Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 09:37 AM EDT

PDB ID	:	3IAF
Title	:	Structure of benzaldehyde lyase A28S mutant with monomethyl benzoylphosphonate
Authors	:	Brandt, G.S.; Petsko, G.A.; Ringe, D.; McLeish, M.J.
Deposited on	:	2009-07-13
Resolution	:	2.80 Å(reported)

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

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

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

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

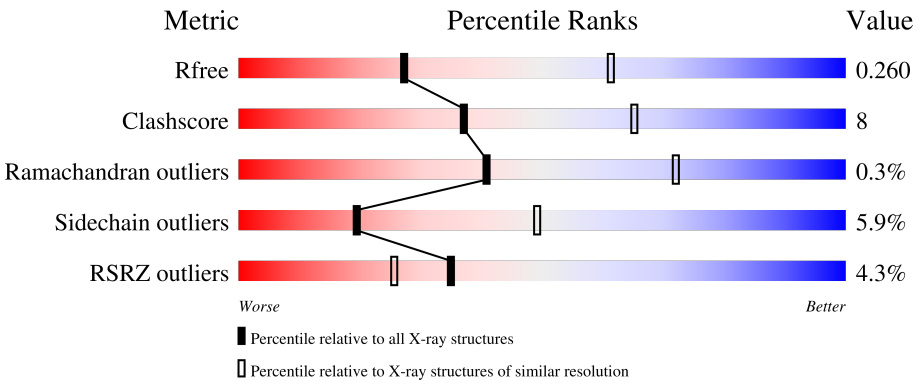
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	570	5% 81% 15% • •
1	B	570	6% 75% 20% • •
1	C	570	3% 80% 16% • •
1	D	570	2% 79% 16% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16626 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 Benzaldehyde lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	554	4084	2576	723	768	1	16	0	0	0
1	B	554	4084	2576	723	768	1	16	0	0	0
1	C	554	4084	2576	723	768	1	16	0	0	0
1	D	554	4084	2576	723	768	1	16	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SEP	ALA	engineered mutation	UNP Q9F4L3
A	563	GLY	-	expression tag	UNP Q9F4L3
A	564	SER	-	expression tag	UNP Q9F4L3
A	565	HIS	-	expression tag	UNP Q9F4L3
A	566	HIS	-	expression tag	UNP Q9F4L3
A	567	HIS	-	expression tag	UNP Q9F4L3
A	568	HIS	-	expression tag	UNP Q9F4L3
A	569	HIS	-	expression tag	UNP Q9F4L3
A	570	HIS	-	expression tag	UNP Q9F4L3
B	28	SEP	ALA	engineered mutation	UNP Q9F4L3
B	563	GLY	-	expression tag	UNP Q9F4L3
B	564	SER	-	expression tag	UNP Q9F4L3
B	565	HIS	-	expression tag	UNP Q9F4L3
B	566	HIS	-	expression tag	UNP Q9F4L3
B	567	HIS	-	expression tag	UNP Q9F4L3
B	568	HIS	-	expression tag	UNP Q9F4L3
B	569	HIS	-	expression tag	UNP Q9F4L3
B	570	HIS	-	expression tag	UNP Q9F4L3
C	28	SEP	ALA	engineered mutation	UNP Q9F4L3
C	563	GLY	-	expression tag	UNP Q9F4L3
C	564	SER	-	expression tag	UNP Q9F4L3

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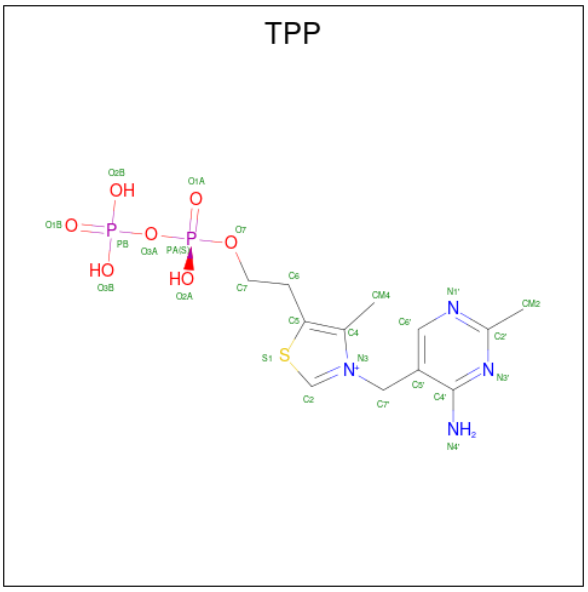
Chain	Residue	Modelled	Actual	Comment	Reference
C	565	HIS	-	expression tag	UNP Q9F4L3
C	566	HIS	-	expression tag	UNP Q9F4L3
C	567	HIS	-	expression tag	UNP Q9F4L3
C	568	HIS	-	expression tag	UNP Q9F4L3
C	569	HIS	-	expression tag	UNP Q9F4L3
C	570	HIS	-	expression tag	UNP Q9F4L3
D	28	SEP	ALA	engineered mutation	UNP Q9F4L3
D	563	GLY	-	expression tag	UNP Q9F4L3
D	564	SER	-	expression tag	UNP Q9F4L3
D	565	HIS	-	expression tag	UNP Q9F4L3
D	566	HIS	-	expression tag	UNP Q9F4L3
D	567	HIS	-	expression tag	UNP Q9F4L3
D	568	HIS	-	expression tag	UNP Q9F4L3
D	569	HIS	-	expression tag	UNP Q9F4L3
D	570	HIS	-	expression tag	UNP Q9F4L3

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	26	12	4	7	2	1	0	0
2	B	1	26	12	4	7	2	1	0	0
2	C	1	26	12	4	7	2	1	0	0
2	D	1	26	12	4	7	2	1	0	0

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

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

- Molecule 4 is water.

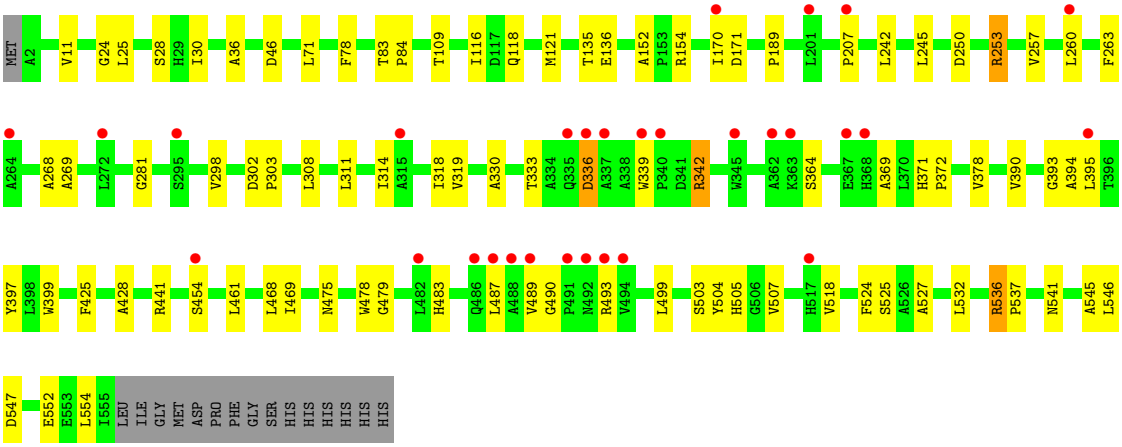
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0
4	B	30	Total O 30 30	0	0
4	C	57	Total O 57 57	0	0
4	D	48	Total O 48 48	0	0

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.

