



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2021 – 04:20 PM EDT

PDB ID : 3DVA  
Title : Snapshots of catalysis in the E1 subunit of the pyruvate dehydrogenase multi-enzyme complex  
Authors : Pei, X.Y.; Titman, C.M.; Frank, R.A.W.; Leeper, F.J.; Luisi, B.F.  
Deposited on : 2008-07-18  
Resolution : 2.35 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](mailto: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.

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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 : 2.23.2  
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) : 2.23.2

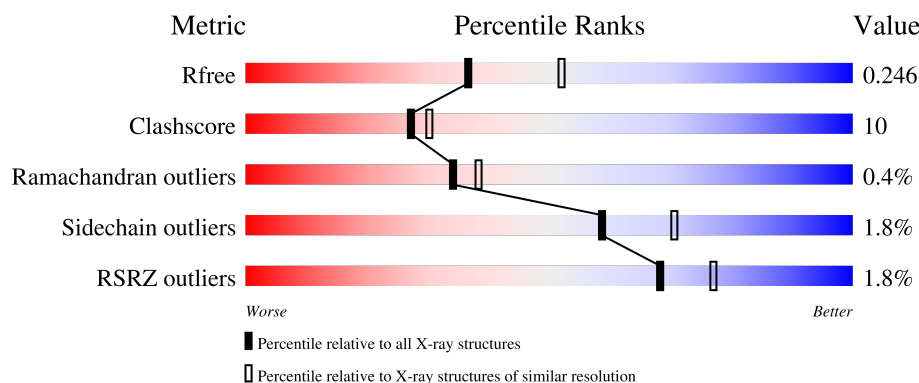
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	369	<div> <div>5%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	369	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	E	369	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	G	369	<div> <div>%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
2	B	325	<div> <div>77%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	325	<div><div></div><div>82%17%.</div></div>
2	F	325	<div><div></div><div>76%23%.</div></div>
2	H	325	<div><div></div><div>82%17%</div></div>
3	I	428	<div><div><div>2%</div><div></div></div><div>. . .90%</div></div>
3	J	428	<div><div><div>2%</div><div></div></div><div>. . .91%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23282 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 Pyruvate dehydrogenase E1 component subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	C	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	E	354	Total	C	N	O	S	0	0	0
			2798	1791	473	526	8			
1	G	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ALA	ILE	engineered mutation	UNP P21873
C	206	ALA	ILE	engineered mutation	UNP P21873
E	206	ALA	ILE	engineered mutation	UNP P21873
G	206	ALA	ILE	engineered mutation	UNP P21873

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	D	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	F	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	H	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			

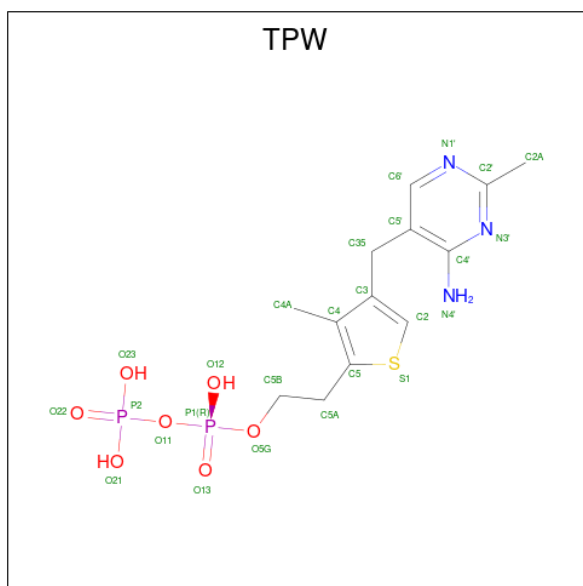
- Molecule 3 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	42	Total	C	N	O	S	0	0	0
			314	195	62	56	1			
3	J	40	Total	C	N	O	S	0	0	0
			294	180	59	54	1			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	E	2	Total	Mg	0	0
			2	2		
4	G	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>3</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
5	C	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
5	E	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	S	
			26	13	3	7	2	1	
								0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	K		
			1	1	0	0
6	D	1	Total	K		
			1	1	0	0

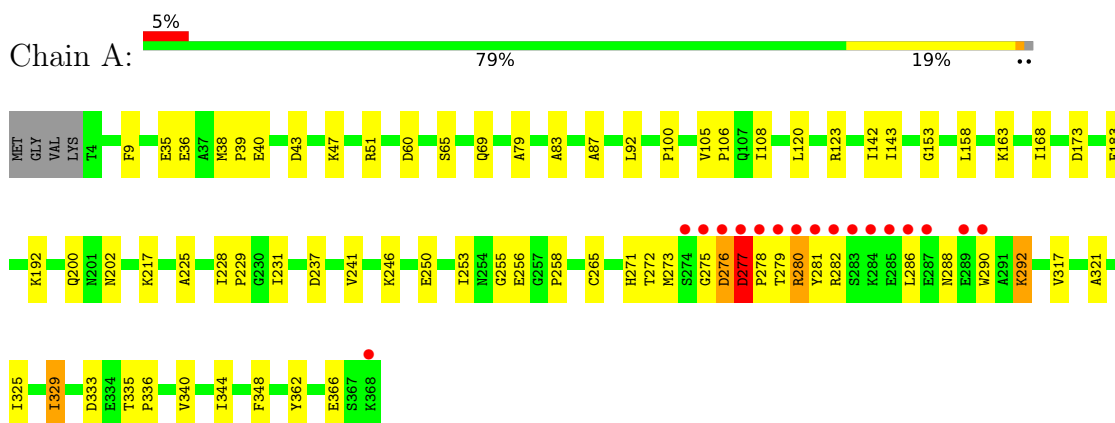
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	150	Total	O		
			150	150	0	0
7	B	139	Total	O		
			139	139	0	0
7	C	148	Total	O		
			148	148	0	0
7	D	161	Total	O		
			161	161	0	0
7	E	100	Total	O		
			100	100	0	0
7	F	126	Total	O		
			126	126	0	0
7	G	139	Total	O		
			139	139	0	0
7	H	155	Total	O		
			155	155	0	0
7	I	5	Total	O		
			5	5	0	0
7	J	4	Total	O		
			4	4	0	0

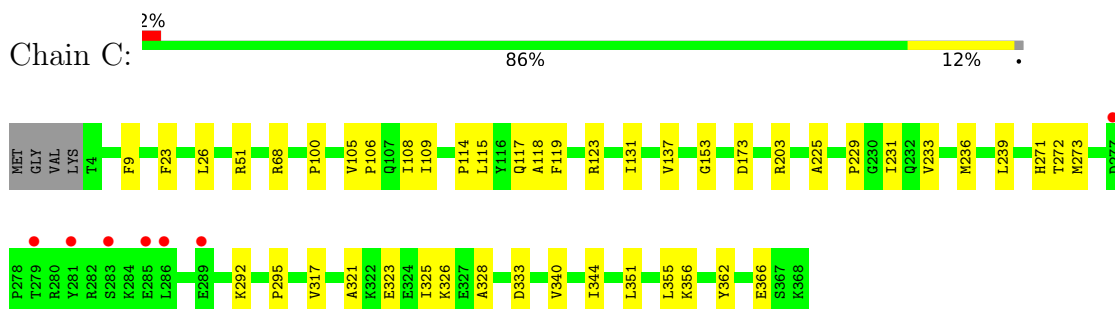
### 3 Residue-property plots [i](#)

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.

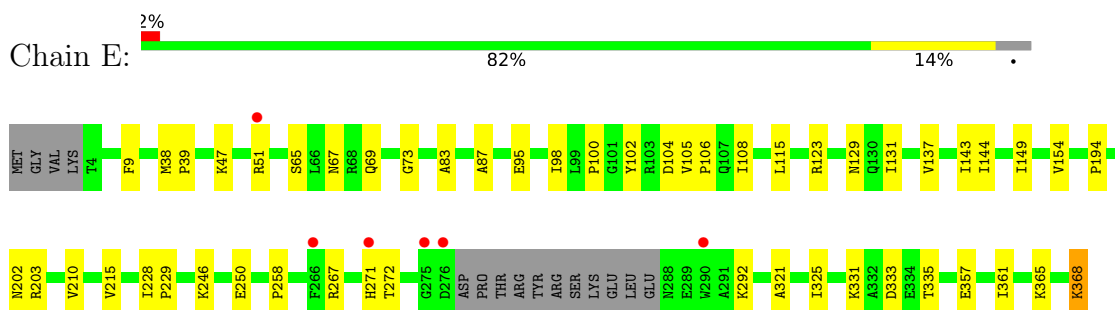
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



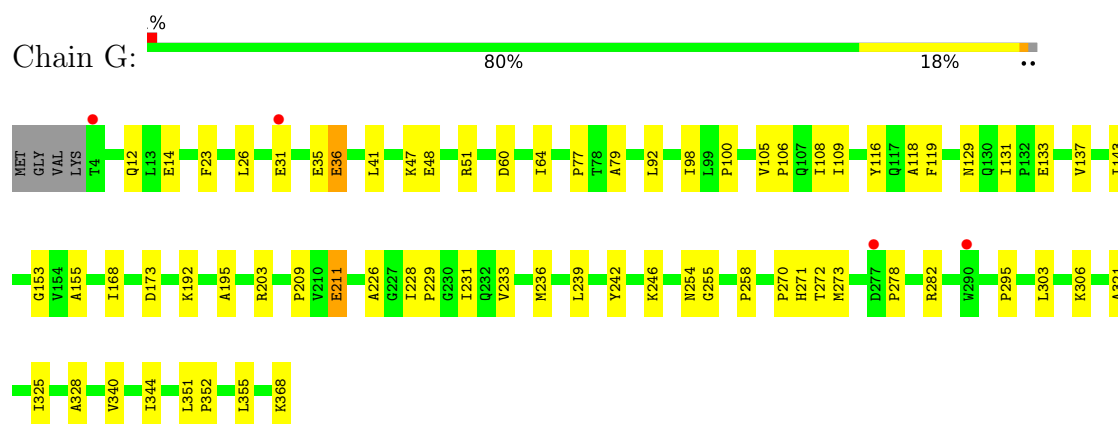
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



