU:HB3	2:F:336:GLU:HB2	2.00	0.43
2:H:80:HIS:HB2	2:H:140:TYR:CZ	2.54	0.43
2:H:185:THR:HA	2:H:186:ARG:NH1	2.34	0.43
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.87	0.43
1:E:257:LEU:HD23	1:E:336:LEU:HD21	2.00	0.43
2:F:82:ASN:ND2	2:F:133:GLN:HB3	2.34	0.43
2:H:109:MET:HB2	3:H:401:39G:H12	2.01	0.43
2:D:75:LEU:HD21	3:D:401:39G:O27	2.19	0.42
2:F:164:LEU:C	2:F:164:LEU:HD23	2.40	0.42
2:F:166:ILE:HG22	2:F:167:LEU:N	2.32	0.42
1:A:305:LEU:HD23	1:A:314:MET:HB3	2.02	0.42
2:B:148:HIS:ND1	2:B:151:LEU:HG	2.34	0.42
2:B:235:ILE:O	2:B:239:VAL:HG22	2.19	0.42
2:B:84:ILE:HD12	2:B:84:ILE:HA	1.97	0.42
1:C:339:SER:O	1:C:343:LYS:HB2	2.20	0.42
2:F:171:LEU:O	2:F:171:LEU:HD12	2.18	0.42
1:G:257:LEU:HA	1:G:336:LEU:HD23	2.00	0.42
2:H:156:LEU:HD21	2:H:166:ILE:HD13	1.99	0.42
1:A:158:PHE:HE2	1:A:163:ALA:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:O	1:A:180:ILE:HG12	2.19	0.42
1:A:268:GLY:O	1:A:269:LEU:HD23	2.20	0.42
2:B:288:MET:O	2:B:296:ARG:HD3	2.20	0.42
2:D:52:VAL:HG22	2:D:105:VAL:HG22	2.02	0.42
2:F:85:GLY:O	2:F:106:THR:HG23	2.18	0.42
2:B:76:LYS:HE2	2:B:348:PHE:HA	2.01	0.42
2:B:84:ILE:HB	2:B:166:ILE:O	2.19	0.42
1:E:386:ARG:NH2	2:F:316:ASP:OD2	2.42	0.42
1:A:124:TYR:HB2	1:A:135:LEU:HB2	2.00	0.42
2:F:247:LEU:HD23	2:F:250:ILE:HD12	2.01	0.42
2:H:131:ILE:HD13	2:H:134:ILE:HD12	2.02	0.42
2:H:195:LEU:HB3	2:H:250:ILE:HG13	2.01	0.42
2:B:142:HIS:NE2	2:B:205:ASP:OD2	2.52	0.42
2:B:206:ILE:HG21	2:B:297:ILE:O	2.20	0.42
2:B:80:HIS:HB2	2:B:140:TYR:HD2	1.81	0.42
1:C:287:PRO:O	1:C:291:TRP:HB2	2.19	0.42
2:D:187:TRP:CE3	2:D:221:THR:HG21	2.55	0.42
2:D:87:LEU:HD21	2:D:107:HIS:NE2	2.35	0.42
2:F:109:MET:HG3	2:F:157:ALA:HB1	2.02	0.42
2:H:148:HIS:O	2:H:149:ARG:HG2	2.19	0.42
1:G:386:ARG:HD3	1:G:386:ARG:HA	1.77	0.42
2:B:70:ARG:NH1	2:B:172:ALA:O	2.53	0.42
2:B:200:TYR:O	2:B:200:TYR:HD1	2.03	0.42
1:C:220:LEU:O	1:C:220:LEU:HD13	2.20	0.42
2:F:146:ILE:HD12	2:F:173:ARG:O	2.20	0.42
2:F:169:PHE:CD1	2:F:169:PHE:N	2.87	0.41
1:G:369:GLN:HB3	2:H:111:ALA:HB2	2.02	0.41
2:H:326:SER:C	2:H:328:GLU:H	2.24	0.41
2:B:187:TRP:CD1	2:B:187:TRP:N	2.88	0.41
2:F:236:LEU:HD22	2:F:242:PRO:HD3	2.01	0.41
1:A:198:ARG:HG3	1:A:198:ARG:H	1.64	0.41
2:B:135:LEU:HA	2:B:138:LEU:HB2	2.01	0.41
2:F:84:ILE:HB	2:F:166:ILE:O	2.21	0.41
2:H:67:ARG:HG3	2:H:70:ARG:HH21	1.85	0.41
2:F:59:PHE:HZ	2:F:341:THR:HG21	1.85	0.41
2:D:187:TRP:HB2	2:D:188:TYR:CE1	2.55	0.41
1:E:327:GLN:HB3	1:E:330:LYS:HG3	2.02	0.41
1:G:389:LYS:HD2	1:G:389:LYS:HA	1.87	0.41
1:G:89:LYS:HE2	1:G:140:CYS:SG	2.59	0.41
1:E:55:LYS:HD2	1:E:124:TYR:HE1	1.85	0.41
2:H:128:GLN:HG2	2:H:307:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:LEU:HD11	2:H:104:LEU:HD22	2.03	0.41
2:H:156:LEU:HA	2:H:156:LEU:HD23	1.77	0.41
1:A:77:LYS:HD2	1:A:79:LEU:HD21	2.03	0.41
2:D:213:MET:O	2:D:217:LEU:HD23	2.20	0.41
1:E:216:SER:HA	1:E:242:LYS:NZ	2.36	0.41
2:H:188:TYR:N	2:H:188:TYR:CD1	2.88	0.41
2:H:346:ILE:HD12	2:H:347:SER:N	2.34	0.41
1:A:88:GLU:HB3	1:A:90:PHE:CE2	2.56	0.41
1:C:55:LYS:NZ	1:C:122:ASP:OD2	2.53	0.41
2:D:284:LEU:O	2:D:288:MET:HG3	2.21	0.41
2:B:141:ILE:O	2:B:146:ILE:HG22	2.21	0.41
1:C:286:PHE:HB3	1:C:291:TRP:CD2	2.56	0.41
2:F:147:ILE:HD11	2:F:175:THR:CG2	2.43	0.41
2:F:333:LEU:HD23	2:F:334:ILE:N	2.35	0.41
2:H:11:GLN:HG2	2:H:13:LEU:HG	2.02	0.41
2:B:131:ILE:HD13	2:B:134:ILE:HD12	2.02	0.41
2:D:89:VAL:HG22	2:D:345:VAL:HG13	2.02	0.41
1:E:97:ASP:OD2	1:E:102:ARG:NH2	2.53	0.41
2:F:235:ILE:O	2:F:239:VAL:HG22	2.20	0.41
2:H:87:LEU:HD21	2:H:107:HIS:CE1	2.56	0.41
2:H:173:ARG:HG2	2:H:174:HIS:H	1.85	0.41
2:H:228:HIS:HA	2:H:231:GLN:HB2	2.02	0.41
2:B:200:TYR:HB2	2:B:204:VAL:CG2	2.50	0.40
2:D:182:PTR:HE1	2:D:189:ARG:HH12	1.86	0.40
2:F:11:GLN:N	2:F:18:TRP:O	2.52	0.40
2:B:194:MET:N	2:B:194:MET:SD	2.86	0.40
2:B:262:LEU:O	2:B:264:GLN:NE2	2.55	0.40
1:C:216:SER:HG	1:C:242:LYS:HZ2	1.55	0.40
1:A:357:THR:HG22	2:B:32:SER:HB3	2.03	0.40
1:A:57:ASN:ND2	1:A:61:ASP:OD2	2.37	0.40
1:A:62:ASP:OD2	1:A:124:TYR:OH	2.31	0.40
2:B:11:GLN:N	2:B:18:TRP:O	2.55	0.40
2:B:284:LEU:O	2:B:288:MET:HG3	2.22	0.40
1:C:101:ALA:O	1:C:105:VAL:HG23	2.21	0.40
2:F:147:ILE:HG13	2:F:175:THR:HG22	1.96	0.40
1:C:304:ASN:OD1	1:C:307:LYS:NZ	2.55	0.40
2:D:222:LEU:HA	2:D:222:LEU:HD23	1.94	0.40
2:F:247:LEU:HD23	2:F:247:LEU:HA	1.93	0.40
1:A:161:ARG:NH2	1:A:331:VAL:O	2.50	0.40
2:D:117:VAL:HG13	2:D:219:GLY:HA2	2.03	0.40
1:G:107:LEU:HD13	1:G:182:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:MET:HG3	1:G:314:MET:O	2.21	0.40
2:H:166:ILE:O	2:H:167:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	341/371 (92%)	320 (94%)	19 (6%)	2 (1%)	25 62
1	C	322/371 (87%)	309 (96%)	13 (4%)	0	100 100
1	E	323/371 (87%)	310 (96%)	13 (4%)	0	100 100
1	G	333/371 (90%)	313 (94%)	20 (6%)	0	100 100
2	B	341/364 (94%)	324 (95%)	17 (5%)	0	100 100
2	D	340/364 (93%)	325 (96%)	14 (4%)	1 (0%)	41 74
2	F	338/364 (93%)	323 (96%)	14 (4%)	1 (0%)	41 74
2	H	340/364 (93%)	322 (95%)	16 (5%)	2 (1%)	25 62
All	All	2678/2940 (91%)	2546 (95%)	126 (5%)	6 (0%)	47 78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	329	SER
2	H	326	SER
1	A	266	ASN
2	H	325	GLN
2	F	185	THR
1	A	265	SER