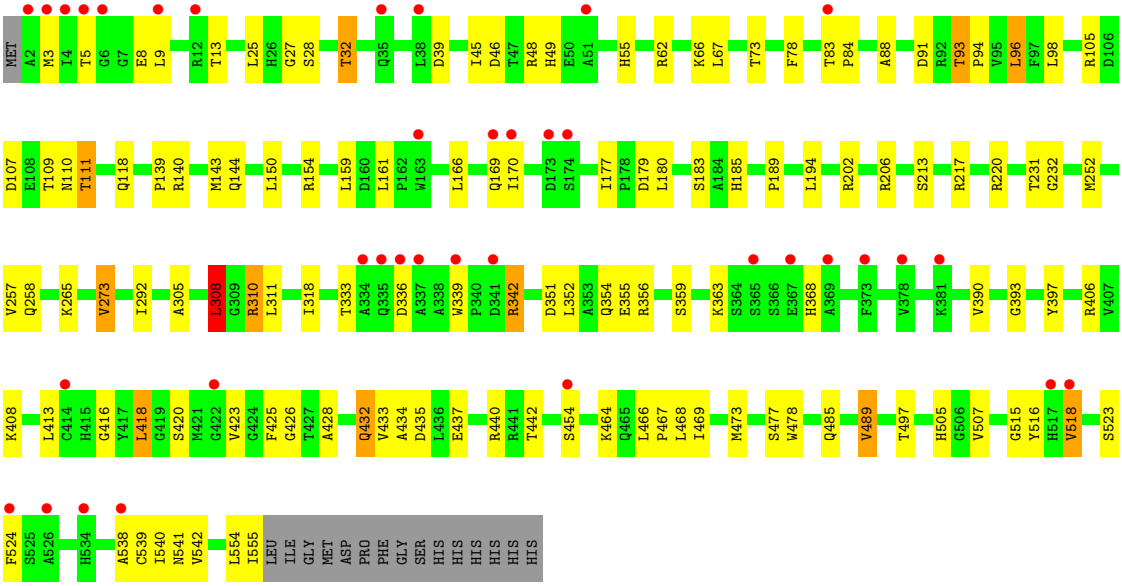
- Molecule 1: Benzaldehyde lyase

Chain A:



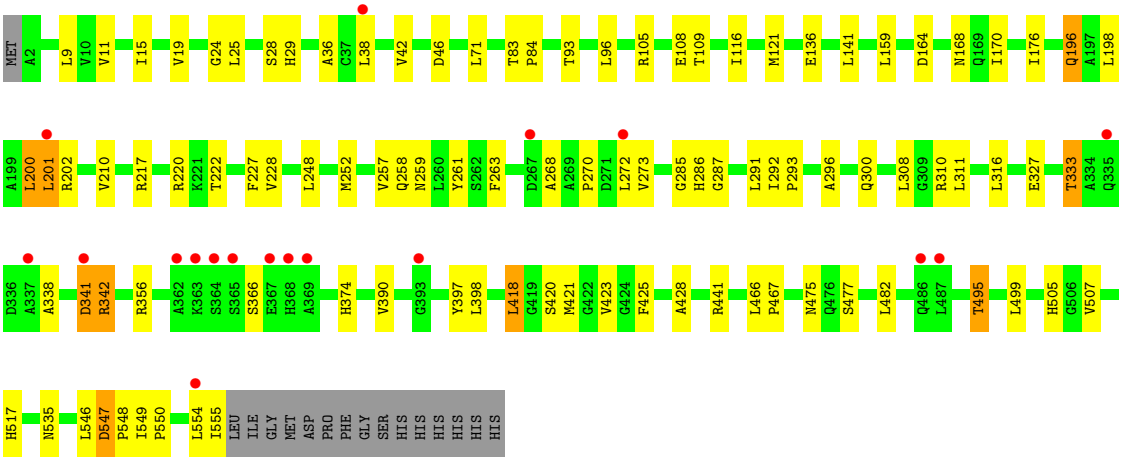
- Molecule 1: Benzaldehyde lyase

Chain B:



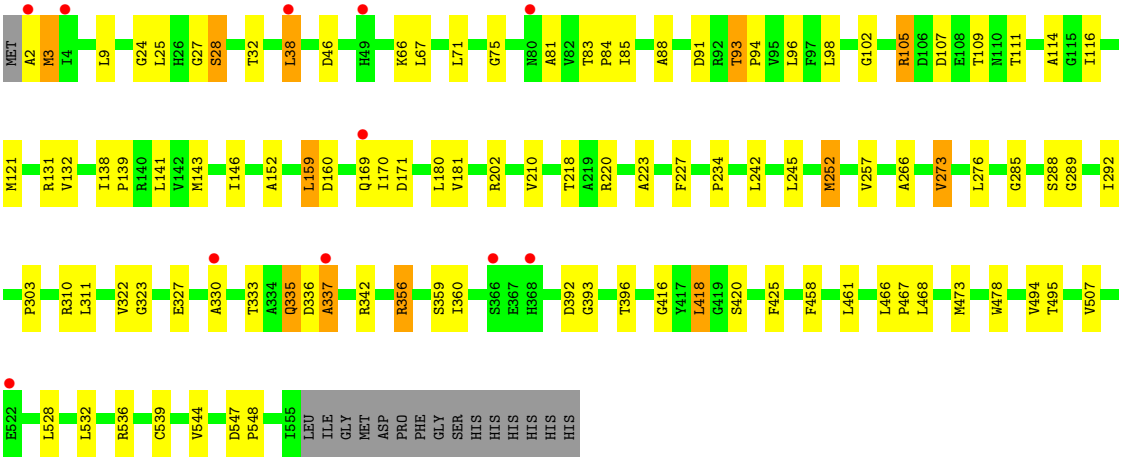
• Molecule 1: Benzaldehyde lyase

Chain C:



• Molecule 1: Benzaldehyde lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.96Å 150.96Å 195.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.89 – 2.80 44.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.89-2.80) 99.4 (44.10-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.260 0.212 , 0.260	Depositor DCC
R_{free} test set	6394 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16626	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0123e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, SEP

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	0.33	0/4156	0.52	0/5667
1	B	0.33	0/4156	0.56	0/5667
1	C	0.34	0/4156	0.56	0/5667
1	D	0.34	0/4156	0.55	1/5667 (0.0%)
All	All	0.34	0/16624	0.55	1/22668 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	266	ALA	CB-CA-C	5.42	118.23	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4084	0	4068	69	0
1	B	4084	0	4068	86	0
1	C	4084	0	4068	55	0
1	D	4084	0	4068	62	0
2	A	26	0	16	6	0
2	B	26	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	26	0	16	0	0
2	D	26	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	47	0	0	1	0
4	B	30	0	0	2	0
4	C	57	0	0	2	0
4	D	48	0	0	0	0
All	All	16626	0	16336	255	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 8.