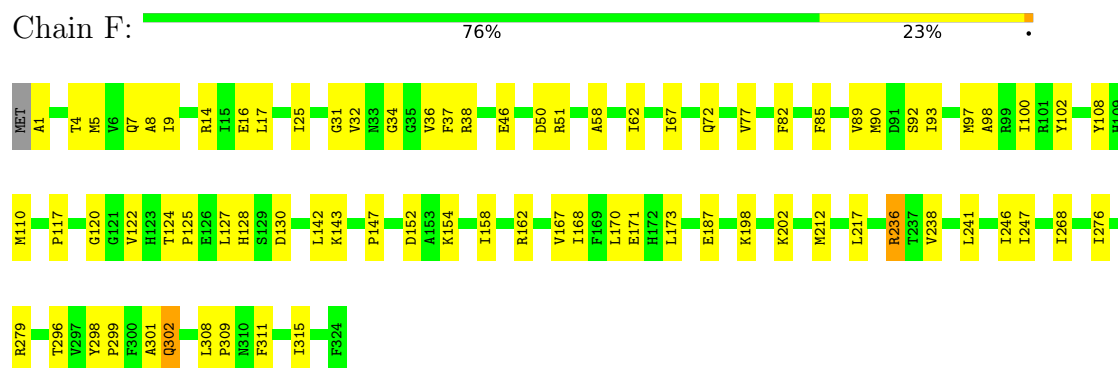
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



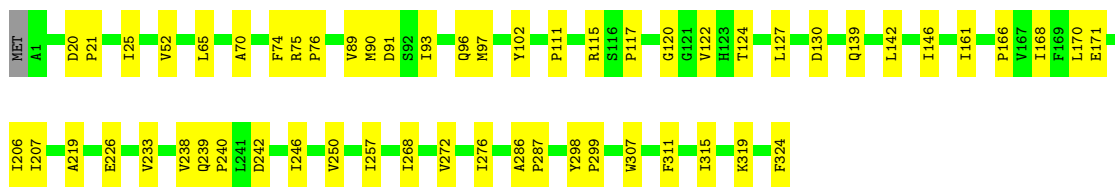
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

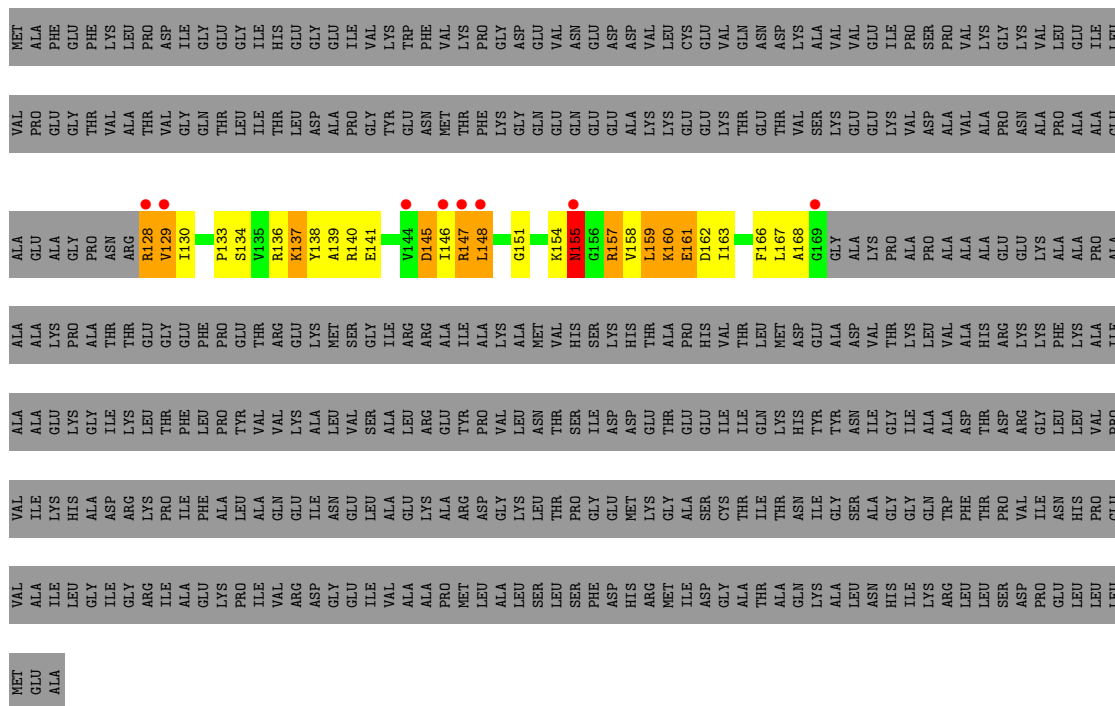


Chain H:



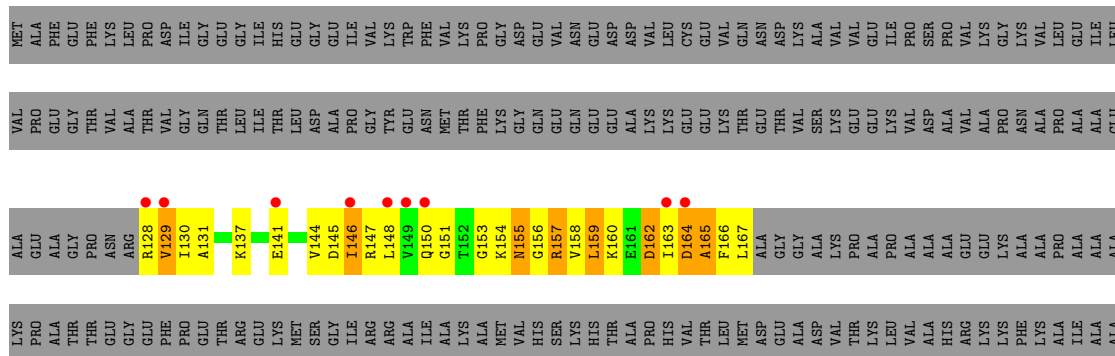
- Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain I:



- Molecule 3: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain J:



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.67Å 232.29Å 91.94Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	72.17 – 2.35 72.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (72.17-2.35) 98.9 (72.08-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.247 0.191 , 0.246	Depositor DCC
$R_{free}$ test set	5906 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: TPW, MG, K