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	282/331 (85%)	274 (97%)	8 (3%)	43	67
1	C	289/331 (87%)	286 (99%)	3 (1%)	76	86
1	E	291/331 (88%)	287 (99%)	4 (1%)	67	82
1	G	288/331 (87%)	281 (98%)	7 (2%)	49	71
2	B	296/320 (92%)	289 (98%)	7 (2%)	49	71
2	D	294/320 (92%)	285 (97%)	9 (3%)	40	65
2	F	294/320 (92%)	285 (97%)	9 (3%)	40	65
2	H	300/320 (94%)	288 (96%)	12 (4%)	31	60
All	All	2334/2604 (90%)	2275 (98%)	59 (2%)	47	70

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ARG
1	A	122	ASP
1	A	149	ARG
1	A	217	HIS
1	A	266	ASN
1	A	269	LEU
1	A	321	ASN
1	A	327	GLN
2	B	73	ARG
2	B	140	TYR
2	B	171	LEU
2	B	194	MET
2	B	198	MET
2	B	222	LEU
2	B	294	ASP
1	C	56	LYS
1	C	149	ARG
1	C	389	LYS
2	D	10	ARG

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Mol	Chain	Res	Type
2	D	99	PHE
2	D	143	SER
2	D	161	ASP
2	D	177	ASP
2	D	186	ARG
2	D	323	TYR
2	D	324	ASP
2	D	331	ASP
1	E	228	TYR
1	E	286	PHE
1	E	301	LEU
1	E	389	LYS
2	F	49	ARG
2	F	99	PHE
2	F	143	SER
2	F	149	ARG
2	F	152	LYS
2	F	189	ARG
2	F	200	TYR
2	F	202	GLN
2	F	323	TYR
1	G	158	PHE
1	G	258	CYS
1	G	260	TYR
1	G	285	GLU
1	G	368	GLU
1	G	376	GLU
1	G	379	SER
2	H	49	ARG
2	H	94	ARG
2	H	99	PHE
2	H	148	HIS
2	H	149	ARG
2	H	152	LYS
2	H	161	ASP
2	H	186	ARG
2	H	198	MET
2	H	267	LYS
2	H	330	ARG
2	H	342	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	GLN