All (255) 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:B:342:ARG:HG2	1:B:342:ARG:HH11	1.01	1.10
1:B:434:ALA:HA	1:B:437:GLU:HB2	1.45	0.98
1:B:518:VAL:HG21	1:B:524:PHE:HB2	1.47	0.96
1:C:342:ARG:HG3	1:C:342:ARG:HH11	1.28	0.95
1:B:342:ARG:HH11	1:B:342:ARG:CG	1.80	0.94
1:B:206:ARG:HH21	1:B:206:ARG:HG3	1.33	0.93
1:D:342:ARG:HG3	1:D:342:ARG:HH11	1.34	0.91
1:B:518:VAL:HG13	1:B:542:VAL:HA	1.50	0.90
1:B:342:ARG:HG2	1:B:342:ARG:NH1	1.81	0.87
1:A:371:HIS:HE1	1:A:399:TRP:CZ3	1.97	0.83
1:B:32:THR:HG21	1:B:166:LEU:HB3	1.62	0.82
1:C:300:GLN:OE1	1:C:308:LEU:HA	1.82	0.80
1:B:554:LEU:O	1:B:555:ILE:HG13	1.85	0.76
1:A:503:SER:HB2	1:A:505:HIS:CE1	2.21	0.76
1:A:207:PRO:HD3	1:A:342:ARG:NH2	2.00	0.76
1:D:2:ALA:O	1:D:171:ASP:HA	1.86	0.76
1:C:342:ARG:HH11	1:C:342:ARG:CG	1.98	0.75
1:C:93:THR:HG22	1:C:217:ARG:NH2	2.00	0.75
1:B:434:ALA:HA	1:B:437:GLU:CB	2.17	0.74
1:A:371:HIS:CE1	1:A:399:TRP:CH2	2.77	0.73
1:A:207:PRO:HD3	1:A:342:ARG:HH21	1.52	0.72
1:D:273:VAL:HG11	1:D:292:ILE:HG23	1.73	0.71
1:A:371:HIS:CE1	1:A:399:TRP:CZ3	2.78	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TRP:HE3	2:A:571:TPP:H72	1.57	0.69
1:B:518:VAL:CG2	1:B:524:PHE:HB2	2.22	0.68
1:A:136:GLU:HG3	1:A:170:ILE:HD13	1.75	0.68
1:C:227:PHE:HA	1:C:333:THR:HG21	1.75	0.68
1:C:495:THR:HG21	1:D:38:LEU:HG	1.75	0.67
1:C:554:LEU:O	1:C:555:ILE:HG13	1.95	0.65
1:C:198:LEU:HA	1:C:201:LEU:HD23	1.78	0.65
1:D:91:ASP:OD1	1:D:416:GLY:HA3	1.97	0.65
1:B:505:HIS:HB3	1:B:541:ASN:HB2	1.79	0.65
1:B:202:ARG:HH22	1:B:336:ASP:CG	2.01	0.64
1:B:418:LEU:CD1	1:B:420:SER:HB2	2.28	0.64
1:A:505:HIS:HB3	1:A:541:ASN:HB2	1.79	0.64
1:B:518:VAL:HG12	1:B:541:ASN:O	1.98	0.64
1:C:270:PRO:HD2	1:C:293:PRO:HG3	1.78	0.63
1:A:478:TRP:CE3	2:A:571:TPP:H72	2.34	0.62
1:A:536:ARG:HG3	1:A:537:PRO:CD	2.29	0.62
1:B:435:ASP:HB3	1:B:440:ARG:O	1.99	0.62
1:D:289:GLY:HA2	1:D:292:ILE:O	1.99	0.61
1:B:478:TRP:HB3	2:B:571:TPP:H61	1.83	0.61
1:B:310:ARG:HG3	1:B:311:LEU:HG	1.83	0.60
1:B:98:LEU:HD22	1:B:161:LEU:HD11	1.83	0.60
1:A:260:LEU:HD12	1:A:263:PHE:CD2	2.36	0.60
1:A:281:GLY:HA3	1:B:110:ASN:HB2	1.84	0.60
1:B:32:THR:HG21	1:B:166:LEU:CB	2.30	0.60
1:B:9:LEU:HD11	1:B:170:ILE:HD11	1.84	0.60
1:C:220:ARG:HD3	1:C:327:GLU:OE1	2.01	0.59
1:C:505:HIS:CE1	1:C:517:HIS:HB2	2.37	0.59
1:A:364:SER:HB2	1:A:371:HIS:CE1	2.37	0.58
1:D:418:LEU:HD13	1:D:420:SER:HB2	1.85	0.58
1:C:285:GLY:HA3	1:C:291:LEU:HD23	1.86	0.58
1:A:135:THR:HB	1:A:170:ILE:HD11	1.84	0.58
1:A:78:PHE:CD2	1:A:118:GLN:HG2	2.39	0.58
1:C:210:VAL:HG13	1:C:257:VAL:HG11	1.86	0.58
1:C:342:ARG:HG3	1:C:342:ARG:NH1	2.09	0.58
1:A:336:ASP:HB2	1:A:339:TRP:NE1	2.19	0.57
1:A:536:ARG:HG3	1:A:537:PRO:HD2	1.86	0.57
1:B:390:VAL:HG21	1:B:428:ALA:HA	1.87	0.57
1:B:418:LEU:HD13	1:B:420:SER:HB2	1.84	0.57
1:C:108:GLU:HG3	1:D:310:ARG:HH12	1.69	0.57
1:B:273:VAL:HG11	1:B:292:ILE:HG23	1.86	0.57
1:C:93:THR:HG22	1:C:217:ARG:HH21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:HG3	1:D:342:ARG:NH1	2.07	0.57
1:D:88:ALA:HA	1:D:93:THR:HG23	1.88	0.56
1:A:507:VAL:HG13	1:B:507:VAL:HG13	1.87	0.56
1:C:108:GLU:HG3	1:D:310:ARG:NH1	2.21	0.56
1:C:507:VAL:HG13	1:D:507:VAL:HG13	1.87	0.56
1:D:528:LEU:O	1:D:532:LEU:HB2	2.05	0.56
1:A:336:ASP:HB2	1:A:339:TRP:HE1	1.71	0.56
1:A:263:PHE:HB3	1:A:269:ALA:HA	1.86	0.56
1:D:3:MET:HG3	1:D:169:GLN:HB3	1.88	0.56
1:B:45:ILE:HD13	1:B:433:VAL:HG21	1.88	0.55
1:B:342:ARG:CG	1:B:342:ARG:NH1	2.49	0.55
1:B:433:VAL:O	1:B:434:ALA:HB3	2.07	0.55
1:C:136:GLU:CD	1:C:136:GLU:H	2.10	0.55
1:D:81:ALA:O	1:D:85:ILE:HG13	2.06	0.55
1:B:518:VAL:HG11	1:B:542:VAL:HG22	1.88	0.55
1:D:478:TRP:HB3	2:D:571:TPP:H61	1.89	0.54
1:D:75:GLY:HA2	1:D:116:ILE:HD11	1.87	0.54
1:D:102:GLY:HA3	1:D:114:ALA:HB2	1.88	0.54
1:B:432:GLN:HG3	1:B:468:LEU:HB2	1.88	0.54
1:B:206:ARG:HG3	1:B:206:ARG:NH2	2.10	0.54
1:B:27:GLY:HA3	1:B:73:THR:HB	1.90	0.54
1:B:232:GLY:O	1:B:342:ARG:HB3	2.08	0.54
1:B:518:VAL:CG1	1:B:541:ASN:O	2.56	0.54
1:C:116:ILE:HB	1:C:121:MET:HE1	1.90	0.54
1:C:228:VAL:HG11	1:C:248:LEU:HD22	1.88	0.54
1:C:273:VAL:HG11	1:C:292:ILE:HG23	1.88	0.54
1:D:392:ASP:OD1	1:D:393:GLY:N	2.39	0.54
1:A:24:GLY:O	1:A:46:ASP:HA	2.09	0.53
1:B:189:PRO:HB3	1:B:318:ILE:HG21	1.90	0.53
1:C:535:ASN:HB2	4:C:585:HOH:O	2.09	0.53
1:D:227:PHE:HA	1:D:333:THR:HG21	1.91	0.53
1:D:131:ARG:HA	1:D:160:ASP:HB3	1.91	0.52
1:B:351:ASP:O	1:B:355:GLU:HB2	2.10	0.52
1:A:263:PHE:HD1	1:A:268:ALA:O	1.93	0.52
1:D:547:ASP:N	1:D:548:PRO:HD2	2.25	0.52
1:B:32:THR:CG2	1:B:166:LEU:HB3	2.38	0.51
1:C:15:ILE:HD11	1:C:42:VAL:HG21	1.93	0.51
1:B:3:MET:HB3	1:B:169:GLN:HB3	1.93	0.51
1:B:516:TYR:HB2	1:B:540:ILE:HG13	1.93	0.51
1:A:260:LEU:HA	1:A:263:PHE:CD2	2.46	0.51
1:A:536:ARG:HG3	1:A:537:PRO:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:CD1	1:C:420:SER:HB2	2.41	0.50
1:D:418:LEU:CD1	1:D:420:SER:HB2	2.41	0.50
1:C:109:THR:HA	1:D:311:LEU:HD21	1.92	0.50
1:A:189:PRO:HB3	1:A:318:ILE:HG21	1.94	0.50
1:A:298:VAL:HB	1:A:314:ILE:HG22	1.94	0.50
1:A:242:LEU:HD12	1:A:245:LEU:HD12	1.94	0.50
1:A:475:ASN:HB2	1:A:546:LEU:HB2	1.92	0.50
1:A:109:THR:HG22	1:B:311:LEU:HD21	1.93	0.49
1:A:504:TYR:HE1	1:B:48:ARG:NH2	2.10	0.49
1:C:200:LEU:HD22	1:C:272:LEU:HD13	1.95	0.49
1:A:250:ASP:HA	1:A:253:ARG:HG3	1.95	0.49
1:B:78:PHE:CD2	1:B:118:GLN:HG2	2.48	0.49
1:B:359:SER:O	1:B:363:LYS:HG2	2.11	0.49
1:B:418:LEU:HD12	1:B:420:SER:HB2	1.94	0.49
1:C:196:GLN:HG2	1:C:316:LEU:HD22	1.95	0.49
1:C:418:LEU:HD13	1:C:420:SER:HB2	1.94	0.49
1:B:94:PRO:HG3	1:B:154:ARG:HG2	1.95	0.48
1:B:478:TRP:CE3	2:B:571:TPP:HM41	2.48	0.48
1:C:547:ASP:N	1:C:548:PRO:HD2	2.27	0.48
1:B:62:ARG:HB3	1:B:413:LEU:HD22	1.96	0.48
1:D:132:VAL:HG22	1:D:141:LEU:HD23	1.95	0.48
1:A:311:LEU:HD21	1:B:109:THR:HG22	1.94	0.48
1:B:96:LEU:HD13	1:B:98:LEU:HG	1.96	0.48
1:D:220:ARG:HA	1:D:220:ARG:NE	2.28	0.48
1:D:234:PRO:HA	1:D:252:MET:O	2.13	0.48
1:B:88:ALA:HA	1:B:93:THR:HG23	1.95	0.48