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	0.38	0/2958	0.53	1/3995 (0.0%)
1	C	0.35	0/2958	0.48	0/3995
1	E	0.33	0/2858	0.45	0/3859
1	G	0.31	0/2958	0.47	0/3995
2	B	0.40	0/2534	0.55	2/3437 (0.1%)
2	D	0.27	0/2534	0.53	1/3437 (0.0%)
2	F	0.26	0/2534	0.52	1/3437 (0.0%)
2	H	0.28	0/2534	0.51	0/3437
3	I	1.44	1/316 (0.3%)	1.17	1/421 (0.2%)
3	J	1.54	0/295	1.16	1/395 (0.3%)
All	All	0.41	1/22479 (0.0%)	0.53	7/30408 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	138	TYR	CD2-CE2	-5.70	1.30	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASP	CB-CG-OD1	-7.67	111.40	118.30
2	B	234	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	236	ARG	CB-CA-C	-5.90	98.59	110.40
2	D	236	ARG	CB-CA-C	-5.84	98.72	110.40
3	J	162	ASP	CB-CG-OD1	-5.63	113.23	118.30
2	F	236	ARG	CB-CA-C	-5.61	99.18	110.40
3	I	145	ASP	N-CA-C	-5.16	97.08	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	2895	0	2871	73	0
1	C	2895	0	2871	34	0
1	E	2798	0	2776	44	0
1	G	2895	0	2871	64	0
2	B	2488	0	2515	47	0
2	D	2488	0	2515	46	0
2	F	2488	0	2515	58	0
2	H	2488	0	2515	47	0
3	I	314	0	322	40	0
3	J	294	0	291	36	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
5	A	26	0	16	1	0
5	C	26	0	16	3	0
5	E	26	0	16	1	0
5	G	26	0	16	3	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	150	0	0	3	0
7	B	139	0	0	5	0
7	C	148	0	0	3	0
7	D	161	0	0	7	0
7	E	100	0	0	6	0
7	F	126	0	0	5	0
7	G	139	0	0	10	0
7	H	155	0	0	2	0
7	I	5	0	0	0	0
7	J	4	0	0	2	0
All	All	23282	0	22126	449	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 (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:CB	1:A:282:ARG:HA	1.57	1.34
2:D:285:GLU:HG3	3:I:140:ARG:NH2	1.56	1.18
3:J:160:LYS:O	3:J:160:LYS:HG2	1.43	1.17
1:A:281:TYR:HB3	1:A:282:ARG:HA	1.30	1.11
1:A:281:TYR:HB2	1:A:282:ARG:HA	1.30	1.07
2:F:127:LEU:HD13	1:G:143:ILE:HD11	1.32	1.06
3:I:154:LYS:O	3:I:155:ASN:HB2	1.62	0.98
3:I:160:LYS:O	3:I:160:LYS:HG2	1.60	0.98
3:I:160:LYS:O	3:I:161:GLU:HG3	1.61	0.98
1:A:281:TYR:CB	1:A:282:ARG:CA	2.44	0.96
2:D:285:GLU:HG3	3:I:140:ARG:HH22	1.25	0.93
1:A:277:ASP:N	1:A:278:PRO:CD	2.30	0.91
3:I:160:LYS:C	3:I:161:GLU:HG3	1.87	0.91
3:J:154:LYS:C	3:J:156:GLY:H	1.74	0.89
3:I:151:GLY:HA2	3:I:162:ASP:OD2	1.73	0.89
3:J:164:ASP:O	3:J:165:ALA:HB2	1.73	0.89
3:I:159:LEU:HB2	3:I:161:GLU:OE1	1.74	0.88
2:F:152:ASP:HB2	7:F:1357:HOH:O	1.73	0.87
1:C:273:MET:HE2	7:C:1510:HOH:O	1.74	0.86
3:I:166:PHE:C	3:I:168:ALA:H	1.80	0.84
1:E:368:LYS:HA	1:E:368:LYS:NZ	1.93	0.84
2:F:247:ILE:HD11	2:F:279:ARG:HD2	1.59	0.83
1:C:321:ALA:O	1:C:325:ILE:HG12	1.77	0.83
1:A:277:ASP:N	1:A:278:PRO:HD2	1.91	0.82
1:A:277:ASP:H	1:A:278:PRO:CD	1.91	0.82
1:A:231:ILE:HD11	1:C:9:PHE:HE1	1.43	0.81
1:A:273:MET:HE2	1:A:273:MET:HA	1.59	0.81
2:D:285:GLU:CG	3:I:140:ARG:NH2	2.41	0.81
3:I:159:LEU:CB	3:I:161:GLU:OE1	2.29	0.80
3:I:160:LYS:O	3:I:161:GLU:CG	2.30	0.80
2:H:122:VAL:HG23	2:H:124:THR:HG23	1.65	0.79
3:J:157:ARG:HG2	3:J:158:VAL:N	1.97	0.79
3:I:160:LYS:O	3:I:160:LYS:CG	2.29	0.78
2:D:32:VAL:HG23	7:D:1518:HOH:O	1.81	0.78
1:A:281:TYR:HB3	1:A:282:ARG:CA	2.09	0.78
1:E:365:LYS:HE3	7:E:1497:HOH:O	1.85	0.77
3:J:144:VAL:HG12	3:J:145:ASP:N	1.98	0.77
2:B:198:LYS:HB3	2:B:217:LEU:HD21	1.65	0.77
2:D:122:VAL:HG23	2:D:124:THR:HG23	1.67	0.77
1:G:23:PHE:HB3	1:G:233:VAL:HG12	1.67	0.76
1:A:277:ASP:HB2	1:A:278:PRO:HD3	1.67	0.76
1:E:321:ALA:O	1:E:325:ILE:HG12	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:137:LYS:HG3	3:I:137:LYS:O	1.86	0.76
3:J:164:ASP:O	3:J:165:ALA:CB	2.30	0.76
2:H:286:ALA:HB1	2:H:287:PRO:HD2	1.66	0.76
1:E:115:LEU:HD21	1:E:325:ILE:HD13	1.66	0.75
1:C:123:ARG:NH1	1:C:333:ASP:OD1	2.20	0.75
1:A:231:ILE:HD11	1:C:9:PHE:CE1	2.21	0.74
1:A:246:LYS:HE2	1:A:250:GLU:OE1	1.88	0.74
2:D:285:GLU:HG3	3:I:140:ARG:HH21	1.52	0.73
2:F:127:LEU:CD1	1:G:143:ILE:HD11	2.15	0.72
3:J:154:LYS:C	3:J:156:GLY:N	2.41	0.72
1:G:36:GLU:HG3	7:G:1416:HOH:O	1.88	0.72
3:I:166:PHE:C	3:I:168:ALA:N	2.44	0.71
2:F:100:ILE:HG13	2:F:110:MET:HE3	1.71	0.70
1:C:109:ILE:HD11	1:C:118:ALA:HB2	1.70	0.70
1:A:292:LYS:N	1:A:292:LYS:HD2	2.07	0.69
2:F:302:GLN:HE21	2:F:302:GLN:HA	1.55	0.69
1:E:9:PHE:HZ	1:G:231:ILE:HD11	1.57	0.69
2:D:271:ASN:ND2	7:D:1427:HOH:O	2.25	0.69
3:J:144:VAL:CG1	3:J:145:ASP:N	2.55	0.68
2:B:89:VAL:O	2:B:89:VAL:HG22	1.94	0.68
1:E:9:PHE:CD1	1:G:229:PRO:HB3	2.29	0.68
1:A:281:TYR:HB2	1:A:282:ARG:CA	2.14	0.67
2:H:324:PHE:O	3:J:137:LYS:HE2	1.93	0.67
2:F:120:GLY:HA3	2:F:298:TYR:OH	1.95	0.67
1:E:131:ILE:H	1:E:131:ILE:HD12	1.60	0.66
2:H:311:PHE:O	2:H:315:ILE:HG12	1.95	0.66
3:I:139:ALA:HB2	3:I:163:ILE:HD12	1.77	0.66
2:D:298:TYR:CG	2:D:299:PRO:HD2	2.31	0.66
3:J:154:LYS:O	3:J:156:GLY:N	2.29	0.66
1:G:129:ASN:O	1:G:131:ILE:HD12	1.96	0.66
1:A:348:PHE:HE1	7:B:1328:HOH:O	1.78	0.65
2:F:5:MET:O	2:F:9:ILE:HG12	1.95	0.65
3:J:163:ILE:HD13	3:J:163:ILE:N	2.10	0.65
2:H:168:ILE:N	2:H:168:ILE:HD12	2.12	0.65
2:H:272:VAL:O	2:H:276:ILE:HG12	1.96	0.65
1:A:277:ASP:H	1:A:278:PRO:HD2	1.55	0.64
1:E:368:LYS:HA	1:E:368:LYS:HZ3	1.62	0.64
1:G:109:ILE:HD11	1:G:118:ALA:HB2	1.79	0.64
1:C:115:LEU:HD21	1:C:325:ILE:HD13	1.79	0.64
2:F:67:ILE:HG23	2:F:110:MET:CE	2.28	0.64
2:D:285:GLU:CG	3:I:140:ARG:HH21	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:ALA:HB1	2:D:287:PRO:HD2	1.81	0.63
1:E:129:ASN:O	1:E:131:ILE:HD12	1.98	0.63
1:A:92:LEU:HD11	1:A:168:ILE:HG21	1.80	0.63
2:B:120:GLY:HA3	2:B:298:TYR:OH	1.99	0.62
2:D:277:ASN:O	2:D:281:ILE:HB	1.99	0.62
1:E:267:ARG:NH2	7:E:1518:HOH:O	2.32	0.62
1:G:192:LYS:HE2	1:G:255:GLY:O	1.99	0.62
3:J:156:GLY:O	3:J:157:ARG:C	2.36	0.62
2:H:319:LYS:HE3	7:H:1574:HOH:O	2.00	0.62
1:E:368:LYS:HA	1:E:368:LYS:HZ2	1.64	0.61
2:F:89:VAL:HG22	2:F:89:VAL:O	2.00	0.61
2:D:142:LEU:HD13	2:D:168:ILE:HD11	1.82	0.61
1:A:40:GLU:H	1:A:40:GLU:CD	2.02	0.61
1:C:123:ARG:NH2	1:C:333:ASP:OD1	2.32	0.61
2:F:25:ILE:HD13	2:F:77:VAL:HB	1.83	0.61
2:F:296:THR:CG2	1:G:344:ILE:HD13	2.31	0.60
2:H:93:ILE:HA	2:H:97:MET:HG2	1.83	0.60
1:A:277:ASP:H	1:A:278:PRO:HD3	1.65	0.60
2:B:117:PRO:HA	2:B:171:GLU:O	2.02	0.60
3:J:156:GLY:C	3:J:157:ARG:O	2.35	0.60
3:J:157:ARG:HG2	3:J:158:VAL:H	1.66	0.59
2:B:74:PHE:O	2:B:76:PRO:HD3	2.03	0.59
2:H:298:TYR:CG	2:H:299:PRO:HD2	2.37	0.59
2:H:89:VAL:HG22	2:H:89:VAL:O	2.02	0.59
2:H:117:PRO:HA	2:H:171:GLU:O	2.03	0.59
1:G:14:GLU:HG3	7:G:1448:HOH:O	2.01	0.59
1:A:273:MET:HE2	1:A:273:MET:CA	2.33	0.59
1:G:64:ILE:HG23	1:G:273:MET:HE3	1.84	0.59
2:D:89:VAL:O	2:D:89:VAL:HG22	2.03	0.58
2:B:57:LEU:HD11	5:C:1370:TPW:H4A3	1.85	0.58
2:B:241:LEU:HD21	2:B:272:VAL:HG22	1.84	0.58
2:F:32:VAL:HG23	7:F:1328:HOH:O	2.02	0.58
3:J:157:ARG:HD2	3:J:159:LEU:HD23	1.86	0.58
2:F:102:TYR:OH	2:H:299:PRO:HA	2.04	0.57
1:A:9:PHE:CD1	1:C:229:PRO:HB3	2.39	0.57
1:A:142:ILE:HG12	2:D:126:GLU:HB3	1.85	0.57
1:A:292:LYS:HD2	1:A:292:LYS:H	1.67	0.57
2:F:37:PHE:CZ	2:F:173:LEU:HD22	2.39	0.57
2:F:67:ILE:HG23	2:F:110:MET:HE3	1.85	0.57
1:A:65:SER:O	1:A:69:GLN:HG3	2.05	0.57
2:B:122:VAL:HG23	2:B:124:THR:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ARG:CZ	1:C:333:ASP:OD1	2.53	0.57
2:H:120:GLY:HA3	2:H:298:TYR:OH	2.04	0.56
1:A:246:LYS:O	1:A:250:GLU:HG3	2.05	0.56
2:F:298:TYR:CG	2:F:299:PRO:HD2	2.41	0.56
1:G:352:PRO:HB3	2:H:240:PRO:HG3	1.86	0.56
1:G:60:ASP:OD2	1:G:79:ALA:HB2	2.06	0.56
2:B:281:ILE:HG13	2:B:281:ILE:O	2.05	0.56