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	H	182	2	15,16,17	1.62	1 (6%)	19,22,24	1.23	4 (21%)
2	PTR	B	182	2	15,16,17	1.35	1 (6%)	19,22,24	0.53	1 (5%)
2	PTR	F	182	2	15,16,17	1.35	1 (6%)	19,22,24	0.55	0
2	TPO	H	180	2	8,10,11	1.08	0	10,14,16	1.13	0
2	PTR	D	182	2	15,16,17	1.37	1 (6%)	19,22,24	0.70	0
2	TPO	D	180	2	8,10,11	1.57	1 (12%)	10,14,16	1.91	1 (10%)
2	TPO	F	180	2	8,10,11	1.09	0	10,14,16	1.18	1 (10%)
2	TPO	B	180	2	8,10,11	1.16	0	10,14,16	1.08	1 (10%)

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	-	1/10/11/13	0/1/1/1
2	PTR	B	182	2	-	0/10/11/13	0/1/1/1
2	PTR	F	182	2	-	2/10/11/13	0/1/1/1
2	TPO	H	180	2	-	6/9/11/13	-
2	PTR	D	182	2	-	0/10/11/13	0/1/1/1
2	TPO	D	180	2	-	2/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	F	180	2	-	3/9/11/13	-
2	TPO	B	180	2	-	4/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	182	PTR	OH-CZ	-5.76	1.27	1.40
2	B	182	PTR	OH-CZ	-4.43	1.30	1.40
2	F	182	PTR	OH-CZ	-4.37	1.30	1.40
2	D	182	PTR	OH-CZ	-4.35	1.30	1.40
2	D	180	TPO	P-O1P	3.40	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	180	TPO	P-OG1-CB	-5.66	106.12	123.21
2	H	182	PTR	O3P-P-OH	2.78	113.95	105.24
2	F	180	TPO	P-OG1-CB	-2.76	114.88	123.21
2	H	182	PTR	P-OH-CZ	-2.75	114.95	123.75
2	H	182	PTR	OH-P-O1P	-2.70	99.13	109.31
2	B	180	TPO	P-OG1-CB	-2.36	116.08	123.21
2	H	182	PTR	O2P-P-OH	2.09	111.78	105.24
2	B	182	PTR	O2P-P-OH	2.06	111.68	105.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	180	TPO	N-CA-CB-CG2
2	H	180	TPO	C-CA-CB-CG2
2	H	180	TPO	O-C-CA-CB
2	H	180	TPO	CG2-CB-OG1-P
2	F	180	TPO	O-C-CA-CB
2	B	180	TPO	CG2-CB-OG1-P
2	B	180	TPO	CB-OG1-P-O3P
2	H	182	PTR	CZ-OH-P-O1P
2	F	180	TPO	CB-OG1-P-O2P
2	D	180	TPO	C-CA-CB-CG2
2	B	180	TPO	CA-CB-OG1-P
2	B	180	TPO	N-CA-CB-CG2
2	H	180	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
2	H	180	TPO	CB-OG1-P-O2P
2	F	180	TPO	CB-OG1-P-O3P
2	F	182	PTR	CA-CB-CG-CD2
2	D	180	TPO	O-C-CA-CB
2	F	182	PTR	CA-CB-CG-CD1

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	182	PTR	3	0
2	B	182	PTR	3	0
2	F	182	PTR	1	0
2	H	180	TPO	1	0
2	D	182	PTR	1	0
2	D	180	TPO	2	0
2	F	180	TPO	2	0
2	B	180	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
3	39G	F	401	-	29,32,32	1.66	7 (24%)	37,46,46	4.16	13 (35%)
3	39G	H	401	-	29,32,32	1.67	7 (24%)	37,46,46	4.17	13 (35%)
3	39G	B	401	-	29,32,32	1.67	7 (24%)	37,46,46	4.11	13 (35%)
3	39G	D	401	-	29,32,32	1.66	7 (24%)	37,46,46	4.19	12 (32%)