1:D:24:GLY:O	1:D:46:ASP:HA	2.14	0.48
1:D:116:ILE:HB	1:D:121:MET:CE	2.44	0.48
1:B:189:PRO:HG2	1:B:194:LEU:HD13	1.96	0.47
1:C:482:LEU:HD22	1:C:546:LEU:HD21	1.95	0.47
1:A:302:ASP:O	1:A:319:VAL:HA	2.13	0.47
1:D:152:ALA:HB1	1:D:303:PRO:HB3	1.97	0.47
1:C:293:PRO:HG2	1:C:296:ALA:HB2	1.97	0.47
1:A:395:LEU:HD13	4:A:596:HOH:O	2.13	0.47
1:B:5:THR:OG1	1:B:8:GLU:HB2	2.15	0.47
1:B:477:SER:HB2	1:B:497:THR:O	2.13	0.47
1:C:342:ARG:CG	1:C:342:ARG:NH1	2.65	0.47
1:D:202:ARG:NH2	1:D:336:ASP:O	2.44	0.47
1:D:242:LEU:HD12	1:D:245:LEU:HD12	1.96	0.47
1:C:257:VAL:O	1:C:291:LEU:HD12	2.14	0.47
1:B:434:ALA:CA	1:B:437:GLU:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HG13	1:D:181:VAL:HG11	1.97	0.46
1:D:210:VAL:HG13	1:D:257:VAL:HG11	1.98	0.46
1:A:30:ILE:HD12	1:A:71:LEU:HG	1.97	0.46
1:C:202:ARG:NH2	1:C:338:ALA:O	2.49	0.46
1:D:333:THR:HA	1:D:336:ASP:OD1	2.15	0.46
1:D:105:ARG:H	1:D:105:ARG:HG2	1.59	0.46
1:A:518:VAL:HG21	1:A:524:PHE:HA	1.98	0.45
1:A:116:ILE:HB	1:A:121:MET:CE	2.46	0.45
1:C:29:HIS:HD2	4:C:606:HOH:O	1.98	0.45
1:C:341:ASP:OD2	1:C:341:ASP:N	2.46	0.45
1:D:27:GLY:O	1:D:28:SEP:CB	2.64	0.45
1:D:342:ARG:NH1	1:D:342:ARG:CG	2.77	0.45
1:A:257:VAL:O	1:A:260:LEU:HB3	2.16	0.45
1:B:342:ARG:HA	1:B:342:ARG:HD3	1.57	0.45
1:C:24:GLY:O	1:C:46:ASP:HA	2.16	0.45
1:A:330:ALA:O	1:A:333:THR:HG22	2.16	0.45
1:B:354:GLN:HG3	4:B:593:HOH:O	2.17	0.45
1:B:55:HIS:HB2	1:B:426:GLY:HA3	1.99	0.45
1:B:67:LEU:HB2	1:B:150:LEU:HD21	1.98	0.45
1:B:231:THR:HG22	1:B:339:TRP:CE2	2.52	0.45
1:C:83:THR:HB	1:C:84:PRO:HD3	1.98	0.45
1:C:259:ASN:C	1:C:261:TYR:H	2.19	0.45
1:A:390:VAL:HG21	1:A:428:ALA:HA	1.98	0.44
1:A:395:LEU:HB3	2:A:571:TPP:PB	2.57	0.44
1:A:364:SER:HB2	1:A:371:HIS:CG	2.53	0.44
1:A:507:VAL:CG1	1:B:507:VAL:HG13	2.48	0.44
1:B:55:HIS:CE1	1:B:423:VAL:HG12	2.52	0.44
1:A:395:LEU:HB3	2:A:571:TPP:O2B	2.17	0.44
1:B:393:GLY:O	1:B:397:TYR:HD2	2.00	0.44
1:A:394:ALA:HA	1:A:397:TYR:CE2	2.53	0.44
1:B:140:ARG:O	1:B:144:GLN:HB2	2.18	0.44
1:D:116:ILE:HB	1:D:121:MET:HE1	2.00	0.44
1:B:183:SER:O	1:B:185:HIS:N	2.46	0.44
1:B:351:ASP:OD2	4:B:575:HOH:O	2.21	0.44
1:C:366:SER:HB2	1:C:374:HIS:ND1	2.33	0.44
1:C:549:ILE:HA	1:C:550:PRO:HD2	1.88	0.44
1:D:88:ALA:HA	1:D:93:THR:CG2	2.48	0.44
1:C:15:ILE:HD11	1:C:42:VAL:CG2	2.48	0.43
1:B:213:SER:O	1:B:217:ARG:HG2	2.18	0.43
1:D:143:MET:HE1	1:D:180:LEU:HB2	2.00	0.43
1:B:515:GLY:HA2	1:B:539:CYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:ARG:O	1:D:360:ILE:HG12	2.18	0.43
1:A:499:LEU:HD22	1:B:48:ARG:HH11	1.82	0.43
1:D:91:ASP:HB2	1:D:93:THR:HG22	2.00	0.43
1:B:45:ILE:HG23	1:B:464:LYS:HG2	2.01	0.43
1:C:105:ARG:HG2	1:C:164:ASP:OD2	2.17	0.43
1:D:67:LEU:HD22	1:D:146:ILE:HG23	1.99	0.43
1:A:393:GLY:O	1:A:397:TYR:HD2	2.02	0.43
1:A:478:TRP:CE3	2:A:571:TPP:HM41	2.53	0.43
1:A:469:ILE:HD13	1:A:532:LEU:HD22	2.00	0.43
1:A:518:VAL:HG11	1:A:527:ALA:HB2	2.00	0.43
1:D:210:VAL:HG13	1:D:257:VAL:CG1	2.48	0.42
1:D:218:THR:HG21	1:D:323:GLY:H	1.85	0.42
1:A:372:PRO:HB2	1:A:399:TRP:CD1	2.53	0.42
1:C:9:LEU:HD11	1:C:170:ILE:HD11	2.02	0.42
1:C:477:SER:HA	1:C:499:LEU:HB2	2.01	0.42
1:A:25:LEU:HD21	1:B:478:TRP:CZ2	2.54	0.42
1:A:369:ALA:HB3	1:A:545:ALA:HB2	2.00	0.42
1:A:83:THR:HB	1:A:84:PRO:HD3	2.00	0.42
1:A:260:LEU:HA	1:A:263:PHE:CE2	2.55	0.42
1:A:479:GLY:HA3	2:A:571:TPP:O1B	2.19	0.42
1:B:109:THR:HG1	1:B:111:THR:HG1	1.61	0.42
1:A:489:VAL:HG12	1:A:493:ARG:HD3	2.02	0.42
1:A:505:HIS:H	1:A:541:ASN:HD22	1.67	0.42
1:B:305:ALA:HA	1:B:308:LEU:HD22	2.02	0.42
1:B:432:GLN:HG2	1:B:442:THR:HB	2.02	0.42
1:C:11:VAL:HG21	1:C:36:ALA:HB3	2.01	0.42
1:D:93:THR:HA	1:D:94:PRO:HD3	1.95	0.42
1:D:285:GLY:O	1:D:288:SER:HB3	2.20	0.42
1:A:394:ALA:HA	1:A:397:TYR:CD2	2.55	0.42
1:A:311:LEU:CD2	1:B:109:THR:HG22	2.50	0.42
1:D:138:ILE:HB	1:D:139:PRO:HD3	2.02	0.42
1:C:420:SER:O	1:C:423:VAL:HG13	2.19	0.42
1:C:475:ASN:O	1:C:546:LEU:HD12	2.20	0.42
1:D:9:LEU:HD11	1:D:170:ILE:HD11	2.02	0.42
1:B:466:LEU:HA	1:B:467:PRO:HD3	1.65	0.41
1:D:210:VAL:CG1	1:D:257:VAL:HG11	2.50	0.41
1:D:461:LEU:HD21	1:D:468:LEU:HD23	2.01	0.41
1:A:170:ILE:HG22	1:A:171:ASP:N	2.35	0.41
1:B:83:THR:HB	1:B:84:PRO:HD3	2.02	0.41
1:B:485:GLN:O	1:B:489:VAL:HG23	2.21	0.41
1:C:390:VAL:HG21	1:C:428:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:LEU:HA	1:C:467:PRO:HD3	1.82	0.41
1:C:286:HIS:NE2	1:D:111:THR:HB	2.36	0.41
1:D:98:LEU:HD23	1:D:159:LEU:HB3	2.03	0.41
1:D:335:GLN:C	1:D:337:ALA:H	2.24	0.41
1:D:458:PHE:CZ	1:D:539:CYS:HB2	2.55	0.41
1:A:154:ARG:H	1:A:154:ARG:HD2	1.85	0.41
1:B:13:THR:HG21	1:B:139:PRO:HA	2.02	0.41
1:B:91:ASP:OD1	1:B:416:GLY:HA3	2.20	0.41
1:D:396:THR:HG23	1:D:473:MET:HG3	2.02	0.41
1:D:276:LEU:HB3	1:D:322:VAL:HG13	2.01	0.41
1:D:223:ALA:O	1:D:330:ALA:HB2	2.20	0.41
1:A:461:LEU:HD21	1:A:468:LEU:HD23	2.02	0.41
1:A:490:GLY:HA3	1:A:493:ARG:HG3	2.03	0.41
1:B:27:GLY:HA3	1:B:73:THR:CB	2.50	0.41
1:B:524:PHE:HE1	1:B:540:ILE:HG21	1.84	0.41
1:D:466:LEU:HA	1:D:467:PRO:HD3	1.74	0.41
1:C:263:PHE:CD1	1:C:268:ALA:HB1	2.57	0.40
1:C:286:HIS:HB3	1:C:287:GLY:H	1.60	0.40
1:A:152:ALA:HB1	1:A:303:PRO:CG	2.51	0.40
1:B:143:MET:HE1	1:B:180:LEU:HB2	2.02	0.40
1:B:433:VAL:O	1:B:434:ALA:CB	2.69	0.40
1:B:469:ILE:HG12	1:B:538:ALA:HB3	2.03	0.40
1:C:311:LEU:HD21	1:D:109:THR:HG22	2.03	0.40
1:D:83:THR:HB	1:D:84:PRO:HD3	2.01	0.40
1:A:11:VAL:HG21	1:A:36:ALA:HB3	2.04	0.40
1:A:378:VAL:HG13	1:A:525:SER:HB3	2.03	0.40
1:B:554:LEU:C	1:B:555:ILE:HG13	2.40	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	551/570 (97%)	512 (93%)	35 (6%)	4 (1%)	22	53
1	B	551/570 (97%)	510 (93%)	40 (7%)	1 (0%)	47	78
1	C	551/570 (97%)	523 (95%)	28 (5%)	0	100	100
1	D	551/570 (97%)	516 (94%)	34 (6%)	1 (0%)	47	78
All	All	2204/2280 (97%)	2061 (94%)	137 (6%)	6 (0%)	41	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ARG
1	A	308	LEU
1	A	336	ASP
1	B	308	LEU
1	D	337	ALA
1	A	552	GLU