2:F:311:PHE:O	2:F:315:ILE:HG12	2.05	0.56
2:B:102:TYR:OH	2:D:299:PRO:HA	2.06	0.56
2:H:206:ILE:HD12	2:H:257:ILE:HD11	1.88	0.56
2:B:37:PHE:CZ	2:B:173:LEU:HD22	2.41	0.55
2:F:299:PRO:HA	2:H:102:TYR:OH	2.06	0.55
3:J:160:LYS:O	3:J:160:LYS:CG	2.30	0.55
2:F:247:ILE:HD11	2:F:279:ARG:CD	2.35	0.55
2:H:207:ILE:HA	2:H:233:VAL:HG13	1.89	0.55
1:C:23:PHE:HB3	1:C:233:VAL:HG12	1.89	0.55
1:C:109:ILE:HD11	1:C:118:ALA:CB	2.36	0.55
3:J:166:PHE:O	3:J:167:LEU:CB	2.54	0.55
2:B:311:PHE:O	2:B:315:ILE:HG12	2.06	0.55
2:H:250:VAL:HG21	2:H:276:ILE:HD12	1.88	0.55
3:I:145:ASP:OD2	3:I:147:ARG:HB2	2.07	0.55
3:J:151:GLY:CA	3:J:158:VAL:HG22	2.37	0.55
2:D:223:LEU:HB3	2:D:228:ILE:HB	1.89	0.55
3:I:159:LEU:O	3:I:161:GLU:N	2.39	0.55
1:E:194:PRO:HG2	7:E:1444:HOH:O	2.07	0.55
3:J:154:LYS:O	3:J:155:ASN:HB2	2.07	0.55
1:A:153:GLY:HA2	2:B:65:LEU:HD12	1.89	0.55
1:A:329:ILE:O	1:A:329:ILE:HD13	2.06	0.55
1:C:271:HIS:CD2	1:C:272:THR:HG23	2.41	0.55
2:F:100:ILE:HG13	2:F:110:MET:CE	2.36	0.55
1:A:43:ASP:O	1:A:47:LYS:HG3	2.07	0.54
2:D:100:ILE:HG13	2:D:110:MET:HE3	1.88	0.54
2:F:241:LEU:HD21	7:F:1373:HOH:O	2.07	0.54
1:A:9:PHE:HZ	1:C:231:ILE:HD11	1.72	0.54
1:A:192:LYS:HE2	1:A:256:GLU:HA	1.88	0.54
1:A:281:TYR:HB2	1:A:282:ARG:HG2	1.89	0.54
1:A:60:ASP:OD2	1:A:79:ALA:HB2	2.08	0.54
1:A:277:ASP:CB	1:A:278:PRO:HD3	2.34	0.54
2:B:254:GLY:HA2	2:B:283:SER:O	2.08	0.54
2:F:246:ILE:CG2	2:F:276:ILE:HD11	2.38	0.54
3:J:151:GLY:HA3	3:J:158:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:GLY:HA3	2:D:298:TYR:OH	2.08	0.54
2:H:238:VAL:HB	2:H:268:ILE:HG12	1.90	0.54
3:J:157:ARG:HD3	7:J:432:HOH:O	2.08	0.54
2:D:142:LEU:HD23	2:D:166:PRO:HB2	1.90	0.53
2:F:117:PRO:HA	2:F:171:GLU:O	2.08	0.53
1:G:47:LYS:HG2	7:G:1474:HOH:O	2.07	0.53
1:G:271:HIS:CD2	1:G:272:THR:HG23	2.44	0.53
7:B:1370:HOH:O	3:I:134:SER:HB3	2.07	0.53
2:F:122:VAL:HG23	2:F:124:THR:HG23	1.91	0.53
1:G:35:GLU:H	1:G:35:GLU:CD	2.11	0.53
1:G:77:PRO:HG3	1:G:273:MET:HE1	1.90	0.53
3:J:147:ARG:HH21	3:J:147:ARG:HG3	1.74	0.53
1:E:144:ILE:HG12	5:E:1370:TPW:N3'	2.24	0.53
5:C:1370:TPW:H2	7:C:1455:HOH:O	2.09	0.53
3:I:129:VAL:CG2	3:I:130:ILE:N	2.72	0.53
3:I:137:LYS:HA	3:I:140:ARG:NH1	2.23	0.52
2:B:5:MET:O	2:B:9:ILE:HG12	2.09	0.52
2:B:298:TYR:CG	2:B:299:PRO:HD2	2.44	0.52
2:F:168:ILE:N	2:F:168:ILE:HD12	2.25	0.52
2:F:100:ILE:HG21	2:F:110:MET:HE2	1.91	0.52
3:J:157:ARG:CD	7:J:432:HOH:O	2.58	0.52
3:J:147:ARG:HG3	3:J:147:ARG:NH2	2.25	0.52
2:H:242:ASP:O	2:H:246:ILE:HG13	2.10	0.52
1:E:102:TYR:HE2	1:E:144:ILE:CD1	2.22	0.51
1:G:77:PRO:HG2	1:G:270:PRO:HD2	1.92	0.51
2:F:14:ARG:NH1	2:F:46:GLU:OE1	2.42	0.51
2:D:271:ASN:HB3	7:D:1420:HOH:O	2.09	0.51
1:E:271:HIS:CD2	1:E:272:THR:HG23	2.45	0.51
1:G:368:LYS:NZ	1:G:368:LYS:HB3	2.26	0.51
2:B:34:GLY:O	2:B:38:ARG:HA	2.11	0.51
1:G:100:PRO:HG3	1:G:108:ILE:HG21	1.93	0.51
1:A:83:ALA:O	1:A:87:ALA:HB3	2.10	0.51
2:H:75:ARG:HD3	2:H:161:ILE:O	2.10	0.51
1:A:100:PRO:HG3	1:A:108:ILE:HG21	1.92	0.51
1:C:100:PRO:HG3	1:C:108:ILE:HG21	1.93	0.51
1:G:153:GLY:HA2	2:H:65:LEU:HD12	1.92	0.51
2:F:125:PRO:HG2	2:F:128:HIS:CE1	2.45	0.51
2:H:146:ILE:HG12	2:H:170:LEU:HB2	1.93	0.51
1:G:109:ILE:HD11	1:G:118:ALA:CB	2.41	0.51
1:G:303:LEU:HD13	7:G:1474:HOH:O	2.10	0.51
1:A:158:LEU:HD23	1:A:163:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HE2	1:A:255:GLY:O	2.11	0.51
2:D:298:TYR:CD2	2:D:299:PRO:HD2	2.45	0.51
1:E:65:SER:O	1:E:69:GLN:HG3	2.10	0.51
7:B:1406:HOH:O	3:I:133:PRO:HD2	2.11	0.50
1:A:286:LEU:O	1:A:290:TRP:HD1	1.94	0.50
1:C:105:VAL:O	1:C:109:ILE:HG12	2.12	0.50
1:G:233:VAL:HB	7:G:1441:HOH:O	2.10	0.50
1:G:271:HIS:CE1	5:G:1370:TPW:H5A2	2.46	0.50
2:F:198:LYS:HB3	2:F:217:LEU:HD21	1.93	0.50
3:J:156:GLY:O	3:J:157:ARG:O	2.29	0.50
1:E:203:ARG:HB2	7:E:1453:HOH:O	2.11	0.50
2:F:246:ILE:HG22	2:F:276:ILE:HD11	1.93	0.50
1:G:352:PRO:HD2	1:G:355:LEU:HB2	1.93	0.50
3:I:148:LEU:O	3:I:166:PHE:CZ	2.64	0.50
3:J:154:LYS:O	3:J:155:ASN:CB	2.59	0.50
1:A:272:THR:O	1:A:273:MET:HE2	2.13	0.49
1:A:142:ILE:HD12	1:A:143:ILE:HG12	1.93	0.49
2:B:134:GLY:O	2:B:138:GLN:HG3	2.12	0.49
1:E:215:VAL:HG12	1:G:226:ALA:O	2.12	0.49
1:G:254:ASN:ND2	7:G:1447:HOH:O	2.45	0.49
2:H:74:PHE:O	2:H:76:PRO:HD3	2.11	0.49
1:A:183:GLU:OE1	2:B:58:ALA:HB1	2.12	0.49
2:F:36:VAL:HG23	2:F:37:PHE:CD2	2.47	0.49
1:A:123:ARG:HB3	2:D:302:GLN:HE21	1.78	0.49
1:A:228:ILE:HG21	1:A:258:PRO:HG2	1.94	0.49
2:B:201:GLY:H	2:B:231:GLU:HB2	1.76	0.49
1:C:68:ARG:HG3	7:C:1510:HOH:O	2.11	0.49
2:H:142:LEU:HD22	2:H:168:ILE:HD11	1.95	0.49
2:D:146:ILE:HG12	2:D:170:LEU:HB2	1.92	0.49
1:A:288:ASN:N	1:A:288:ASN:HD22	2.10	0.49
2:D:207:ILE:HA	2:D:233:VAL:HG13	1.94	0.49
1:G:133:GLU:HG2	7:H:1500:HOH:O	2.13	0.49
1:A:335:THR:HG22	7:A:1501:HOH:O	2.13	0.49
2:F:17:LEU:O	2:F:51:ARG:NH1	2.45	0.49
1:E:331:LYS:O	1:E:335:THR:HG23	2.12	0.49
2:F:170:LEU:HD13	7:F:1332:HOH:O	2.13	0.48
5:A:1370:TPW:H4A3	2:D:57:LEU:HD11	1.95	0.48
2:D:117:PRO:HA	2:D:171:GLU:O	2.12	0.48
1:E:100:PRO:HB2	1:E:104:ASP:HB2	1.95	0.48
2:H:226:GLU:OE1	2:H:319:LYS:NZ	2.45	0.48
1:E:228:ILE:HG21	1:E:258:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:299:PRO:HD3	2:H:307:TRP:CD2	2.48	0.48
1:E:357:GLU:O	1:E:361:ILE:HG12	2.13	0.48
2:F:98:ALA:HB2	2:F:142:LEU:HD21	1.95	0.48
2:B:299:PRO:HA	2:D:102:TYR:OH	2.14	0.48
1:C:105:VAL:N	1:C:106:PRO:CD	2.77	0.48
2:D:11:ASP:O	2:D:15:ILE:HG12	2.13	0.48
2:F:4:THR:OG1	2:F:7:GLN:HG3	2.13	0.48
1:A:51:ARG:HG3	1:A:317:VAL:HG22	1.96	0.48
2:B:36:VAL:HG23	2:B:37:PHE:CD2	2.48	0.48
1:E:228:ILE:HB	1:E:229:PRO:HD2	1.96	0.48
2:D:109:HIS:HE1	7:D:1436:HOH:O	1.96	0.48
2:D:311:PHE:O	2:D:315:ILE:HG13	2.14	0.48
1:G:271:HIS:HE1	5:G:1370:TPW:H5A2	1.78	0.48
1:G:278:PRO:HB3	1:G:282:ARG:HE	1.79	0.48
3:J:129:VAL:HG11	3:J:146:ILE:HG23	1.95	0.48
2:F:8:ALA:HB1	2:F:154:LYS:HB2	1.96	0.47
1:G:143:ILE:HD12	2:H:96:GLN:NE2	2.29	0.47
1:G:143:ILE:HD13	2:H:91:ASP:OD1	2.14	0.47
2:B:125:PRO:HG2	2:B:128:HIS:CE1	2.49	0.47
2:B:324:PHE:O	3:I:157:ARG:NH2	2.40	0.47
2:F:93:ILE:HA	2:F:97:MET:HG2	1.96	0.47
3:I:162:ASP:N	3:I:162:ASP:OD1	2.44	0.47
1:A:51:ARG:HG3	1:A:317:VAL:CG2	2.45	0.47
1:A:123:ARG:NH2	1:A:329:ILE:HD11	2.29	0.47
1:A:228:ILE:HB	1:A:229:PRO:HD2	1.96	0.47
1:G:340:VAL:O	1:G:344:ILE:HG12	2.14	0.47
1:A:271:HIS:CD2	1:A:272:THR:HG23	2.50	0.47
2:D:299:PRO:HD3	2:D:307:TRP:CD2	2.49	0.47
1:G:31:GLU:N	1:G:31:GLU:OE1	2.48	0.47
2:B:206:ILE:HD12	2:B:257:ILE:HD11	1.97	0.47
1:C:119:PHE:HE2	1:C:328:ALA:HB3	1.80	0.47
1:E:202:ASN:O	1:E:203:ARG:HB3	2.15	0.47
3:J:144:VAL:CG1	3:J:145:ASP:H	2.25	0.47
1:E:100:PRO:HG3	1:E:108:ILE:HG21	1.97	0.47
1:E:246:LYS:NZ	1:E:250:GLU:OE2	2.48	0.47
2:F:212:MET:HE2	2:F:212:MET:HA	1.97	0.46
1:G:119:PHE:HE2	1:G:328:ALA:HB3	1.80	0.46
1:A:278:PRO:O	1:A:279:THR:CG2	2.63	0.46
1:A:278:PRO:C	1:A:279:THR:HG23	2.35	0.46
2:D:8:ALA:HB1	2:D:154:LYS:HB2	1.98	0.46
2:H:142:LEU:HD23	2:H:166:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:ILE:HG21	2:D:187:GLU:HB3	1.98	0.46
1:E:143:ILE:HD11	2:H:127:LEU:HD13	1.98	0.46
2:F:268:ILE:C	2:F:268:ILE:HD12	2.36	0.46
2:D:318:ALA:O	2:D:322:MET:HG2	2.16	0.46
1:E:47:LYS:HE3	1:E:51:ARG:HH12	1.80	0.46
1:G:321:ALA:O	1:G:325:ILE:HG13	2.16	0.46
1:A:38:MET:SD	1:A:39:PRO:HD2	2.55	0.46
2:B:159:SER:OG	2:B:189:THR:HB	2.16	0.46
1:C:26:LEU:HG	1:C:239:LEU:HD12	1.98	0.46
1:G:64:ILE:HG12	1:G:273:MET:CE	2.45	0.46
