Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2024 – 02:59 pm BST

PDB ID	:	8R3P
Title	:	Transketolase from Enterococcus faecium in complex with thiamin pyrophosphate
Authors	:	Ballut, L.; Georges, R.N.; Aghajari, N.; Hecquet, L.; Charmantray, F.; Doumeche, B.
Deposited on	:	2023-11-10
Resolution	:	2.90 Å(reported)

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

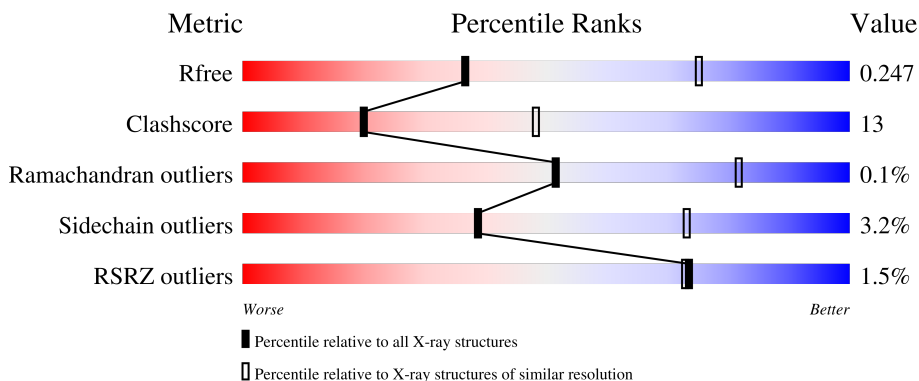|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		3.2%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	680	% 74% 24% •
1	B	680	% 70% 26% • •
1	C	680	3% 68% 29% • •
1	D	680	% 72% 24% • •

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 20625 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5155	3260	862	1011	22			
1	B	666	Total	C	N	O	S	0	0	0
			5106	3227	854	1002	23			
1	C	668	Total	C	N	O	S	0	0	0
			5122	3237	857	1005	23			
1	D	668	Total	C	N	O	S	0	0	0
			5119	3235	857	1005	22			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	666	GLU	-	expression tag	UNP I3U1P7
A	667	ASN	-	expression tag	UNP I3U1P7
A	668	LEU	-	expression tag	UNP I3U1P7
A	669	TYR	-	expression tag	UNP I3U1P7
A	670	PHE	-	expression tag	UNP I3U1P7
A	671	GLN	-	expression tag	UNP I3U1P7
A	672	GLY	-	expression tag	UNP I3U1P7
A	673	LEU	-	expression tag	UNP I3U1P7
A	674	GLU	-	expression tag	UNP I3U1P7
A	675	HIS	-	expression tag	UNP I3U1P7
A	676	HIS	-	expression tag	UNP I3U1P7
A	677	HIS	-	expression tag	UNP I3U1P7
A	678	HIS	-	expression tag	UNP I3U1P7
A	679	HIS	-	expression tag	UNP I3U1P7
A	680	HIS	-	expression tag	UNP I3U1P7
B	666	GLU	-	expression tag	UNP I3U1P7
B	667	ASN	-	expression tag	UNP I3U1P7
B	668	LEU	-	expression tag	UNP I3U1P7
B	669	TYR	-	expression tag	UNP I3U1P7
B	670	PHE	-	expression tag	UNP I3U1P7
B	671	GLN	-	expression tag	UNP I3U1P7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	672	GLY	-	expression tag	UNP I3U1P7
B	673	LEU	-	expression tag	UNP I3U1P7
B	674	GLU	-	expression tag	UNP I3U1P7
B	675	HIS	-	expression tag	UNP I3U1P7
B	676	HIS	-	expression tag	UNP I3U1P7
B	677	HIS	-	expression tag	UNP I3U1P7
B	678	HIS	-	expression tag	UNP I3U1P7
B	679	HIS	-	expression tag	UNP I3U1P7
B	680	HIS	-	expression tag	UNP I3U1P7
C	666	GLU	-	expression tag	UNP I3U1P7
C	667	ASN	-	expression tag	UNP I3U1P7
C	668	LEU	-	expression tag	UNP I3U1P7
C	669	TYR	-	expression tag	UNP I3U1P7
C	670	PHE	-	expression tag	UNP I3U1P7
C	671	GLN	-	expression tag	UNP I3U1P7
C	672	GLY	-	expression tag	UNP I3U1P7
C	673	LEU	-	expression tag	UNP I3U1P7
C	674	GLU	-	expression tag	UNP I3U1P7
C	675	HIS	-	expression tag	UNP I3U1P7
C	676	HIS	-	expression tag	UNP I3U1P7
C	677	HIS	-	expression tag	UNP I3U1P7
C	678	HIS	-	expression tag	UNP I3U1P7
C	679	HIS	-	expression tag	UNP I3U1P7
C	680	HIS	-	expression tag	UNP I3U1P7
D	666	GLU	-	expression tag	UNP I3U1P7
D	667	ASN	-	expression tag	UNP I3U1P7
D	668	LEU	-	expression tag	UNP I3U1P7
D	669	TYR	-	expression tag	UNP I3U1P7
D	670	PHE	-	expression tag	UNP I3U1P7
D	671	GLN	-	expression tag	UNP I3U1P7
D	672	GLY	-	expression tag	UNP I3U1P7
D	673	LEU	-	expression tag	UNP I3U1P7
D	674	GLU	-	expression tag	UNP I3U1P7
D	675	HIS	-	expression tag	UNP I3U1P7
D	676	HIS	-	expression tag	UNP I3U1P7
D	677	HIS	-	expression tag	UNP I3U1P7
D	678	HIS	-	expression tag	UNP I3U1P7
D	679	HIS	-	expression tag	UNP I3U1P7
D	680	HIS	-	expression tag	UNP I3U1P7