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
3	39G	F	401	-	-	9/25/27/27	0/3/3/3
3	39G	H	401	-	-	12/25/27/27	0/3/3/3
3	39G	B	401	-	-	4/25/27/27	0/3/3/3
3	39G	D	401	-	-	9/25/27/27	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	401	39G	C20-S25	4.41	1.82	1.76
3	D	401	39G	C20-S25	4.37	1.82	1.76
3	F	401	39G	C20-S25	4.32	1.82	1.76
3	B	401	39G	C20-S25	4.31	1.82	1.76
3	B	401	39G	C15-N17	4.02	1.46	1.35
3	F	401	39G	C15-N17	4.01	1.46	1.35
3	D	401	39G	C15-N17	3.95	1.46	1.35
3	H	401	39G	C15-N17	3.92	1.46	1.35
3	H	401	39G	O26-S25	3.17	1.47	1.43
3	D	401	39G	O26-S25	3.14	1.47	1.43
3	B	401	39G	O26-S25	3.10	1.47	1.43
3	F	401	39G	O26-S25	3.05	1.46	1.43
3	B	401	39G	O27-S25	2.99	1.46	1.43
3	H	401	39G	O27-S25	2.98	1.46	1.43
3	H	401	39G	S25-N28	2.90	1.72	1.62
3	F	401	39G	O27-S25	2.85	1.46	1.43
3	F	401	39G	S25-N28	2.84	1.71	1.62
3	B	401	39G	S25-N28	2.83	1.71	1.62
3	D	401	39G	S25-N28	2.83	1.71	1.62
3	D	401	39G	O27-S25	2.76	1.46	1.43
3	B	401	39G	C18-N17	2.39	1.46	1.41
3	F	401	39G	C18-N17	2.35	1.46	1.41
3	D	401	39G	C18-N17	2.33	1.46	1.41
3	D	401	39G	O16-C15	-2.25	1.18	1.23
3	B	401	39G	O16-C15	-2.25	1.18	1.23
3	H	401	39G	O16-C15	-2.24	1.18	1.23
3	F	401	39G	O16-C15	-2.23	1.18	1.23
3	H	401	39G	C18-N17	2.20	1.46	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	39G	C24-C23-C18	17.53	141.08	121.25
3	F	401	39G	C24-C23-C18	17.43	140.97	121.25
3	H	401	39G	C24-C23-C18	17.41	140.94	121.25
3	B	401	39G	C24-C23-C18	17.30	140.82	121.25
3	H	401	39G	O27-S25-O26	-11.33	101.16	119.52
3	F	401	39G	O27-S25-O26	-11.25	101.28	119.52
3	D	401	39G	O27-S25-O26	-11.20	101.37	119.52
3	B	401	39G	O27-S25-O26	-11.10	101.53	119.52
3	D	401	39G	C24-C23-C22	-10.99	98.86	120.31
3	B	401	39G	C24-C23-C22	-10.95	98.94	120.31
3	F	401	39G	C24-C23-C22	-10.90	99.04	120.31
3	H	401	39G	C24-C23-C22	-10.74	99.35	120.31
3	H	401	39G	C18-N17-C15	-4.12	115.62	126.93
3	D	401	39G	C18-N17-C15	-4.11	115.66	126.93
3	F	401	39G	C18-N17-C15	-3.57	117.14	126.93
3	B	401	39G	C18-N17-C15	-3.18	118.21	126.93
3	F	401	39G	C6-N7-N8	3.11	108.01	103.93
3	D	401	39G	C5-C15-N17	3.08	121.94	116.06
3	H	401	39G	C6-N7-N8	3.05	107.93	103.93
3	F	401	39G	O27-S25-C20	2.98	111.82	108.05
3	B	401	39G	C22-C23-C18	2.97	120.24	117.44
3	D	401	39G	C6-N7-N8	2.86	107.68	103.93
3	D	401	39G	C22-C23-C18	2.79	120.06	117.44
3	B	401	39G	C6-N7-N8	2.78	107.57	103.93
3	D	401	39G	O27-S25-C20	2.71	111.48	108.05
3	F	401	39G	C22-C23-C18	2.71	119.99	117.44
3	B	401	39G	O27-S25-C20	2.68	111.44	108.05
3	D	401	39G	O16-C15-N17	-2.68	117.60	123.71
3	F	401	39G	C5-C15-N17	2.65	121.12	116.06
3	H	401	39G	C5-C15-N17	2.64	121.10	116.06
3	B	401	39G	C5-C15-N17	2.60	121.03	116.06
3	H	401	39G	O16-C15-N17	-2.59	117.81	123.71
3	B	401	39G	O26-S25-C20	2.57	111.30	108.05
3	D	401	39G	O26-S25-C20	2.56	111.29	108.05
3	H	401	39G	O27-S25-C20	2.49	111.20	108.05
3	H	401	39G	C22-C23-C18	2.41	119.71	117.44
3	F	401	39G	O16-C15-N17	-2.39	118.25	123.71
3	H	401	39G	O26-S25-C20	2.31	110.97	108.05
3	D	401	39G	C29-N28-C30	2.29	119.43	114.79
3	H	401	39G	C29-N28-C30	2.29	119.42	114.79
3	B	401	39G	O16-C15-N17	-2.21	118.67	123.71
3	F	401	39G	C29-N28-C30	2.19	119.22	114.79
3	D	401	39G	O26-S25-N28	2.16	111.43	106.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	39G	C29-N28-C30	2.15	119.14	114.79
3	B	401	39G	O27-S25-N28	2.14	111.40	106.85
3	B	401	39G	O26-S25-N28	2.14	111.39	106.85
3	H	401	39G	C5-C4-N8	-2.11	107.98	110.18
3	F	401	39G	O27-S25-N28	2.10	111.31	106.85
3	H	401	39G	O27-S25-N28	2.09	111.29	106.85
3	F	401	39G	O26-S25-N28	2.08	111.27	106.85
3	F	401	39G	O26-S25-C20	2.06	110.65	108.05

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	401	39G	C10-C9-N8-C4
3	F	401	39G	C14-C9-N8-C4
3	F	401	39G	C30-N28-S25-C20
3	F	401	39G	C30-N28-S25-O26
3	H	401	39G	C10-C9-N8-C4
3	H	401	39G	C14-C9-N8-C4
3	H	401	39G	C30-N28-S25-C20
3	H	401	39G	C30-N28-S25-O26
3	H	401	39G	C30-N28-S25-O27
3	B	401	39G	C30-N28-S25-O26
3	D	401	39G	C30-N28-S25-C20
3	D	401	39G	C30-N28-S25-O26
3	F	401	39G	C29-N28-S25-O26
3	F	401	39G	C30-N28-S25-O27
3	D	401	39G	C30-N28-S25-O27
3	D	401	39G	C1-C2-C3-C4
3	H	401	39G	C19-C18-N17-C15
3	D	401	39G	C23-C18-N17-C15
3	H	401	39G	C23-C18-N17-C15
3	H	401	39G	C1-C2-C3-C4
3	D	401	39G	C19-C18-N17-C15
3	H	401	39G	C29-N28-S25-O26
3	B	401	39G	C30-N28-S25-C20
3	B	401	39G	C30-N28-S25-O27
3	D	401	39G	C29-N28-S25-O26
3	D	401	39G	C10-C9-N8-N7
3	D	401	39G	C14-C9-N8-N7
3	F	401	39G	C23-C18-N17-C15
3	F	401	39G	C19-C18-N17-C15

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Mol	Chain	Res	Type	Atoms
3	H	401	39G	C14-C9-N8-N7
3	B	401	39G	C29-N28-S25-O26
3	H	401	39G	C21-C20-S25-O26
3	H	401	39G	C19-C20-S25-O26
3	F	401	39G	C14-C9-N8-N7

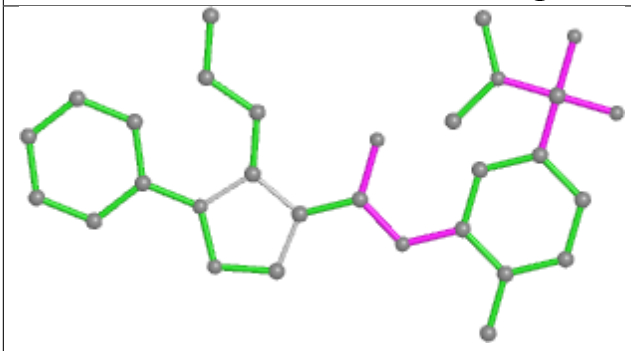
There are no ring outliers.