2:B:1:ALA:N	2:B:183:VAL:O	2.48	0.46
1:C:362:TYR:O	1:C:366:GLU:HG3	2.16	0.46
2:D:177:ARG:HD3	7:D:1466:HOH:O	2.16	0.46
1:E:292:LYS:H	1:E:292:LYS:HD2	1.80	0.46
2:F:147:PRO:HD2	2:F:170:LEU:O	2.16	0.46
1:G:105:VAL:N	1:G:106:PRO:CD	2.78	0.46
3:J:130:ILE:O	3:J:131:ALA:HB2	2.15	0.46
1:A:123:ARG:NH2	1:A:333:ASP:OD1	2.46	0.46
2:B:268:ILE:C	2:B:268:ILE:HD12	2.36	0.46
2:B:75:ARG:HD3	2:B:161:ILE:O	2.16	0.45
2:F:90:MET:HG3	2:H:90:MET:HG3	1.98	0.45
1:E:9:PHE:CZ	1:G:231:ILE:HD11	2.44	0.45
2:F:102:TYR:HH	2:H:299:PRO:HA	1.79	0.45
1:A:280:ARG:HA	1:A:280:ARG:HD3	1.72	0.45
1:G:105:VAL:O	1:G:108:ILE:HG12	2.17	0.45
3:J:157:ARG:HD2	3:J:159:LEU:CD2	2.46	0.45
1:E:149:ILE:HG21	7:E:1527:HOH:O	2.16	0.45
1:G:41:LEU:HD21	1:G:242:TYR:CZ	2.52	0.45
2:D:282:LEU:HG	7:D:1485:HOH:O	2.16	0.45
1:G:98:ILE:HB	1:G:137:VAL:HG12	1.99	0.45
1:A:105:VAL:N	1:A:106:PRO:CD	2.79	0.45
1:C:340:VAL:O	1:C:344:ILE:HG13	2.16	0.45
2:D:37:PHE:CZ	2:D:173:LEU:HD22	2.52	0.45
2:B:299:PRO:HD3	2:B:307:TRP:CD2	2.52	0.45
1:E:100:PRO:HG3	1:E:108:ILE:CG2	2.47	0.45
2:F:143:LYS:HB2	2:F:167:VAL:HG22	1.99	0.45
2:B:25:ILE:HD13	2:B:77:VAL:HB	1.98	0.45
1:C:109:ILE:CD1	1:C:118:ALA:HB2	2.44	0.45
2:H:286:ALA:HB1	2:H:287:PRO:CD	2.43	0.45
2:H:298:TYR:CD2	2:H:299:PRO:HD2	2.52	0.45
1:A:225:ALA:HB2	1:C:225:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:ILE:HA	2:D:97:MET:HG2	1.99	0.45
2:H:115:ARG:NE	2:H:171:GLU:OE2	2.48	0.45
3:J:137:LYS:O	3:J:141:GLU:HG3	2.16	0.45
1:G:155:ALA:HB2	1:G:195:ALA:HB2	1.98	0.44
3:I:166:PHE:O	3:I:168:ALA:N	2.50	0.44
1:C:51:ARG:HG2	1:C:317:VAL:HG21	1.99	0.44
1:E:67:ASN:ND2	1:E:73:GLY:O	2.51	0.44
2:B:8:ALA:HB1	2:B:154:LYS:HB2	1.98	0.44
1:C:351:LEU:O	1:C:356:LYS:HE3	2.17	0.44
3:I:157:ARG:HG2	3:I:159:LEU:HD23	2.00	0.44
2:F:1:ALA:HB3	7:F:1442:HOH:O	2.17	0.44
2:H:268:ILE:HD12	2:H:268:ILE:C	2.37	0.44
1:E:105:VAL:N	1:E:106:PRO:CD	2.79	0.44
2:D:74:PHE:O	2:D:76:PRO:HD3	2.18	0.44
2:D:268:ILE:C	2:D:268:ILE:HD12	2.37	0.44
2:F:98:ALA:HB2	2:F:142:LEU:CD2	2.48	0.44
2:F:162:ARG:NH2	2:F:187:GLU:OE1	2.47	0.44
7:E:1463:HOH:O	1:G:12:GLN:HB2	2.17	0.44
2:F:34:GLY:O	2:F:38:ARG:HA	2.17	0.44
2:F:202:LYS:NZ	2:F:202:LYS:HB3	2.33	0.44
2:F:238:VAL:HB	2:F:268:ILE:HG12	1.99	0.44
1:G:306:LYS:NZ	1:G:306:LYS:HB3	2.33	0.44
2:H:168:ILE:HD12	2:H:168:ILE:H	1.83	0.44
2:B:12:ALA:HB3	2:B:157:LEU:HD23	1.99	0.44
1:C:153:GLY:HA2	2:D:65:LEU:HD12	2.00	0.44
1:C:236:MET:CE	1:C:295:PRO:HD3	2.48	0.44
1:G:209:PRO:HB2	1:G:211:GLU:OE2	2.18	0.44
1:G:254:ASN:HB3	7:G:1465:HOH:O	2.16	0.44
3:I:128:ARG:HB3	3:I:129:VAL:H	1.53	0.44
1:A:202:ASN:HA	1:A:265:CYS:O	2.18	0.43
2:B:17:LEU:O	2:B:51:ARG:NH1	2.46	0.43
2:H:70:ALA:HB1	2:H:111:PRO:HD2	2.00	0.43
3:I:159:LEU:CD1	3:I:161:GLU:OE1	2.66	0.43
1:E:123:ARG:NH2	1:E:333:ASP:OD1	2.49	0.43
3:I:146:ILE:HD11	3:I:158:VAL:HG22	2.00	0.43
2:B:277:ASN:O	2:B:281:ILE:HB	2.17	0.43
2:D:20:ASP:HA	2:D:21:PRO:HD2	1.88	0.43
1:E:131:ILE:HD13	2:F:108:TYR:HE2	1.84	0.43
1:E:203:ARG:O	1:E:210:VAL:N	2.50	0.43
2:D:277:ASN:HB2	7:D:1494:HOH:O	2.19	0.43
2:F:299:PRO:HA	2:H:102:TYR:HH	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ARG:HE	3:I:147:ARG:HB3	1.12	0.43
1:A:362:TYR:O	1:A:366:GLU:HG3	2.19	0.43
2:B:29:ASP:HB3	7:B:1373:HOH:O	2.19	0.43
1:G:211:GLU:H	1:G:211:GLU:CD	2.22	0.43
2:H:20:ASP:HA	2:H:21:PRO:HD2	1.87	0.43
1:C:131:ILE:HD13	1:C:137:VAL:HG23	2.01	0.43
1:G:92:LEU:HD11	1:G:168:ILE:HG21	2.01	0.43
2:B:124:THR:HB	2:B:125:PRO:HD2	1.99	0.43
1:E:98:ILE:HB	1:E:137:VAL:HG12	2.00	0.43
1:E:38:MET:SD	1:E:39:PRO:HD2	2.59	0.43
1:G:271:HIS:CE1	5:G:1370:TPW:S1	3.12	0.43
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.79	0.42
2:B:202:LYS:HG3	7:B:1454:HOH:O	2.19	0.42
1:G:228:ILE:HG21	1:G:258:PRO:HG2	2.01	0.42
1:G:246:LYS:HE3	7:G:1478:HOH:O	2.19	0.42
1:A:200:GLN:NE2	7:A:1378:HOH:O	2.52	0.42
1:A:321:ALA:O	1:A:325:ILE:HG13	2.19	0.42
1:E:95:GLU:H	1:E:95:GLU:HG2	1.60	0.42
1:A:275:GLY:HA2	1:A:276:ASP:HA	1.54	0.42
3:I:154:LYS:O	3:I:155:ASN:CB	2.46	0.42
3:J:146:ILE:CG2	3:J:147:ARG:N	2.81	0.42
1:A:237:ASP:O	1:A:241:VAL:HG23	2.20	0.42
2:F:308:LEU:HA	2:F:309:PRO:HD3	1.91	0.42
1:G:60:ASP:O	1:G:64:ILE:HG13	2.19	0.42
3:I:129:VAL:HG22	3:I:130:ILE:N	2.34	0.42
3:J:153:GLY:O	3:J:156:GLY:N	2.52	0.42
1:C:114:PRO:HD2	1:C:117:GLN:OE1	2.19	0.42
2:D:18:LYS:HE3	2:D:18:LYS:HA	2.01	0.42
2:D:255:ARG:NH2	2:D:285:GLU:HG2	2.35	0.42
3:J:131:ALA:HA	3:J:157:ARG:HG3	2.01	0.42
1:A:253:ILE:C	1:A:253:ILE:HD12	2.40	0.42
1:A:255:GLY:HA2	7:A:1498:HOH:O	2.20	0.42
1:C:355:LEU:HD23	1:C:355:LEU:HA	1.94	0.42
1:G:116:TYR:OH	7:G:1489:HOH:O	2.21	0.42
2:H:219:ALA:HA	2:H:315:ILE:HD11	2.02	0.42
1:A:120:LEU:HD11	1:A:335:THR:HG21	2.00	0.42
2:B:199:ARG:O	2:B:231:GLU:HA	2.20	0.42
3:I:159:LEU:HB3	3:I:161:GLU:OE1	2.15	0.42
1:A:292:LYS:N	1:A:292:LYS:CD	2.77	0.42
2:F:82:PHE:HB2	2:F:85:PHE:CE2	2.55	0.42
2:B:242:ASP:O	2:B:246:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:HA	1:A:336:PRO:HD3	1.91	0.41
1:C:203:ARG:HA	1:C:203:ARG:HD2	1.83	0.41
1:A:229:PRO:HB2	1:C:9:PHE:CD1	2.56	0.41
2:B:238:VAL:HB	2:B:268:ILE:HG12	2.01	0.41
1:E:83:ALA:O	1:E:87:ALA:HB3	2.21	0.41
2:F:58:ALA:O	2:F:62:ILE:HG13	2.19	0.41
2:B:201:GLY:N	2:B:231:GLU:HB2	2.35	0.41
1:G:351:LEU:HA	1:G:352:PRO:HD3	1.86	0.41
2:H:139:GLN:HB3	2:H:142:LEU:HD12	2.02	0.41
2:H:168:ILE:N	2:H:168:ILE:CD1	2.82	0.41
2:D:281:ILE:HG23	2:D:282:LEU:N	2.35	0.41
1:G:129:ASN:O	1:G:131:ILE:CD1	2.67	0.41
2:H:25:ILE:O	2:H:52:VAL:HA	2.21	0.41
3:J:162:ASP:OD1	3:J:162:ASP:N	2.50	0.41
2:F:16:GLU:OE2	2:F:158:ILE:HG23	2.20	0.41
1:G:143:ILE:HD12	2:H:96:GLN:HE21	1.85	0.41
1:A:123:ARG:HH21	1:A:329:ILE:HD11	1.86	0.41
2:B:282:LEU:HA	3:I:134:SER:HB2	2.03	0.41
1:G:26:LEU:HG	1:G:239:LEU:HD12	2.03	0.41
3:J:145:ASP:OD1	3:J:145:ASP:C	2.58	0.41
1:G:64:ILE:HG12	1:G:273:MET:HE2	2.03	0.41
1:G:48:GLU:HG3	1:G:51:ARG:HH21	1.86	0.40
1:G:236:MET:CE	1:G:295:PRO:HD3	2.50	0.40
1:A:340:VAL:O	1:A:344:ILE:HG13	2.22	0.40
1:E:123:ARG:NH1	1:E:333:ASP:OD1	2.51	0.40
1:G:203:ARG:HG3	7:G:1399:HOH:O	2.21	0.40
2:B:92:SER:O	2:B:97:MET:HG2	2.22	0.40
2:B:142:LEU:HD23	2:B:166:PRO:HB2	2.04	0.40
2:H:239:GLN:HA	2:H:240:PRO:HA	1.97	0.40
2:B:57:LEU:CD1	5:C:1370:TPW:H4A3	2.51	0.40
1:C:323:GLU:O	1:C:326:LYS:HB3	2.21	0.40
1:E:102:TYR:HE2	1:E:144:ILE:HD11	1.87	0.40
2:F:92:SER:O	2:F:97:MET:HG2	2.21	0.40
3:I:157:ARG:HG2	3:I:159:LEU:CD2	2.52	0.40
3:I:157:ARG:HH11	3:I:157:ARG:HD2	1.73	0.40
2:B:239:GLN:HA	2:B:240:PRO:HA	1.84	0.40
1:E:154:VAL:HG13	2:F:72:GLN:HE21	1.86	0.40
3:I:139:ALA:HB2	3:I:163:ILE:CD1	2.46	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	363/369 (98%)	352 (97%)	11 (3%)	0	100	100
1	C	363/369 (98%)	350 (96%)	13 (4%)	0	100	100
1	E	350/369 (95%)	339 (97%)	11 (3%)	0	100	100
1	G	363/369 (98%)	353 (97%)	10 (3%)	0	100	100
2	B	322/325 (99%)	315 (98%)	6 (2%)	1 (0%)	41	47
2	D	322/325 (99%)	312 (97%)	9 (3%)	1 (0%)	41	47
2	F	322/325 (99%)	307 (95%)	12 (4%)	3 (1%)	17	17
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	40/428 (9%)	31 (78%)	4 (10%)	5 (12%)	0	0
3	J	38/428 (9%)	30 (79%)	6 (16%)	2 (5%)	2	0
All	All	2805/3632 (77%)	2696 (96%)	97 (4%)	12 (0%)	34	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	ARG
3	J	165	ALA
2	F	301	ALA
3	I	161	GLU
3	I	167	LEU
2	D	236	ARG
2	F	236	ARG
3	I	136	ARG
3	I	160	LYS
3	I	155	ASN
3	J	157	ARG
2	F	31	GLY