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

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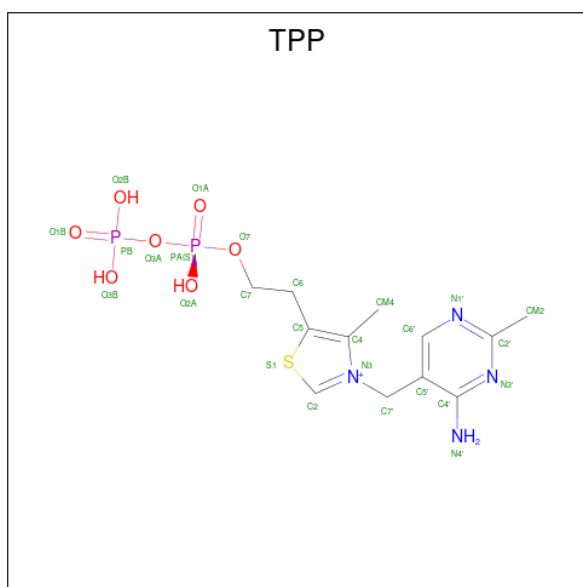
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total 6	O 6	0	0
4	C	2	Total 2	O 2	0	0
4	D	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

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: Transketolase

- Molecule 1: Transketolase

• Molecule 1: Transketolase

Chain C:

• Molecule 1: Transketolase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.66Å 68.22Å 165.46Å 90.00° 110.71° 90.00°	Depositor
Resolution (Å)	34.94 – 2.90 34.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.94-2.90) 98.5 (34.94-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.243 0.210 , 0.247	Depositor DCC
R_{free} test set	2875 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20625	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0/5275	0.53	0/7162
1	B	0.34	0/5224	0.55	0/7092
1	C	0.34	0/5240	0.55	0/7114
1	D	0.33	0/5237	0.55	0/7111
All	All	0.33	0/20976	0.54	0/28479

There are no bond length outliers.

There are no bond angle outliers.

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	5155	0	4995	120	0
1	B	5106	0	4956	133	0
1	C	5122	0	4973	149	0
1	D	5119	0	4965	129	0
2	A	26	0	16	3	0
2	B	26	0	16	2	0
2	C	26	0	16	2	0
2	D	26	0	16	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	6	0	0	2	0
4	C	2	0	0	0	0
4	D	5	0	0	2	0
All	All	20625	0	19953	510	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 13.