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	412/426 (97%)	403 (98%)	9 (2%)	52	83
1	B	412/426 (97%)	375 (91%)	37 (9%)	9	28
1	C	412/426 (97%)	384 (93%)	28 (7%)	16	42
1	D	412/426 (97%)	389 (94%)	23 (6%)	21	51
All	All	1648/1704 (97%)	1551 (94%)	97 (6%)	19	49

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	ARG
1	A	425	PHE
1	A	441	ARG
1	A	454	SER
1	A	483	HIS

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Mol	Chain	Res	Type
1	A	487	LEU
1	A	536	ARG
1	A	547	ASP
1	A	554	LEU
1	B	25	LEU
1	B	32	THR
1	B	39	ASP
1	B	46	ASP
1	B	49	HIS
1	B	66	LYS
1	B	93	THR
1	B	96	LEU
1	B	105	ARG
1	B	107	ASP
1	B	111	THR
1	B	159	LEU
1	B	177	ILE
1	B	179	ASP
1	B	220	ARG
1	B	252	MET
1	B	257	VAL
1	B	258	GLN
1	B	265	LYS
1	B	273	VAL
1	B	308	LEU
1	B	310	ARG
1	B	333	THR
1	B	342	ARG
1	B	352	LEU
1	B	356	ARG
1	B	368	HIS
1	B	406	ARG
1	B	408	LYS
1	B	418	LEU
1	B	425	PHE
1	B	432	GLN
1	B	454	SER
1	B	473	MET
1	B	489	VAL
1	B	518	VAL
1	B	523	SER
1	C	19	VAL

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Mol	Chain	Res	Type
1	C	25	LEU
1	C	38	LEU
1	C	71	LEU
1	C	96	LEU
1	C	141	LEU
1	C	159	LEU
1	C	168	ASN
1	C	176	ILE
1	C	196	GLN
1	C	200	LEU
1	C	201	LEU
1	C	222	THR
1	C	252	MET
1	C	258	GLN
1	C	310	ARG
1	C	333	THR
1	C	341	ASP
1	C	342	ARG
1	C	356	ARG
1	C	397	TYR
1	C	398	LEU
1	C	418	LEU
1	C	421	MET
1	C	425	PHE
1	C	441	ARG
1	C	495	THR
1	C	547	ASP
1	D	3	MET
1	D	25	LEU
1	D	32	THR
1	D	38	LEU
1	D	66	LYS
1	D	71	LEU
1	D	93	THR
1	D	96	LEU
1	D	105	ARG
1	D	107	ASP
1	D	159	LEU
1	D	252	MET
1	D	273	VAL
1	D	327	GLU
1	D	335	GLN

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Mol	Chain	Res	Type
1	D	356	ARG
1	D	359	SER
1	D	418	LEU
1	D	425	PHE
1	D	494	VAL
1	D	495	THR
1	D	536	ARG
1	D	544	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	HIS
1	B	168	ASN
1	B	196	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
1	SEP	B	28	1	8,9,10	1.60	1 (12%)	8,12,14	1.58	2 (25%)
1	SEP	A	28	1	8,9,10	1.61	1 (12%)	8,12,14	1.59	1 (12%)
1	SEP	D	28	1	8,9,10	1.63	1 (12%)	8,12,14	2.75	2 (25%)
1	SEP	C	28	1	8,9,10	1.62	1 (12%)	8,12,14	1.28	1 (12%)

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
1	SEP	B	28	1	-	2/5/8/10	-
1	SEP	A	28	1	-	1/5/8/10	-
1	SEP	D	28	1	-	0/5/8/10	-
1	SEP	C	28	1	-	1/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	28	SEP	P-O1P	3.54	1.62	1.50
1	B	28	SEP	P-O1P	3.54	1.62	1.50
1	A	28	SEP	P-O1P	3.48	1.61	1.50
1	C	28	SEP	P-O1P	3.36	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	28	SEP	OG-CB-CA	6.26	114.23	108.14
1	D	28	SEP	P-OG-CB	-4.17	106.80	118.30
1	A	28	SEP	OG-CB-CA	3.25	111.31	108.14
1	B	28	SEP	P-OG-CB	-2.94	110.18	118.30
1	B	28	SEP	OG-CB-CA	2.62	110.69	108.14
1	C	28	SEP	P-OG-CB	-2.42	111.63	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	28	SEP	N-CA-CB-OG
1	A	28	SEP	CA-CB-OG-P
1	C	28	SEP	CA-CB-OG-P
1	B	28	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	28	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	TPP	A	571	3	22,27,27	1.56	5 (22%)	29,40,40	2.12	9 (31%)
2	TPP	D	571	3	22,27,27	1.49	5 (22%)	29,40,40	2.03	9 (31%)
2	TPP	B	571	3	22,27,27	1.48	4 (18%)	29,40,40	2.09	8 (27%)
2	TPP	C	571	3	22,27,27	1.55	6 (27%)	29,40,40	2.07	7 (24%)