### 5.3.2 Protein sidechains ⓘ

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	301/304 (99%)	293 (97%)	8 (3%)	44	55
1	C	301/304 (99%)	299 (99%)	2 (1%)	84	91
1	E	290/304 (95%)	289 (100%)	1 (0%)	92	96
1	G	301/304 (99%)	298 (99%)	3 (1%)	76	85
2	B	263/264 (100%)	260 (99%)	3 (1%)	73	84
2	D	263/264 (100%)	260 (99%)	3 (1%)	73	84
2	F	263/264 (100%)	260 (99%)	3 (1%)	73	84
2	H	263/264 (100%)	262 (100%)	1 (0%)	91	95
3	I	30/341 (9%)	21 (70%)	9 (30%)	0	0
3	J	28/341 (8%)	20 (71%)	8 (29%)	0	0
All	All	2303/2954 (78%)	2262 (98%)	41 (2%)	59	70

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	36	GLU
1	A	173	ASP
1	A	276	ASP
1	A	277	ASP
1	A	280	ARG
1	A	292	LYS
1	A	329	ILE
2	B	78	PRO
2	B	130	ASP
2	B	241	LEU
1	C	173	ASP
1	C	292	LYS
2	D	50	ASP
2	D	130	ASP
2	D	187	GLU

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Mol	Chain	Res	Type
1	E	368	LYS
2	F	50	ASP
2	F	130	ASP
2	F	302	GLN
1	G	36	GLU
1	G	173	ASP
1	G	211	GLU
2	H	130	ASP
3	I	128	ARG
3	I	129	VAL
3	I	137	LYS
3	I	141	GLU
3	I	147	ARG
3	I	148	LEU
3	I	155	ASN
3	I	157	ARG
3	I	159	LEU
3	J	128	ARG
3	J	129	VAL
3	J	146	ILE
3	J	148	LEU
3	J	150	GLN
3	J	155	ASN
3	J	159	LEU
3	J	164	ASP

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	288	ASN
2	B	33	ASN
2	B	123	HIS
2	B	239	GLN
1	C	19	GLN
1	C	69	GLN
2	D	72	GLN
2	D	109	HIS
2	D	123	HIS
2	D	271	ASN
1	E	81	GLN
1	E	288	ASN

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Mol	Chain	Res	Type
2	F	72	GLN
2	F	214	HIS
2	F	302	GLN
1	G	69	GLN
1	G	271	HIS
2	H	271	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	$\# Z  > 2$
5	TPW	E	1370	4	23,27,27	1.64	3 (13%)	30,40,40	1.88	8 (26%)
5	TPW	C	1370	4	23,27,27	1.83	3 (13%)	30,40,40	1.92	9 (30%)
5	TPW	A	1370	4	23,27,27	1.48	3 (13%)	30,40,40	1.84	9 (30%)
5	TPW	G	1370	4	23,27,27	1.85	3 (13%)	30,40,40	1.81	9 (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
5	TPW	E	1370	4	-	0/16/17/17	0/2/2/2
5	TPW	C	1370	4	-	2/16/17/17	0/2/2/2
5	TPW	A	1370	4	-	3/16/17/17	0/2/2/2
5	TPW	G	1370	4	-	5/16/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1370	TPW	C5A-C5	6.08	1.53	1.50
5	C	1370	TPW	C5A-C5	5.95	1.53	1.50
5	E	1370	TPW	C5A-C5	4.16	1.52	1.50
5	E	1370	TPW	C2-C3	-3.65	1.34	1.37
5	C	1370	TPW	C2-C3	-3.50	1.34	1.37
5	E	1370	TPW	P2-O22	3.48	1.61	1.50
5	G	1370	TPW	P2-O22	3.39	1.61	1.50
5	G	1370	TPW	C2-C3	-3.39	1.35	1.37
5	A	1370	TPW	C5A-C5	3.34	1.52	1.50
5	C	1370	TPW	P2-O22	3.34	1.61	1.50
5	A	1370	TPW	P2-O22	3.32	1.61	1.50
5	A	1370	TPW	C2-C3	-3.14	1.35	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1370	TPW	C3-C2-S1	-3.88	108.13	112.26
5	C	1370	TPW	C35-C5'-C6'	-3.72	116.58	121.73
5	A	1370	TPW	C3-C2-S1	-3.61	108.42	112.26
5	E	1370	TPW	C3-C2-S1	-3.59	108.44	112.26
5	G	1370	TPW	P1-O11-P2	-3.57	120.58	132.83
5	C	1370	TPW	P1-O11-P2	-3.42	121.10	132.83
5	A	1370	TPW	C35-C5'-C6'	-3.39	117.04	121.73
5	G	1370	TPW	C35-C5'-C6'	-3.32	117.14	121.73
5	G	1370	TPW	C3-C2-S1	-3.31	108.73	112.26
5	C	1370	TPW	C6'-N1'-C2'	3.29	121.56	115.96
5	E	1370	TPW	P1-O11-P2	-3.25	121.66	132.83
5	A	1370	TPW	O21-P2-O11	3.23	115.46	104.64
5	E	1370	TPW	C35-C5'-C6'	-3.18	117.33	121.73
5	E	1370	TPW	C6'-N1'-C2'	3.09	121.22	115.96
5	C	1370	TPW	N1'-C2'-N3'	-3.06	120.28	125.54
5	A	1370	TPW	C6'-N1'-C2'	2.99	121.04	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1370	TPW	N1'-C2'-N3'	-2.98	120.41	125.54
5	E	1370	TPW	O21-P2-O11	2.97	114.59	104.64
5	C	1370	TPW	C35-C5'-C4'	2.93	126.22	122.17
5	C	1370	TPW	O21-P2-O11	2.91	114.40	104.64
5	A	1370	TPW	N1'-C2'-N3'	-2.91	120.53	125.54
5	G	1370	TPW	C6'-N1'-C2'	2.86	120.83	115.96
5	A	1370	TPW	P1-O11-P2	-2.85	123.03	132.83
5	G	1370	TPW	O21-P2-O11	2.84	114.17	104.64
5	G	1370	TPW	N1'-C2'-N3'	-2.73	120.84	125.54
5	A	1370	TPW	C2A-C2'-N1'	2.70	120.11	117.14
5	A	1370	TPW	C35-C5'-C4'	2.49	125.60	122.17
5	E	1370	TPW	C35-C5'-C4'	2.25	125.28	122.17
5	E	1370	TPW	C2A-C2'-N1'	2.17	119.52	117.14
5	G	1370	TPW	C35-C5'-C4'	2.14	125.13	122.17
5	C	1370	TPW	C2A-C2'-N3'	2.13	120.47	117.15
5	A	1370	TPW	C5'-C6'-N1'	-2.06	120.39	123.82
5	C	1370	TPW	C5'-C6'-N1'	-2.06	120.39	123.82
5	G	1370	TPW	C5'-C6'-N1'	-2.04	120.43	123.82
5	G	1370	TPW	C2A-C2'-N1'	2.01	119.35	117.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1370	TPW	P1-O11-P2-O21
5	A	1370	TPW	P1-O11-P2-O23
5	C	1370	TPW	C5-C5A-C5B-O5G
5	G	1370	TPW	C5-C5A-C5B-O5G
5	G	1370	TPW	C5B-O5G-P1-O12
5	G	1370	TPW	C5B-O5G-P1-O13
5	G	1370	TPW	P2-O11-P1-O5G
5	C	1370	TPW	P2-O11-P1-O5G
5	A	1370	TPW	P1-O11-P2-O22
5	G	1370	TPW	C5B-O5G-P1-O11

There are no ring outliers.