All (510) 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:602:VAL:HG12	1:A:603:LEU:HD22	1.28	1.13
1:D:189:ASP:O	1:D:190:ILE:HD12	1.65	0.97
1:C:361:LYS:HB2	1:C:386:ASN:HB3	1.52	0.92
1:B:189:ASP:O	1:B:190:ILE:HD12	1.71	0.90
1:B:523:LEU:HD11	1:B:561:SER:HA	1.54	0.88
1:A:602:VAL:HG12	1:A:603:LEU:CD2	2.07	0.84
1:A:35:ALA:HB2	1:A:186:ASP:OD1	1.79	0.83
1:B:429:ILE:HD11	1:B:455:VAL:HG22	1.62	0.81
1:B:357:ARG:HD3	1:B:520:ARG:HA	1.63	0.81
1:A:491:ILE:HD13	1:A:587:SER:HB2	1.63	0.79
1:C:6:ASP:OD1	1:C:295:ARG:NH1	2.15	0.78
1:A:284:PRO:HG2	1:A:287:THR:HG21	1.65	0.78
1:B:242:THR:OG1	4:B:801:HOH:O	2.00	0.78
1:C:74:LEU:HG	1:C:78:LEU:HD11	1.64	0.77
1:C:446:ARG:HB2	1:C:485:MET:HE1	1.65	0.77
1:B:192:LEU:HD12	1:B:263:HIS:HE1	1.50	0.76
1:D:348:TYR:HD2	1:D:496:GLY:HA3	1.50	0.76
1:B:59:ASP:OD1	1:B:148:MET:HE3	1.87	0.75
1:C:492:ARG:NH2	1:C:562:GLU:OE1	2.18	0.75
1:A:380:ASP:OD2	1:B:192:LEU:HB3	1.87	0.74
1:A:609:LYS:NZ	1:A:670:PHE:HB3	2.02	0.74
1:D:429:ILE:HD11	1:D:455:VAL:HG22	1.67	0.74
1:D:348:TYR:CD2	1:D:496:GLY:HA3	2.23	0.74
1:A:156:CYS:SG	1:A:161:LEU:HD11	2.28	0.74
1:C:555:ILE:HD11	1:C:604:PRO:HD2	1.70	0.73
1:C:483:ARG:HG2	1:C:490:VAL:HG21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLU:OE1	4:D:801:HOH:O	2.06	0.72
1:D:361:LYS:HB2	1:D:386:ASN:HB3	1.72	0.72
1:A:298:GLN:NE2	1:A:302:GLU:OE1	2.18	0.71
1:D:357:ARG:HD3	1:D:520:ARG:HA	1.73	0.71
1:D:593:LYS:NZ	4:D:802:HOH:O	2.22	0.71
1:B:556:LEU:HD13	1:B:580:VAL:HG21	1.73	0.71
1:B:654:VAL:O	1:B:658:VAL:HG23	1.90	0.71
1:A:553:GLU:OE1	1:A:579:ASP:N	2.17	0.69
1:C:46:HIS:HE1	1:C:228:SER:HB2	1.58	0.69
1:C:74:LEU:O	1:C:78:LEU:HD12	1.92	0.69
1:C:545:SER:HB3	1:C:582:VAL:HG22	1.74	0.69
1:C:14:ARG:NH1	1:C:33:MET:O	2.26	0.68
1:C:256:LYS:O	1:C:259:THR:OG1	2.10	0.68
1:D:556:LEU:HG	1:D:580:VAL:HG11	1.74	0.68
1:C:29:PRO:O	1:C:33:MET:HG3	1.94	0.68
1:C:380:ASP:OD1	1:D:191:SER:HB3	1.94	0.68
1:B:138:ALA:HB1	1:B:401:GLU:HG3	1.75	0.68
1:D:39:ALA:HB1	1:D:77:LEU:HD11	1.76	0.68
1:C:2:PHE:HA	1:C:6:ASP:OD2	1.94	0.67
1:A:302:GLU:HG3	1:A:303:GLU:N	2.08	0.67
1:B:555:ILE:HG23	1:B:610:ARG:HG2	1.76	0.66
1:D:132:ALA:HB2	1:D:421:ILE:HG23	1.78	0.65
1:A:14:ARG:HG2	1:A:33:MET:HA	1.79	0.64
1:C:14:ARG:HD3	1:C:33:MET:HA	1.78	0.64
1:C:146:ASN:ND2	1:C:149:ASP:HB2	2.12	0.64