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	TPP	A	571	3	-	2/16/17/17	0/2/2/2
2	TPP	D	571	3	-	1/16/17/17	0/2/2/2
2	TPP	B	571	3	-	1/16/17/17	0/2/2/2
2	TPP	C	571	3	-	1/16/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	571	TPP	C4-N3	-4.03	1.36	1.39
2	B	571	TPP	C4-N3	-3.37	1.36	1.39
2	C	571	TPP	C4-N3	-3.25	1.36	1.39
2	D	571	TPP	C4-N3	-2.99	1.37	1.39
2	D	571	TPP	C2'-N3'	2.95	1.39	1.34
2	D	571	TPP	C4'-N3'	2.93	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	571	TPP	C2'-N3'	2.81	1.39	1.34
2	B	571	TPP	C4'-N3'	2.73	1.38	1.35
2	A	571	TPP	C2'-N1'	2.66	1.38	1.34
2	C	571	TPP	C2'-N3'	2.64	1.38	1.34
2	C	571	TPP	C4'-N3'	2.62	1.38	1.35
2	B	571	TPP	C2'-N1'	2.60	1.38	1.34
2	C	571	TPP	C2'-N1'	2.52	1.38	1.34
2	A	571	TPP	C4'-N3'	2.48	1.38	1.35
2	A	571	TPP	C2'-N3'	2.44	1.38	1.34
2	D	571	TPP	C2'-N1'	2.39	1.38	1.34
2	C	571	TPP	C6'-N1'	2.24	1.39	1.34
2	D	571	TPP	C7'-N3	-2.13	1.44	1.48
2	A	571	TPP	C6'-N1'	2.09	1.38	1.34
2	C	571	TPP	C6-C5	2.08	1.51	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	571	TPP	C6-C5-C4	7.20	133.21	127.43
2	C	571	TPP	C6-C5-C4	6.55	132.69	127.43
2	D	571	TPP	C6-C5-C4	6.42	132.59	127.43
2	A	571	TPP	C6-C5-C4	6.10	132.33	127.43
2	A	571	TPP	CM2-C2'-N1'	4.28	121.84	117.14
2	A	571	TPP	PA-O3A-PB	-3.71	120.10	132.83
2	B	571	TPP	PA-O3A-PB	-3.48	120.89	132.83
2	D	571	TPP	CM4-C4-N3	3.41	126.88	122.53
2	C	571	TPP	N1'-C2'-N3'	-3.38	119.72	125.54
2	C	571	TPP	CM2-C2'-N1'	3.37	120.85	117.14
2	C	571	TPP	PA-O3A-PB	-3.31	121.46	132.83
2	D	571	TPP	N1'-C2'-N3'	-3.24	119.96	125.54
2	B	571	TPP	N1'-C2'-N3'	-3.07	120.26	125.54
2	A	571	TPP	N1'-C2'-N3'	-3.06	120.27	125.54
2	C	571	TPP	CM4-C4-N3	2.97	126.32	122.53
2	A	571	TPP	CM4-C4-N3	2.93	126.26	122.53
2	D	571	TPP	C6'-C5'-C4'	2.89	119.65	115.72
2	B	571	TPP	C6'-C5'-C4'	2.88	119.64	115.72
2	B	571	TPP	CM4-C4-N3	2.82	126.12	122.53
2	A	571	TPP	C5'-C7'-N3	2.81	117.95	113.28
2	D	571	TPP	PA-O3A-PB	-2.61	123.87	132.83
2	A	571	TPP	C6'-C5'-C4'	2.51	119.13	115.72
2	D	571	TPP	C6'-N1'-C2'	2.43	120.09	115.96
2	D	571	TPP	CM2-C2'-N3'	2.36	120.83	117.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	571	TPP	C6'-C5'-C4'	2.34	118.91	115.72
2	B	571	TPP	C6'-N1'-C2'	2.32	119.91	115.96
2	C	571	TPP	C6'-N1'-C2'	2.24	119.78	115.96
2	A	571	TPP	C6'-N1'-C2'	2.22	119.74	115.96
2	B	571	TPP	CM2-C2'-N3'	2.12	120.46	117.15
2	B	571	TPP	C5'-C6'-N1'	-2.07	120.37	123.82
2	D	571	TPP	N4'-C4'-N3'	2.02	119.89	117.03
2	D	571	TPP	C5'-C6'-N1'	-2.02	120.46	123.82
2	A	571	TPP	C5'-C6'-N1'	-2.01	120.47	123.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	571	TPP	C5-C6-C7-O7
2	A	571	TPP	PB-O3A-PA-O7
2	B	571	TPP	PB-O3A-PA-O7
2	C	571	TPP	PB-O3A-PA-O7
2	D	571	TPP	PA-O3A-PB-O3B

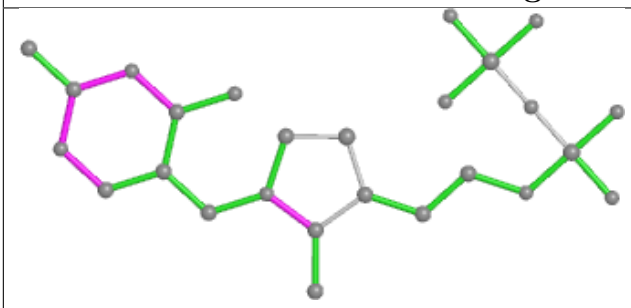
There are no ring outliers.

3 monomers are involved in 9 short contacts:

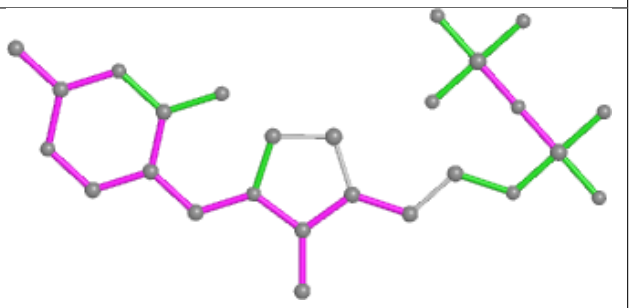
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	571	TPP	6	0
2	D	571	TPP	1	0
2	B	571	TPP	2	0

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.