4 monomers are involved in 8 short contacts:

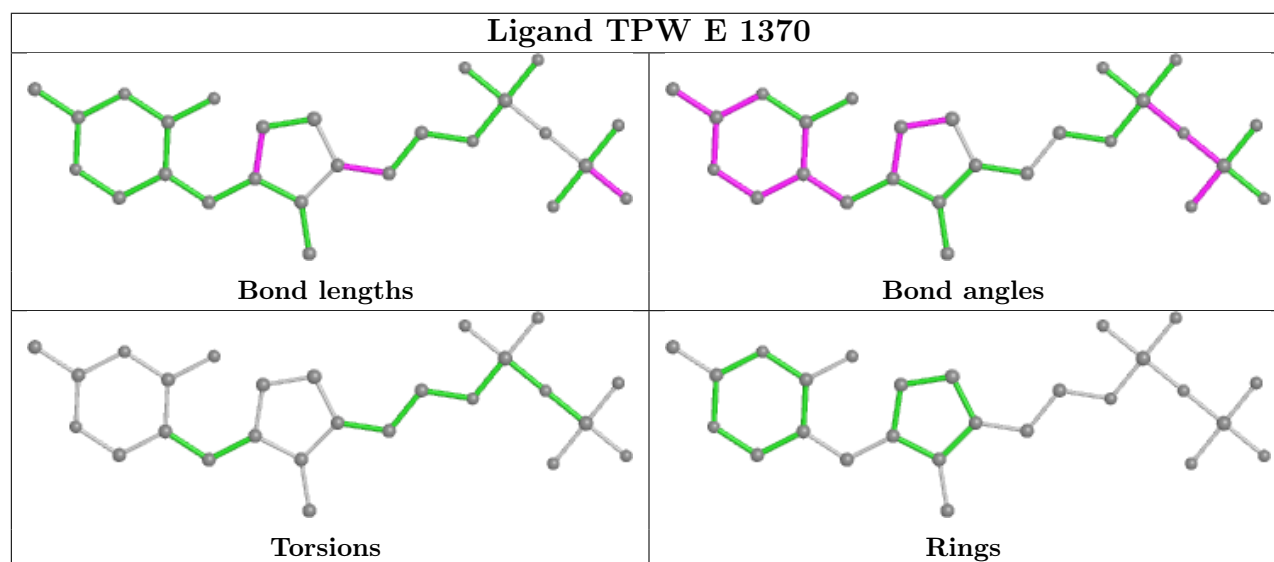
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1370	TPW	1	0
5	C	1370	TPW	3	0

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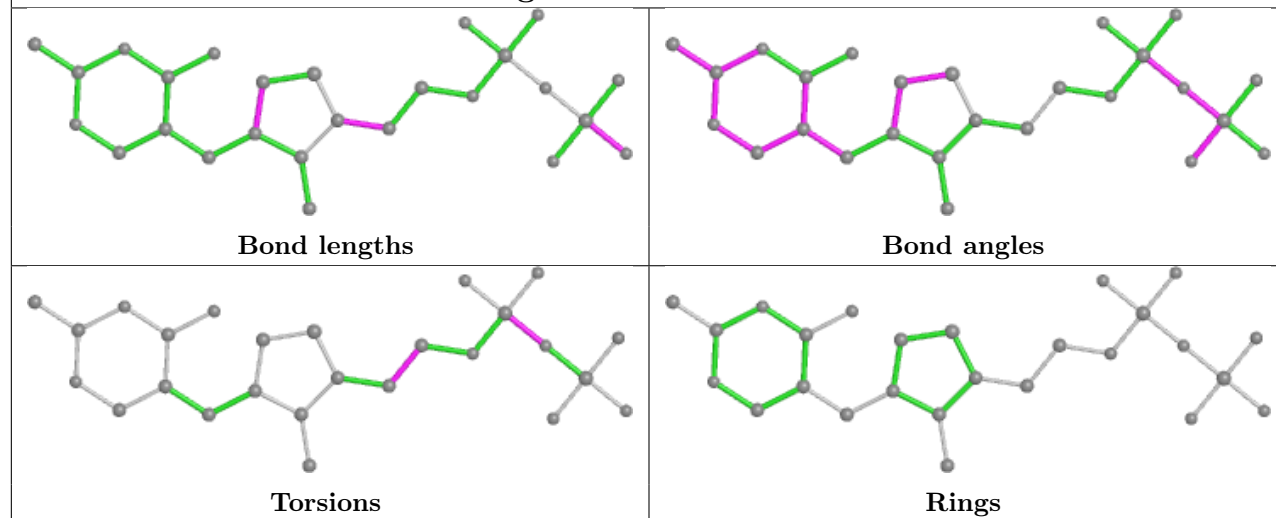
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1370	TPW	1	0
5	G	1370	TPW	3	0

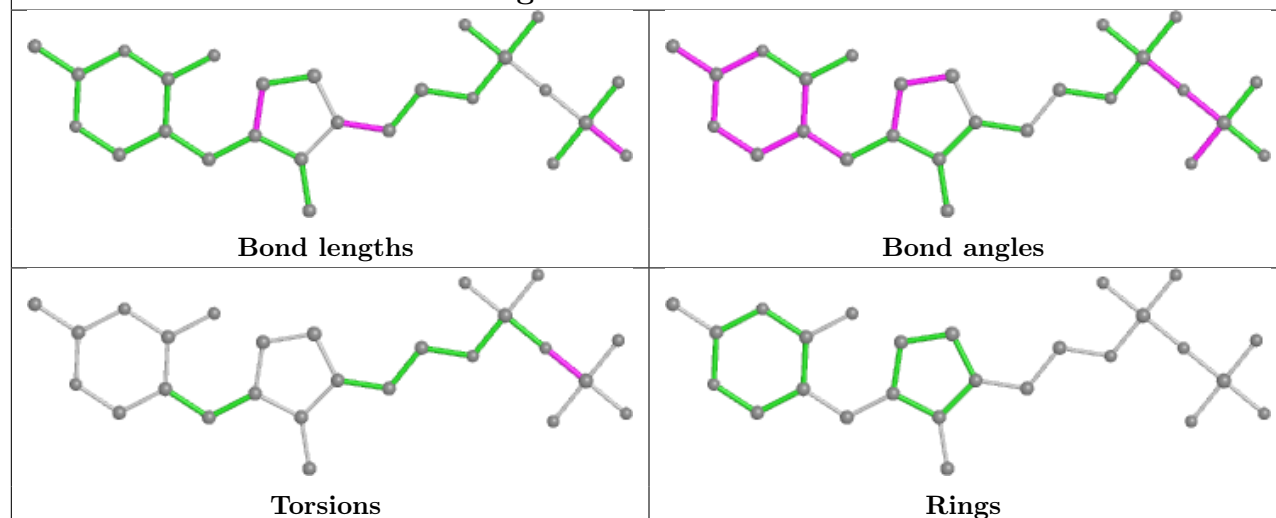
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