1:A:269:GLU:CD	1:A:269:GLU:H	2.01	0.64
1:D:356:SER:HB2	1:D:519:SER:H	1.63	0.64
1:A:212:GLY:O	1:A:240:LYS:HG2	1.98	0.64
1:D:31:LEU:HD22	1:D:70:GLY:HA3	1.78	0.64
1:D:188:ASN:ND2	2:D:701:TPP:O2B	2.31	0.63
1:D:147:VAL:HA	1:D:314:MET:HE1	1.79	0.63
1:A:535:GLU:OE2	1:A:535:GLU:N	2.31	0.63
1:C:187:SER:HB3	1:C:247:LYS:HD2	1.80	0.63
1:B:356:SER:HB2	1:B:519:SER:H	1.64	0.62
1:C:435:PHE:O	1:C:438:VAL:HG12	2.00	0.62
1:C:486:PRO:HB2	1:D:637:PHE:CE1	2.34	0.62
1:B:39:ALA:HB1	1:B:77:LEU:HD11	1.82	0.62
1:A:66:SER:OG	1:A:160:ASP:OD2	2.17	0.61
1:A:39:ALA:HB1	1:A:77:LEU:HD11	1.82	0.61
1:B:435:PHE:O	1:B:438:VAL:HG12	2.01	0.61
1:D:192:LEU:HD12	1:D:263:HIS:CD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:O	4:B:801:HOH:O	2.16	0.61
1:C:396:THR:HG23	1:C:399:HIS:H	1.66	0.61
1:D:527:PRO:HD2	1:D:544:LEU:HD21	1.83	0.61
1:A:411:GLU:HB3	1:A:441:LEU:HD23	1.83	0.60
1:A:407:PHE:CG	1:A:414:MET:HG3	2.36	0.60
1:C:172:MET:O	1:C:176:MET:HG3	2.01	0.60
1:B:632:ILE:CD1	1:B:657:VAL:HG12	2.31	0.60
1:A:188:ASN:ND2	2:A:701:TPP:O1B	2.34	0.60
1:C:61:ASP:HB3	1:C:153:TYR:HE2	1.67	0.60
1:C:458:VAL:HG23	1:C:518:LEU:HD12	1.84	0.60
1:D:417:ALA:O	1:D:421:ILE:HG13	2.02	0.60
1:A:187:SER:HB3	1:A:247:LYS:HD2	1.84	0.59
1:B:125:MET:O	1:B:129:MET:HG3	2.01	0.59
1:B:654:VAL:O	1:B:657:VAL:HG22	2.02	0.59
1:B:229:LYS:O	1:B:233:GLU:HG3	2.02	0.59
1:C:1:MET:HG2	1:C:45:LYS:HE2	1.83	0.59
1:B:182:ILE:HD12	1:B:234:ALA:HB1	1.83	0.59
1:C:237:GLU:HG2	1:C:240:LYS:HB2	1.84	0.59
1:D:429:ILE:HD12	1:D:429:ILE:O	2.02	0.59
1:B:342:ASP:HA	1:B:345:LEU:HD13	1.85	0.59
1:C:291:GLU:CD	1:C:291:GLU:H	2.05	0.59
1:C:39:ALA:HB1	1:C:77:LEU:HD11	1.85	0.58
1:B:361:LYS:HD2	1:B:386:ASN:HB3	1.85	0.58
1:A:269:GLU:OE2	1:A:269:GLU:N	2.29	0.58
1:A:418:MET:HG2	1:A:429:ILE:HG12	1.84	0.58
1:D:573:LEU:HD13	1:D:580:VAL:HG21	1.85	0.58
1:A:227:ILE:O	1:A:231:ILE:HG13	2.04	0.57
1:D:192:LEU:HD12	1:D:263:HIS:NE2	2.19	0.57
1:D:28:HIS:CG	1:D:69:HIS:HB2	2.39	0.57
1:A:552:PRO:HG2	1:A:607:VAL:HG21	1.86	0.57
1:C:291:GLU:OE2	1:C:291:GLU:N	2.30	0.57
1:D:17:SER:O	1:D:21:VAL:HG23	2.04	0.57
1:A:33:MET:HE2	1:A:251:GLY:HA2	1.86	0.57
1:D:526:LEU:HD11	1:D:563:VAL:HG11	1.85	0.57
1:C:127:VAL:HG21	1:C:169:ALA:HB1	1.87	0.57
1:C:603:LEU:HD12	1:C:603:LEU:O	2.03	0.57
1:B:501:ALA:HB1	1:B:537:VAL:HG21	1.85	0.57