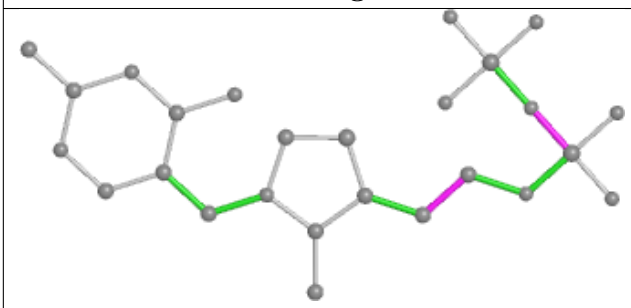
Ligand TPP A 571



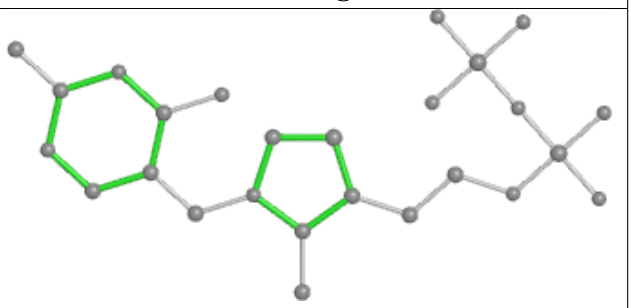
Bond lengths



Bond angles

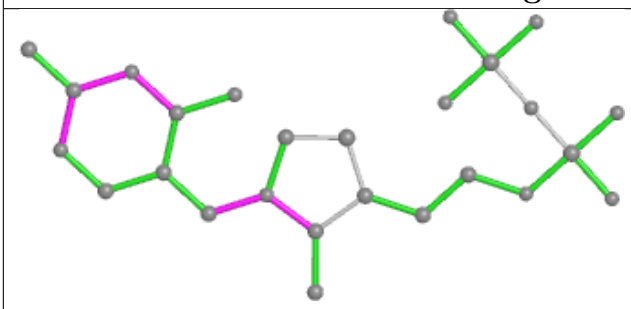


Torsions

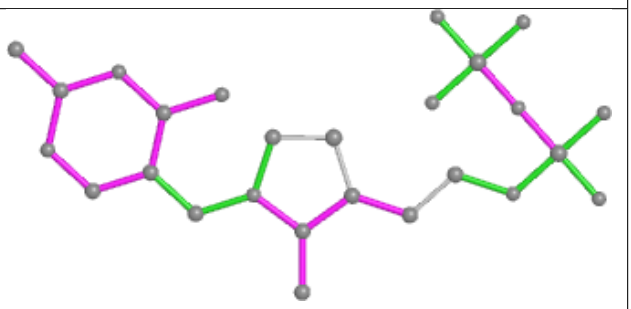


Rings

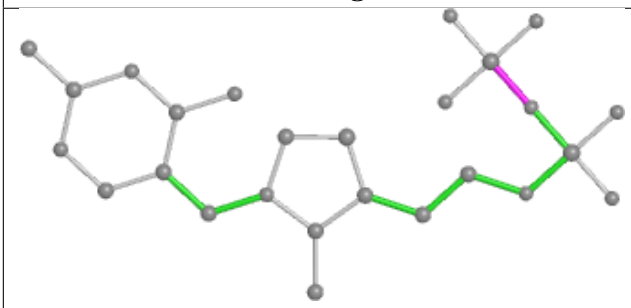
Ligand TPP D 571



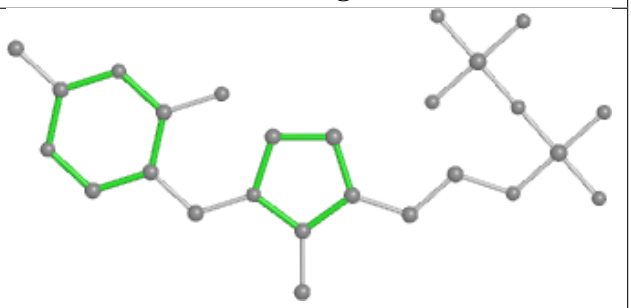
Bond lengths



Bond angles

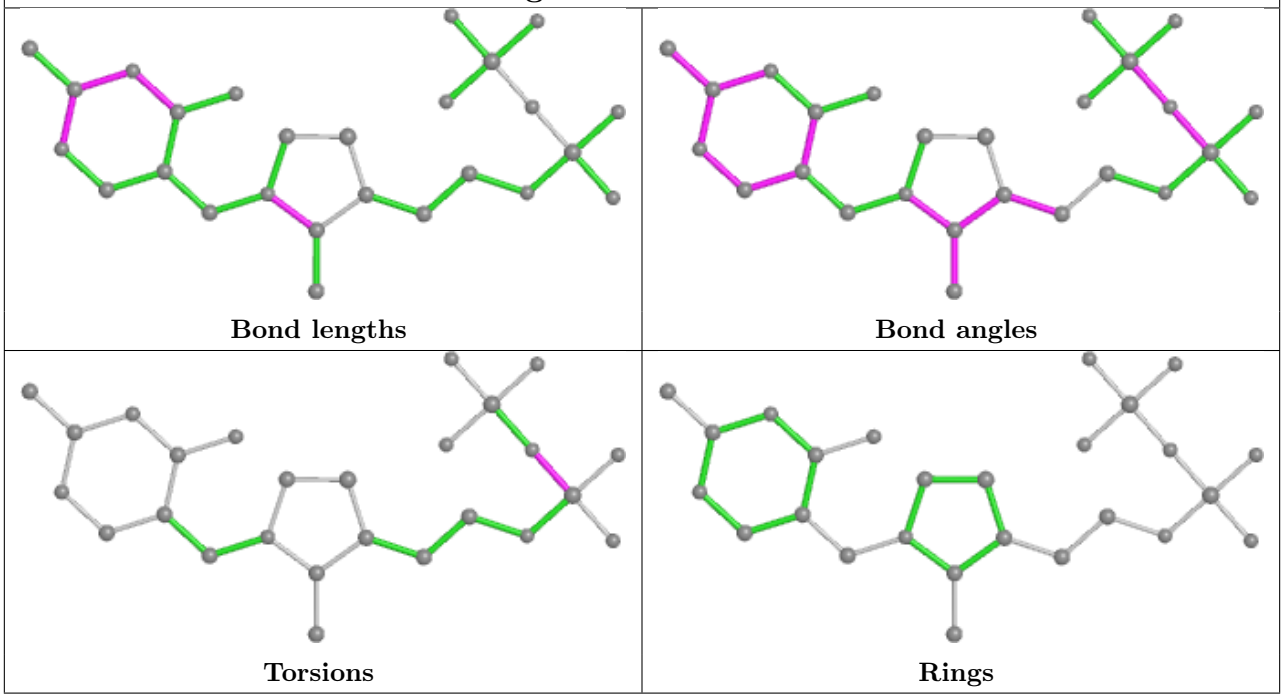


Torsions

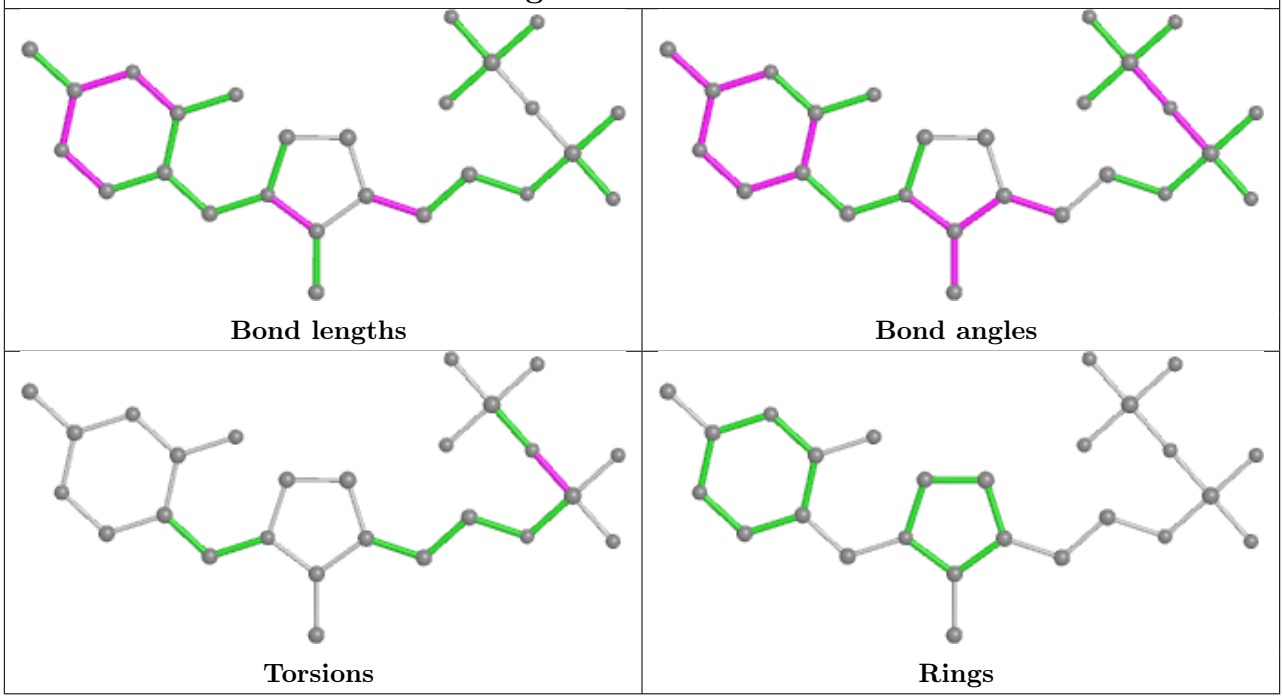


Rings

Ligand TPP B 571



Ligand TPP C 571



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	553/570 (97%)	0.19	30 (5%)	25	17	35, 80, 136, 154	0
1	B	553/570 (97%)	0.39	37 (6%)	17	10	44, 82, 116, 131	0
1	C	553/570 (97%)	-0.04	18 (3%)	46	36	36, 63, 113, 128	0
1	D	553/570 (97%)	0.11	11 (1%)	65	56	43, 69, 95, 120	0
All	All	2212/2280 (97%)	0.16	96 (4%)	35	25	35, 73, 122, 154	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ALA	5.6
1	B	334	ALA	5.1
1	C	368	HIS	4.8
1	D	2	ALA	4.6
1	C	337	ALA	4.5
1	A	362	ALA	4.4
1	B	337	ALA	4.3
1	D	368	HIS	4.1
1	C	369	ALA	4.0
1	B	170	ILE	4.0
1	B	335	GLN	3.9
1	A	487	LEU	3.9
1	B	538	ALA	3.8
1	A	201	LEU	3.7
1	B	378	VAL	3.7
1	B	2	ALA	3.6
1	C	487	LEU	3.6
1	B	341	ASP	3.5
1	B	454	SER	3.4
1	A	260	LEU	3.3
1	B	38	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	454	SER	3.3
1	A	367	GLU	3.2
1	B	5	THR	3.2
1	C	554	LEU	3.2
1	B	35	GLN	3.2
1	B	336	ASP	3.2
1	A	491	PRO	3.1
1	D	330	ALA	3.1
1	C	341	ASP	2.9
1	B	174	SER	2.8
1	C	335	GLN	2.8
1	B	526	ALA	2.8
1	A	489	VAL	2.8
1	B	173	ASP	2.8
1	C	367	GLU	2.8
1	A	486	GLN	2.8
1	A	368	HIS	2.7
1	A	339	TRP	2.7
1	B	3	MET	2.7
1	B	518	VAL	2.7
1	D	38	LEU	2.7
1	D	4	ILE	2.6
1	B	169	GLN	2.6
1	B	12	ARG	2.6
1	C	201	LEU	2.6
1	A	395	LEU	2.6
1	C	272	LEU	2.6
1	C	362	ALA	2.5
1	A	494	VAL	2.5
1	D	337	ALA	2.5
1	A	492	ASN	2.5
1	B	517	HIS	2.5
1	C	364	SER	2.5
1	B	339	TRP	2.5
1	C	365	SER	2.4
1	D	366	SER	2.4
1	A	336	ASP	2.4
1	C	486	GLN	2.4
1	B	163	TRP	2.4
1	B	524	PHE	2.4
1	B	422	GLY	2.4
1	B	534	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	345	TRP	2.3
1	A	493	ARG	2.3
1	A	264	ALA	2.3
1	A	207	PRO	2.3
1	A	517	HIS	2.3
1	B	367	GLU	2.3
1	B	369	ALA	2.3
1	C	267	ASP	2.3
1	A	315	ALA	2.3
1	C	393	GLY	2.3
1	C	38	LEU	2.3
1	A	340	PRO	2.2
1	B	9	LEU	2.2
1	B	381	LYS	2.2
1	B	4	ILE	2.2
1	A	335	GLN	2.2
1	D	80	ASN	2.2
1	B	51	ALA	2.2
1	B	83	THR	2.1
1	D	49	HIS	2.1
1	B	6	GLY	2.1
1	B	414	CYS	2.1
1	C	363	LYS	2.1
1	A	272	LEU	2.1
1	B	365	SER	2.1
1	D	169	GLN	2.1
1	A	482	LEU	2.0
1	A	170	ILE	2.0
1	A	363	LYS	2.0
1	B	373	PHE	2.0
1	A	295	SER	2.0
1	A	488	ALA	2.0
1	D	522	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	B	28	10/11	0.85	0.21	88,89,91,91	0
1	SEP	D	28	10/11	0.88	0.17	68,69,75,75	0
1	SEP	C	28	10/11	0.96	0.10	44,45,49,50	0
1	SEP	A	28	10/11	0.97	0.11	47,48,51,51	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