3 monomers are involved in 4 short contacts:

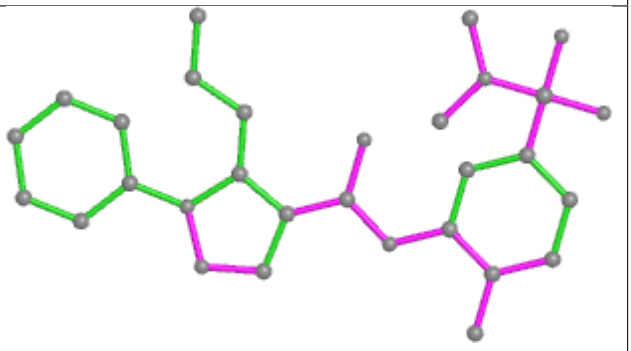
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	39G	1	0
3	H	401	39G	2	0
3	D	401	39G	1	0

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.

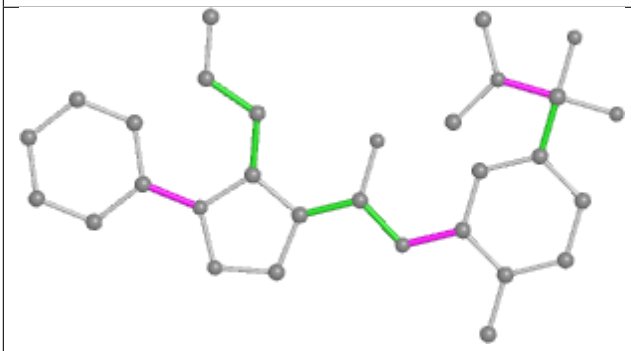
Ligand 39G F 401



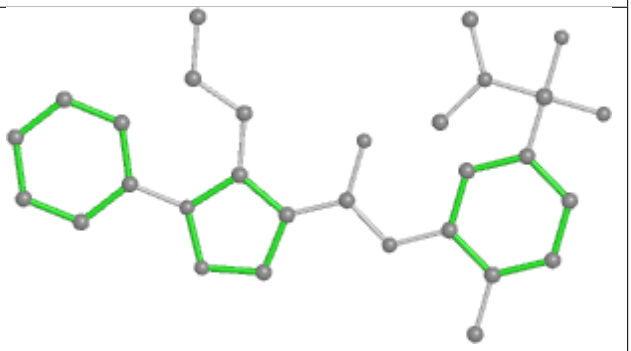
Bond lengths



Bond angles

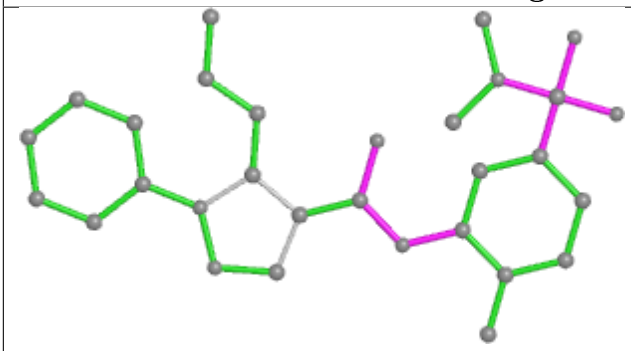


Torsions

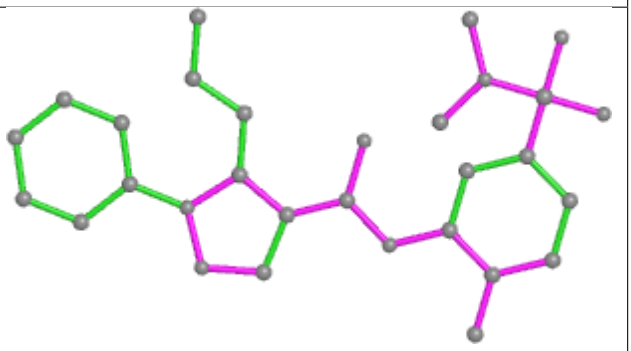


Rings

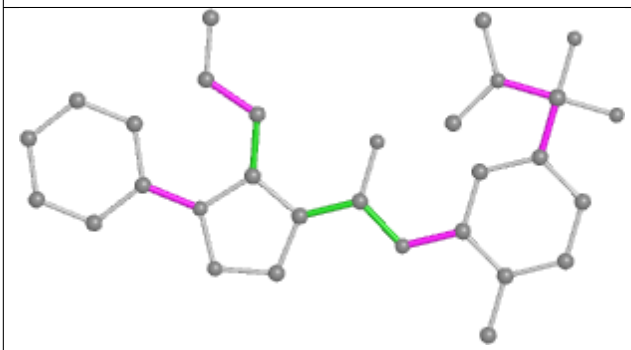
Ligand 39G H 401



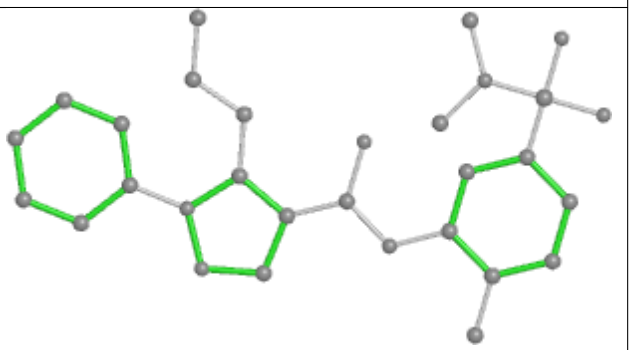
Bond lengths



Bond angles

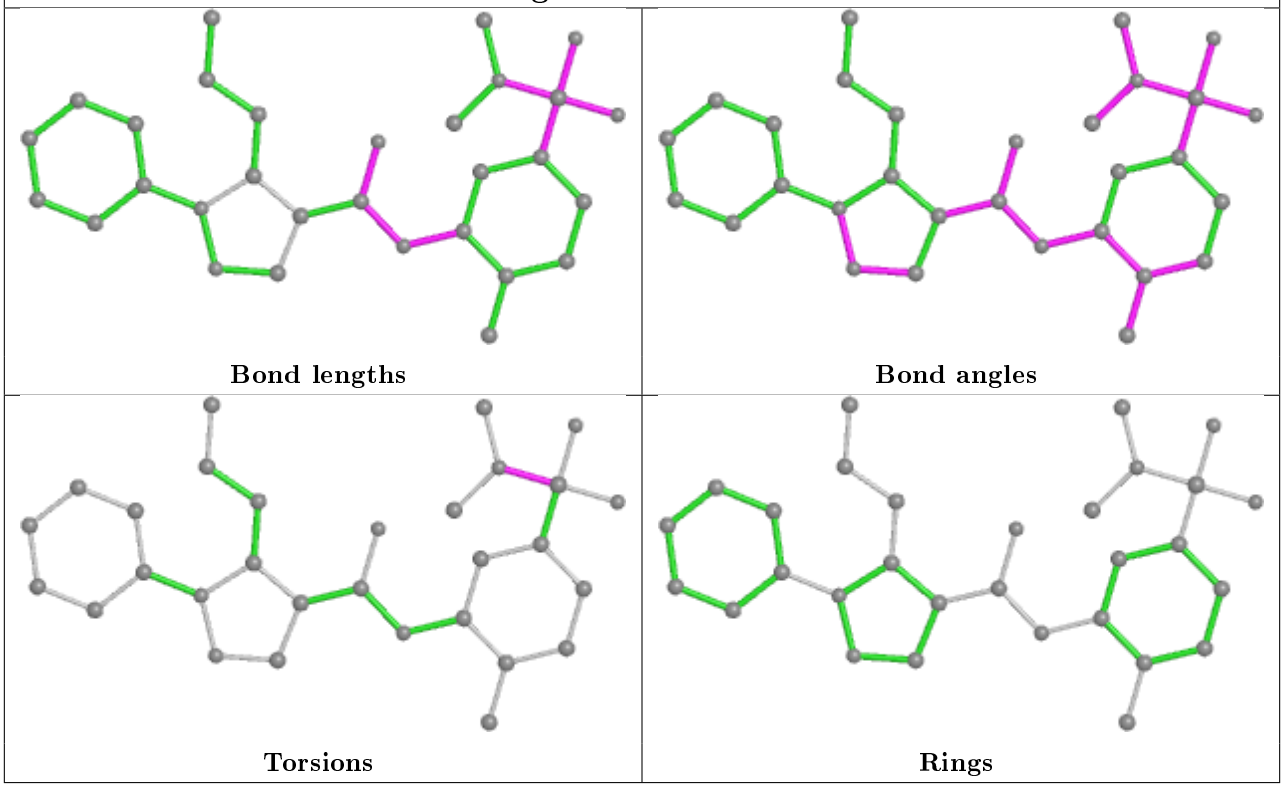


Torsions

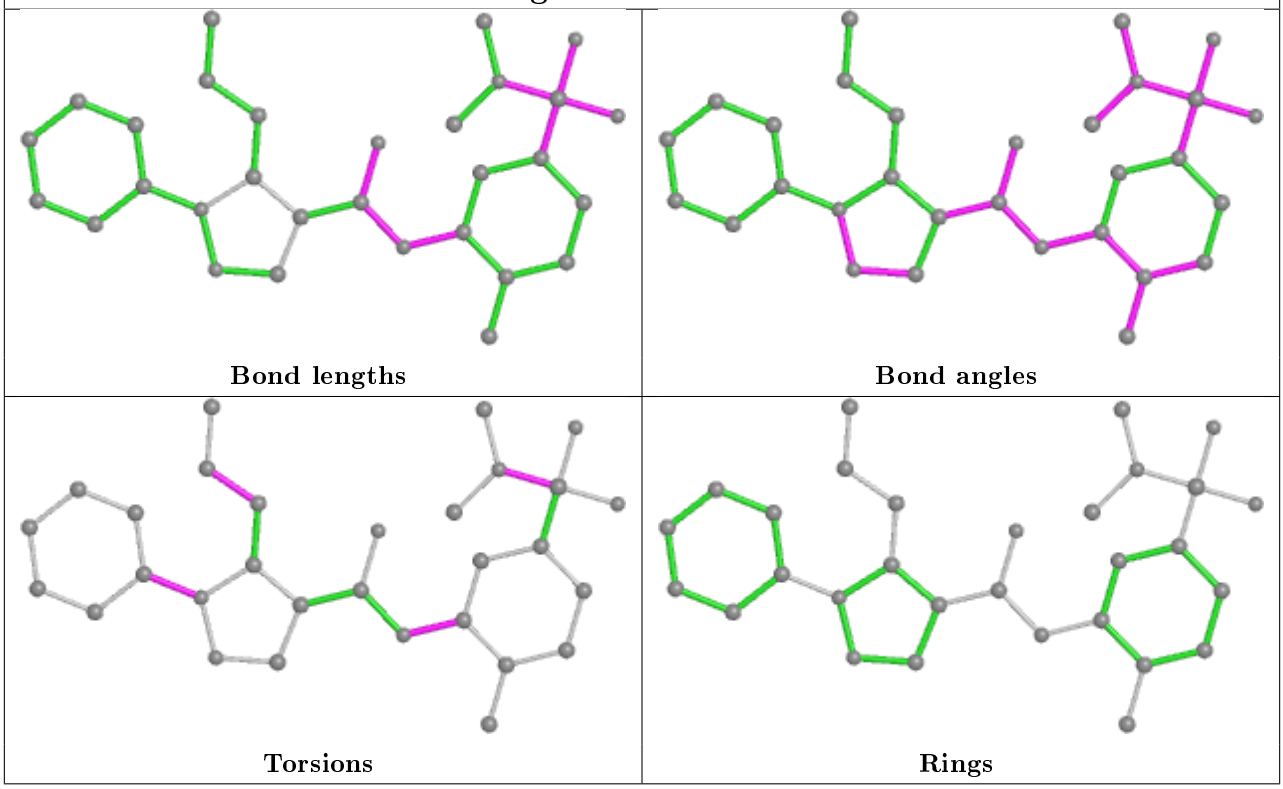


Rings

Ligand 39G B 401



Ligand 39G D 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	345/371 (92%)	-0.15	1 (0%) 94 90	91, 115, 143, 166	0
1	C	326/371 (87%)	-0.07	4 (1%) 79 69	115, 158, 216, 272	0
1	E	327/371 (88%)	0.11	9 (2%) 53 40	125, 153, 199, 227	0
1	G	337/371 (90%)	0.35	29 (8%) 10 8	123, 215, 267, 312	0
2	B	344/364 (94%)	-0.10	1 (0%) 94 90	92, 114, 149, 162	0