1:D:438:VAL:HA	1:D:441:LEU:HD21	1.87	0.57
1:B:158:ASP:O	1:B:162:MET:HG3	2.05	0.56
1:D:355:ALA:HB3	1:D:358:VAL:HG23	1.86	0.56
1:B:151:TYR:CE2	1:B:235:LYS:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:HIS:ND1	1:B:401:GLU:OE1	2.38	0.56
1:C:268:GLY:O	1:C:271:GLY:N	2.39	0.56
1:C:505:VAL:O	1:C:509:THR:HG23	2.06	0.56
1:B:57:TRP:O	1:B:60:ARG:HG2	2.05	0.56
1:D:29:PRO:O	1:D:33:MET:HG3	2.05	0.56
1:C:33:MET:SD	1:C:267:LEU:HD11	2.46	0.56
1:C:123:ILE:O	1:C:127:VAL:HG23	2.06	0.56
1:D:114:ALA:HB1	1:D:125:MET:HE1	1.88	0.56
1:D:345:LEU:HD23	1:D:366:GLU:HB3	1.88	0.56
1:A:407:PHE:CD2	1:A:414:MET:HG3	2.41	0.56
1:B:1:MET:SD	1:D:594:GLN:NE2	2.73	0.56
1:C:609:LYS:HE3	1:C:665:SER:HA	1.86	0.56
1:B:557:ILE:O	1:B:612:ALA:HA	2.06	0.55
1:B:162:MET:HG2	1:B:200:PHE:CE1	2.41	0.55
1:B:188:ASN:ND2	2:B:701:TPP:O2B	2.37	0.55
1:C:298:GLN:HA	1:C:302:GLU:HG3	1.88	0.55
1:C:94:ARG:HG2	1:C:102:GLY:HA2	1.88	0.55
1:D:418:MET:HB3	1:D:429:ILE:HD13	1.88	0.55
1:B:602:VAL:HG12	1:B:603:LEU:HD22	1.88	0.55
1:C:414:MET:O	1:C:418:MET:HG3	2.05	0.55
1:A:121:GLN:O	1:A:125:MET:HG3	2.06	0.55
1:C:43:TRP:CD2	1:C:77:LEU:HD22	2.42	0.55
1:C:458:VAL:HG23	1:C:518:LEU:CD1	2.37	0.55
1:B:28:HIS:CG	1:B:69:HIS:HB2	2.41	0.55
1:D:441:LEU:HD23	1:D:441:LEU:H	1.71	0.55
1:D:121:GLN:O	1:D:125:MET:HG3	2.07	0.55
1:B:33:MET:SD	1:B:251:GLY:HA2	2.46	0.55
1:B:63:PHE:CE1	1:B:155:ILE:HD12	2.42	0.55
1:D:50:ASN:HD21	1:D:305:GLN:NE2	2.05	0.55
1:C:368:SER:CB	1:C:389:VAL:HG11	2.37	0.54
1:B:192:LEU:HD12	1:B:263:HIS:CE1	2.37	0.54
1:C:172:MET:HG2	1:C:176:MET:SD	2.47	0.54
1:C:530:LYS:HG3	1:C:531:GLU:OE2	2.07	0.54
1:B:417:ALA:O	1:B:421:ILE:HG13	2.06	0.54
1:C:498:GLU:HG2	1:C:537:VAL:CG2	2.38	0.54
1:B:131:MET:HE2	1:B:421:ILE:HD11	1.90	0.54
1:C:520:ARG:HH11	1:C:520:ARG:HG2	1.72	0.54
1:A:214:GLN:HB3	1:A:242:THR:HG23	1.90	0.54
1:B:375:TRP:O	1:B:429:ILE:HA	2.08	0.54
1:A:94:ARG:HD3	1:B:468:GLU:HB3	1.89	0.53
1:A:537:VAL:HG13	1:A:586:PRO:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:PHE:CZ	1:C:443:PRO:HB2	2.43	0.53
1:A:31:LEU:HD22	1:A:70:GLY:HA3	1.90	0.53
1:D:188:ASN:HB2	1:D:250:ILE:HB	1.90	0.53
1:D:529:THR:HG23	1:D:544:LEU:HD11	1.89	0.53
1:B:121:GLN:O	1:B:125:MET:HG3	2.08	0.53
1:C:189:ASP:O	1:C:190:ILE:HD12	2.08	0.53