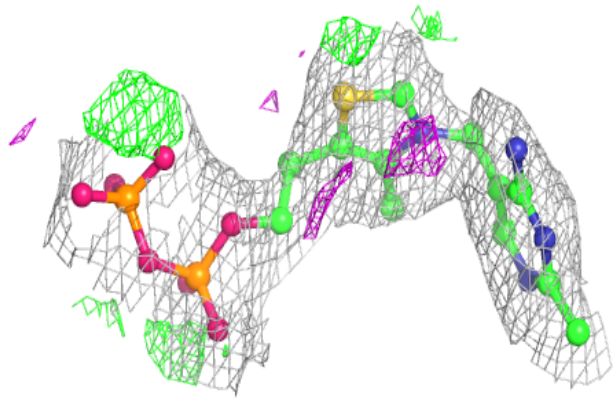
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

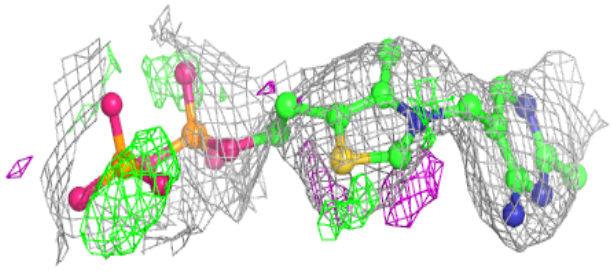
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	572	1/1	0.74	0.21	87,87,87,87	0
3	MG	C	572	1/1	0.88	0.22	61,61,61,61	0
2	TPP	A	571	26/26	0.91	0.23	98,99,100,100	0
3	MG	D	572	1/1	0.94	0.10	77,77,77,77	0
3	MG	B	572	1/1	0.95	0.12	69,69,69,69	0
2	TPP	C	571	26/26	0.97	0.17	58,64,67,67	0
2	TPP	D	571	26/26	0.98	0.10	39,46,53,53	0
2	TPP	B	571	26/26	0.99	0.12	53,61,66,66	0

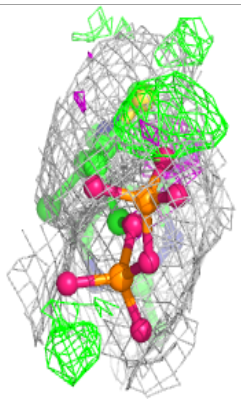
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 571:

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

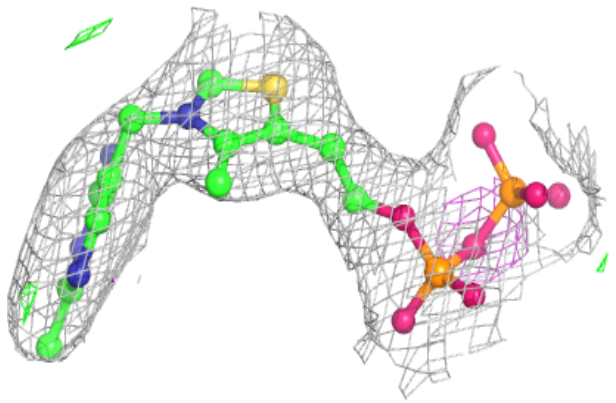


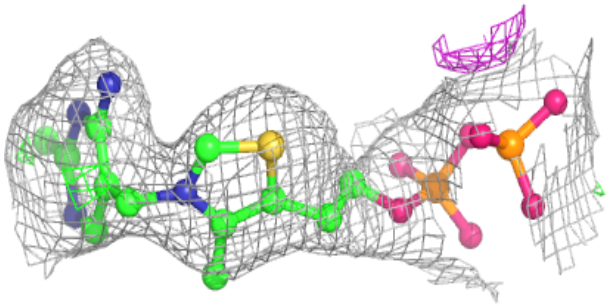


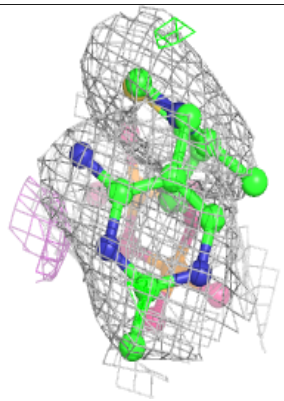


Electron density around TPP C 571:

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

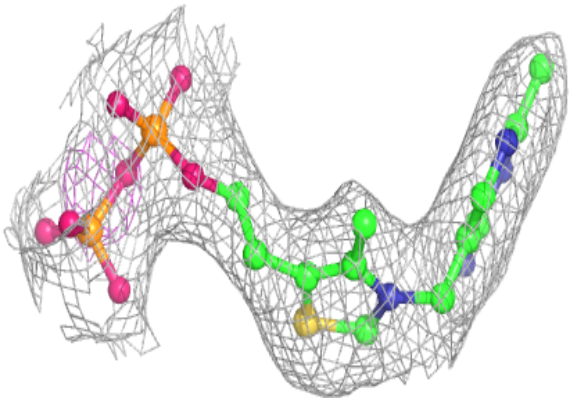


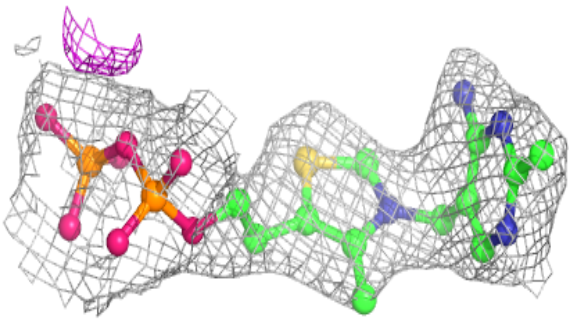


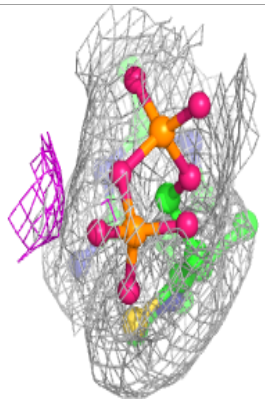


Electron density around TPP D 571:

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

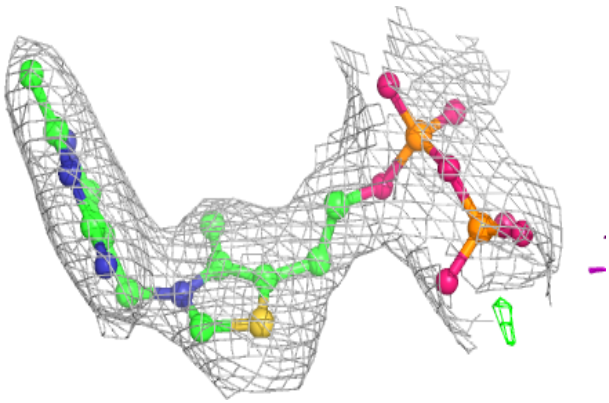


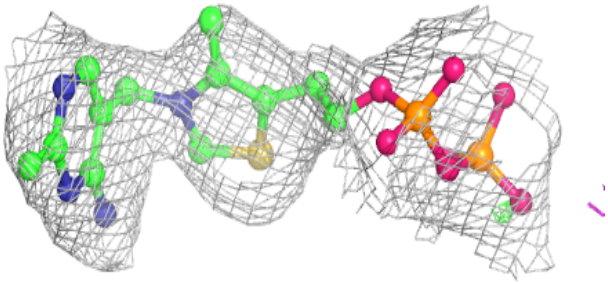


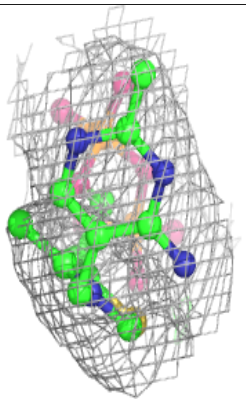


Electron density around TPP B 571:

$2mF_o$-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.