2	D	344/364 (94%)	-0.00	8 (2%) 60 48	100, 135, 181, 206	0
2	F	342/364 (93%)	0.05	6 (1%) 68 57	131, 165, 204, 216	0
2	H	344/364 (94%)	-0.02	1 (0%) 94 90	94, 123, 149, 177	0
All	All	2709/2940 (92%)	0.02	59 (2%) 62 50	91, 141, 229, 312	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	69	VAL	8.2
1	E	224	CYS	5.6
2	D	195	LEU	4.4
1	G	147	PHE	4.1
1	G	70	LEU	4.0
1	E	225	TYR	3.9
1	G	189	PRO	3.8
1	E	219	SER	3.7
1	G	140	CYS	3.7
1	C	231	ALA	3.7
1	G	266	ASN	3.6
1	G	76	GLY	3.6
2	F	274	PHE	3.5
1	G	55	LYS	3.4
1	G	68	GLN	3.2
1	G	59	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	386	ARG	3.1
1	A	235	LEU	3.0
1	G	182	ILE	3.0
1	G	138	MET	3.0
1	G	71	GLY	2.9
1	G	66	THR	2.9
2	F	50	VAL	2.8
1	E	139	GLU	2.8
2	D	194	MET	2.8
2	H	135	LEU	2.7
2	D	242	PRO	2.7
1	G	337	HIS	2.7
1	G	245	ASP	2.6
2	F	289	LEU	2.5
2	F	278	ASN	2.5
1	G	160	GLU	2.5
1	G	167	MET	2.5
1	C	263	PHE	2.5
2	D	308	PHE	2.4
1	G	150	ILE	2.4
2	D	241	THR	2.4
1	E	218	ASN	2.4
2	D	102	VAL	2.3
2	F	236	LEU	2.2
2	B	27	LEU	2.2
1	E	107	LEU	2.2
1	C	377	ASP	2.2
1	G	291	TRP	2.2
2	D	202	GLN	2.1
1	G	52	LEU	2.1
1	G	131	ARG	2.1