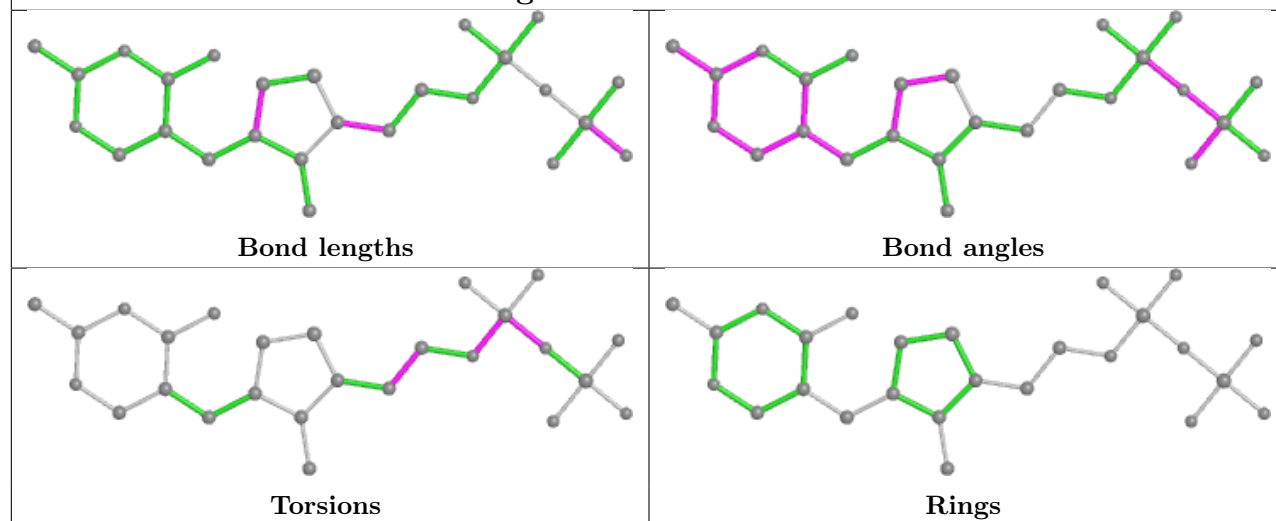
## Ligand TPW C 1370



## Ligand TPW A 1370



## Ligand TPW G 1370





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	365/369 (98%)	0.05	17 (4%) 31 44	15, 25, 44, 58	2 (0%)
1	C	365/369 (98%)	-0.07	7 (1%) 66 76	14, 24, 45, 58	2 (0%)
1	E	354/369 (95%)	0.01	6 (1%) 70 78	21, 32, 48, 60	2 (0%)
1	G	365/369 (98%)	-0.08	4 (1%) 80 87	20, 29, 48, 55	2 (0%)
2	B	324/325 (99%)	-0.28	0 100 100	16, 24, 34, 38	0
2	D	324/325 (99%)	-0.23	0 100 100	15, 20, 27, 30	0
2	F	324/325 (99%)	-0.17	0 100 100	21, 27, 34, 36	0
2	H	324/325 (99%)	-0.17	0 100 100	21, 25, 31, 32	0
3	I	42/428 (9%)	1.12	8 (19%) 1 2	22, 62, 70, 74	0
3	J	40/428 (9%)	0.98	9 (22%) 0 1	20, 53, 75, 78	0
All	All	2827/3632 (77%)	-0.08	51 (1%) 68 77	14, 26, 47, 78	8 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	8.1
1	A	281	TYR	6.0
1	A	286	LEU	5.9
1	A	280	ARG	5.3
3	I	128	ARG	5.3
1	C	286	LEU	5.2
1	A	276	ASP	5.1
3	I	148	LEU	4.8
1	E	290	TRP	4.1
1	A	284	LYS	3.8
1	G	277	ASP	3.7
3	I	155	ASN	3.5
1	E	276	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	282	ARG	3.4
1	A	289	GLU	3.3
1	A	275	GLY	3.1
1	A	287	GLU	3.0
3	J	149	VAL	3.0
3	J	129	VAL	2.9
1	G	4	THR	2.9
1	A	274	SER	2.8
3	I	129	VAL	2.8
1	A	277	ASP	2.8
3	J	150	GLN	2.7
1	E	271	HIS	2.6
1	A	285	GLU	2.6
3	J	128	ARG	2.6
1	C	277	ASP	2.6
3	I	146	ILE	2.5
1	A	290	TRP	2.5
1	C	281	TYR	2.5
3	J	163	ILE	2.4
1	E	266	PHE	2.4
3	J	141	GLU	2.4
1	A	278	PRO	2.4
1	C	279	THR	2.4
1	E	51	ARG	2.3
1	A	368	LYS	2.3
1	E	275	GLY	2.3
1	G	31	GLU	2.3
3	I	169	GLY	2.2
1	C	283	SER	2.2
3	J	164	ASP	2.2
1	C	285	GLU	2.2
1	A	279	THR	2.2
3	I	147	ARG	2.1
3	J	148	LEU	2.1
1	C	289	GLU	2.1
3	I	144	VAL	2.1
3	J	146	ILE	2.0
1	G	290	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

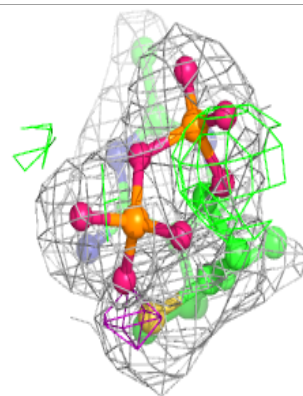
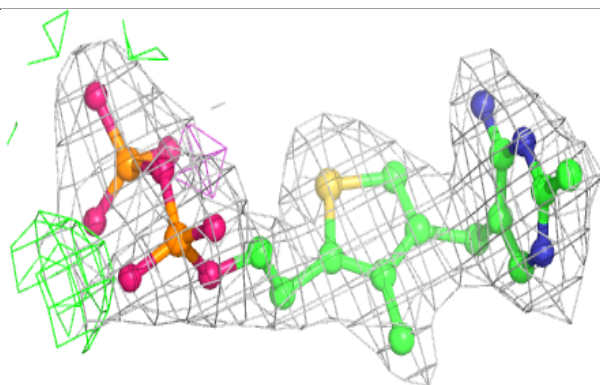
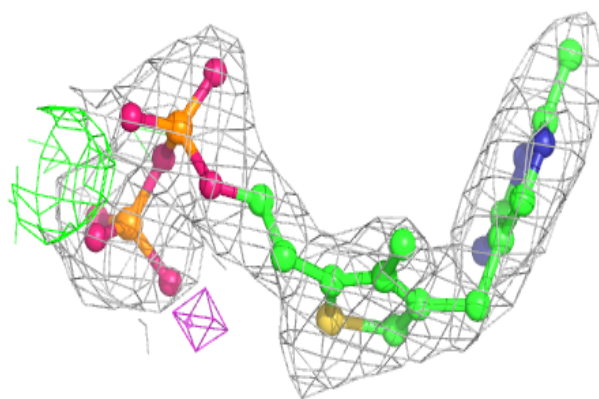
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	E	369	1/1	0.65	0.32	45,45,45,45	0
4	MG	A	1326	1/1	0.85	0.20	30,30,30,30	0
4	MG	G	369	1/1	0.93	0.11	16,16,16,16	0
4	MG	E	370	1/1	0.94	0.08	33,33,33,33	0
4	MG	A	1368	1/1	0.97	0.13	3,3,3,3	0
5	TPW	E	1370	26/26	0.97	0.10	19,20,20,20	0
5	TPW	G	1370	26/26	0.97	0.12	23,23,24,24	0
5	TPW	A	1370	26/26	0.98	0.12	13,13,15,15	0
5	TPW	C	1370	26/26	0.98	0.10	12,12,13,13	0
4	MG	C	1368	1/1	0.99	0.11	7,7,7,7	0
6	K	B	1325	1/1	0.99	0.04	16,16,16,16	0
6	K	D	1325	1/1	0.99	0.06	10,10,10,10	0

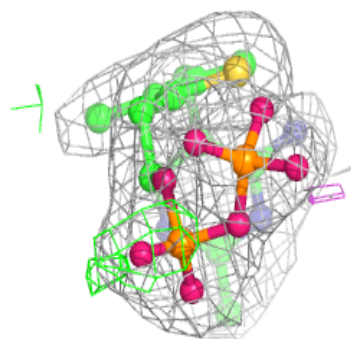
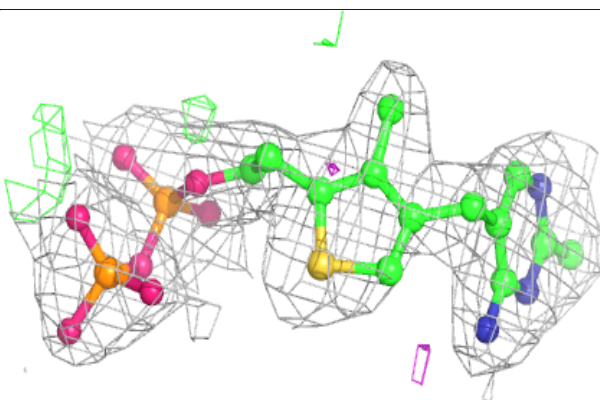
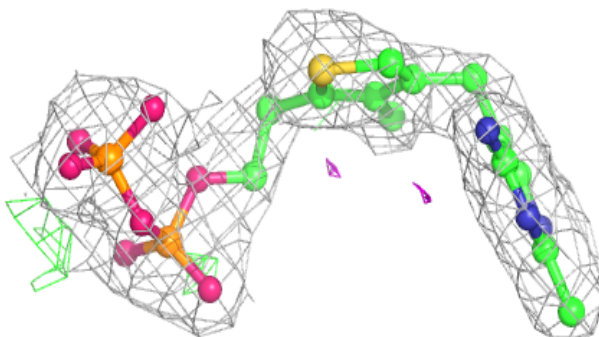
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPW E 1370:**

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

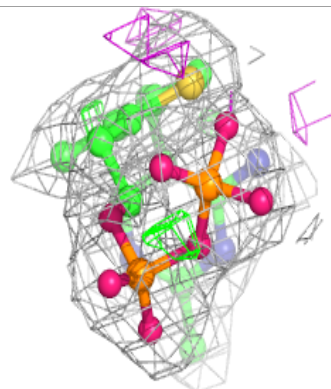
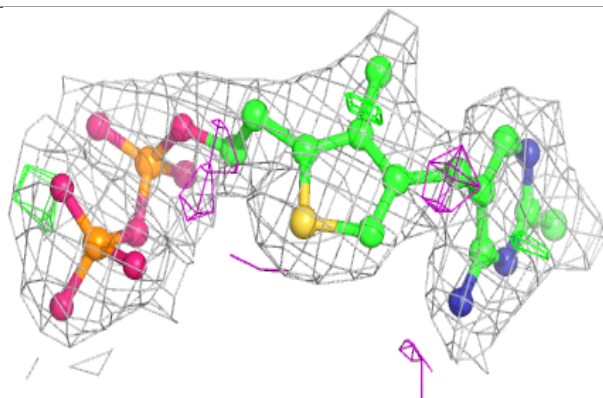
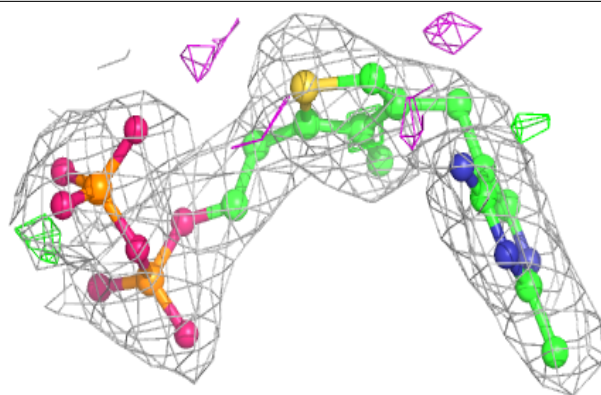
**Electron density around TPW G 1370:**

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

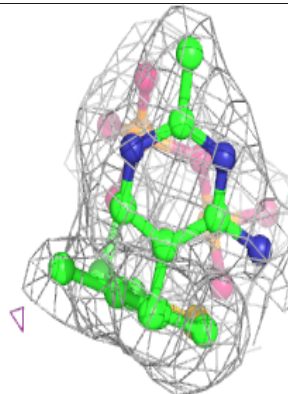
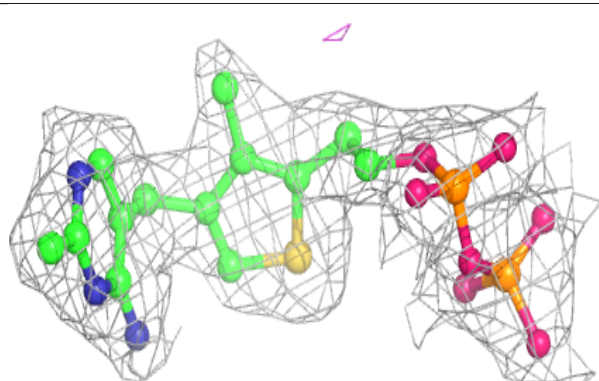
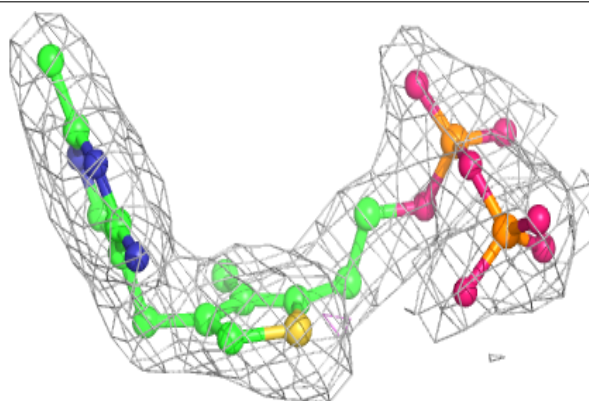


**Electron density around TPW A 1370:**

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

**Electron density around TPW C 1370:**

$2mF_o-DF_c$  (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.