2	D	307	TYR	2.1
1	G	88	GLU	2.1
1	G	329	THR	2.1
1	E	320	MET	2.1
1	G	257	LEU	2.1
1	E	167	MET	2.0
1	C	123	VAL	2.0
1	G	61	ASP	2.0
1	G	102	ARG	2.0
1	G	254	TYR	2.0
2	F	216	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	154	GLY	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	D	182	16/17	0.79	0.22	159,175,178,179	0
2	TPO	D	180	11/12	0.84	0.14	174,179,183,185	0
2	TPO	H	180	11/12	0.85	0.14	120,128,131,135	0
2	TPO	F	180	11/12	0.85	0.19	168,171,175,175	0
2	PTR	F	182	16/17	0.89	0.17	152,161,173,175	0
2	PTR	H	182	16/17	0.90	0.13	127,142,153,155	0
2	PTR	B	182	16/17	0.93	0.18	109,118,124,124	0
2	TPO	B	180	11/12	0.94	0.14	110,115,123,123	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

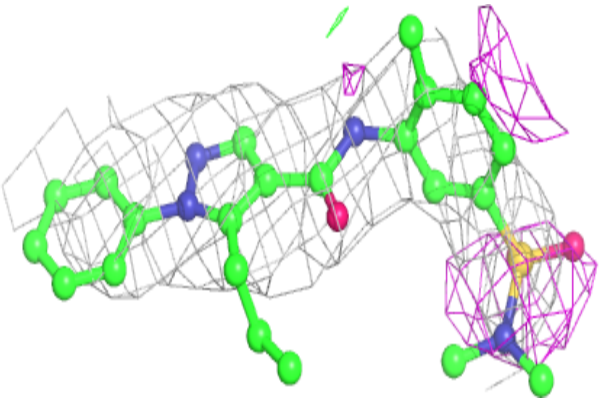
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

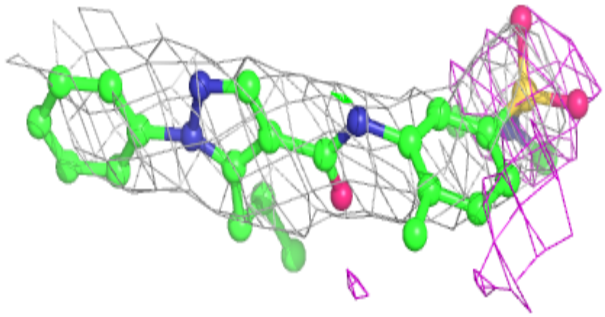
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	39G	H	401	30/30	0.79	0.66	108,111,115,119	0
3	39G	F	401	30/30	0.81	0.78	150,152,157,160	0
3	39G	B	401	30/30	0.90	0.50	102,105,109,113	0
3	39G	D	401	30/30	0.90	0.53	118,121,125,129	0

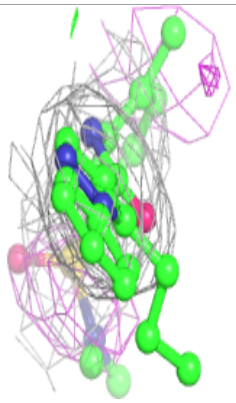
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 39G H 401:

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

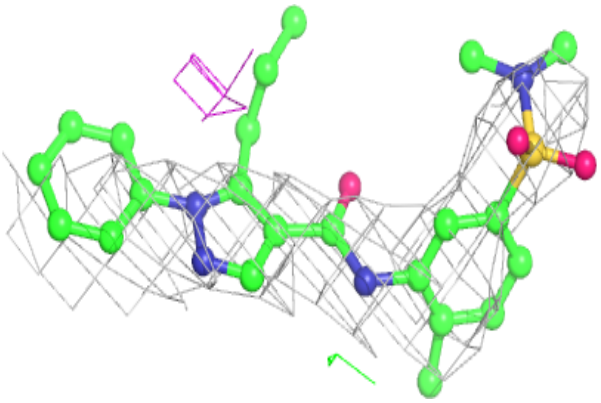


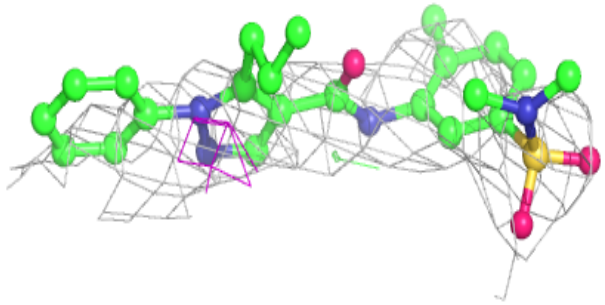


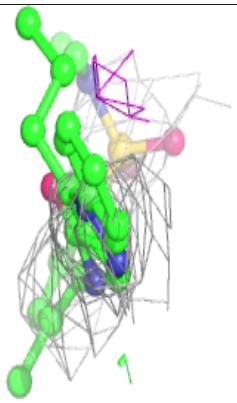


Electron density around 39G F 401:

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

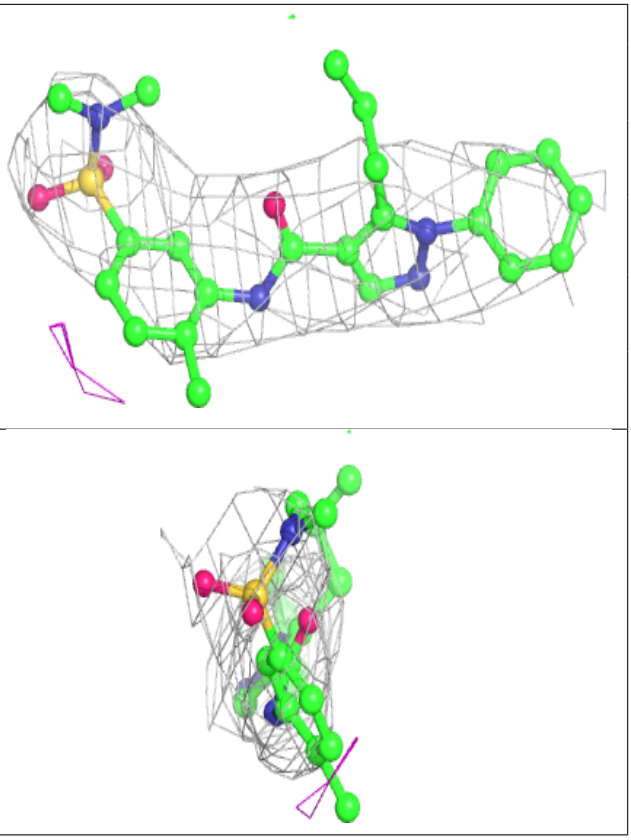






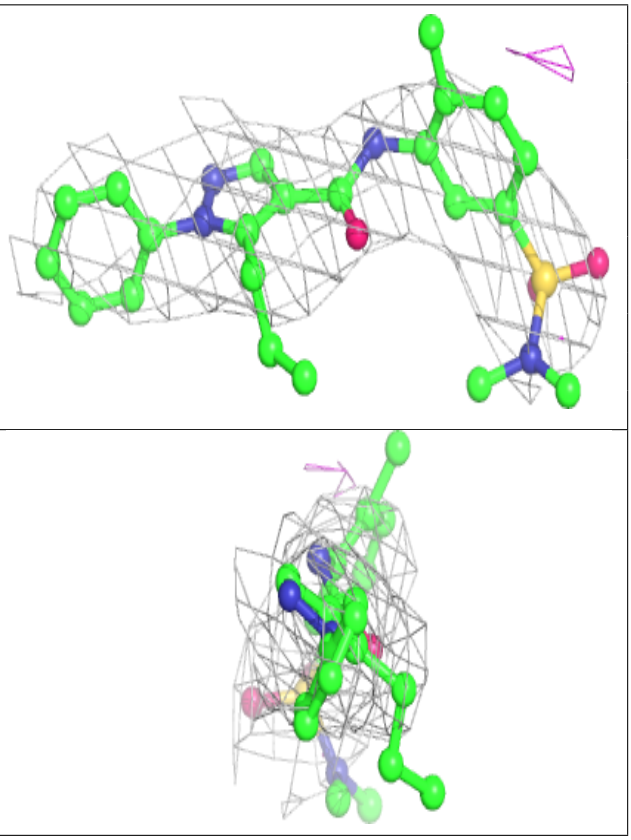
Electron density around 39G B 401:

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



Electron density around 39G D 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.