1:B:162:MET:HG2	1:B:200:PHE:CD1	2.44	0.53
1:C:381:LEU:HD23	1:D:192:LEU:HD22	1.91	0.53
1:A:446:ARG:O	1:A:450:ILE:HG13	2.09	0.53
1:C:40:TYR:CE2	1:C:44:THR:HG21	2.44	0.53
1:B:63:PHE:HE1	1:B:155:ILE:HD12	1.73	0.52
1:B:14:ARG:HG2	1:B:33:MET:HA	1.90	0.52
1:C:275:ALA:O	1:C:278:VAL:HG22	2.09	0.52
1:D:430:TYR:HA	1:D:456:VAL:O	2.09	0.52
1:D:557:ILE:O	1:D:612:ALA:HA	2.10	0.52
1:A:237:GLU:HG3	1:A:240:LYS:HB2	1.92	0.52
1:B:358:VAL:O	1:B:362:GLU:HG3	2.09	0.52
1:D:125:MET:O	1:D:129:MET:HG3	2.09	0.52
1:A:380:ASP:OD1	1:B:191:SER:HB2	2.09	0.52
1:B:501:ALA:CB	1:B:537:VAL:HG21	2.39	0.52
1:B:526:LEU:HB3	1:B:527:PRO:HD2	1.90	0.52
1:C:456:VAL:HG11	1:C:503:TRP:CH2	2.44	0.52
1:C:553:GLU:HG3	1:C:579:ASP:O	2.10	0.52
1:B:418:MET:HE3	1:B:429:ILE:HD13	1.91	0.52
1:A:136:LEU:HD22	1:A:140:TYR:HE2	1.74	0.51
1:D:543:VAL:HG23	1:D:543:VAL:O	2.09	0.51
1:D:560:GLY:O	1:D:563:VAL:HG12	2.10	0.51
1:D:568:LYS:O	1:D:571:LYS:HG3	2.09	0.51
1:A:47:LEU:HG	1:A:49:VAL:HG13	1.93	0.51
1:B:196:THR:OG1	1:B:200:PHE:HB3	2.11	0.51
1:D:436:VAL:HG21	1:D:472:THR:O	2.10	0.51
1:A:191:SER:HB3	1:B:380:ASP:OD2	2.10	0.51
1:A:609:LYS:HZ2	1:A:670:PHE:HB3	1.72	0.51
1:B:432:GLY:HA2	1:B:458:VAL:O	2.10	0.51
1:C:570:GLN:HG3	1:C:580:VAL:HG23	1.93	0.51
1:C:604:PRO:HB2	1:C:607:VAL:HG12	1.92	0.51
1:A:64:VAL:O	1:A:154:ALA:HA	2.11	0.51
1:D:526:LEU:HD11	1:D:563:VAL:CG1	2.40	0.51
1:C:123:ILE:HD11	1:C:156:CYS:SG	2.51	0.51
1:C:557:ILE:HD11	1:C:610:ARG:HD2	1.91	0.51
1:B:281:TRP:CE2	1:B:283:TYR:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:PRO:HB2	1:B:554:GLY:O	2.11	0.51
1:C:155:ILE:HA	1:C:184:LEU:O	2.10	0.51
1:C:377:GLY:HA3	1:C:405:ILE:O	2.10	0.51
1:D:172:MET:HG2	1:D:176:MET:HE3	1.92	0.51
1:B:433:THR:HG22	1:B:459:LEU:HD22	1.93	0.51
1:B:533:ALA:O	1:B:537:VAL:HG22	2.11	0.51
1:A:29:PRO:O	1:A:33:MET:HG3	2.10	0.50
1:A:375:TRP:NE1	1:A:427:THR:HB	2.25	0.50
1:C:196:THR:OG1	1:C:200:PHE:HB3	2.11	0.50
1:D:336:LYS:HD2	1:D:337:LEU:O	2.10	0.50
1:A:479:LEU:HD11	1:A:492:ARG:HD2	1.93	0.50
1:C:31:LEU:HD22	1:C:70:GLY:HA3	1.94	0.50
1:D:189:ASP:C	1:D:190:ILE:HD12	2.30	0.50
1:C:163:GLU:OE2	2:C:701:TPP:HM23	2.12	0.50
1:C:193:ASP:HB3	1:D:406:TRP:CZ3	2.46	0.50
1:C:228:SER:O	1:C:232:GLU:HG3	2.12	0.50
1:C:385:ASN:ND2	1:C:460:THR:OG1	2.44	0.50
1:B:298:GLN:O	1:B:303:GLU:HG2	2.11	0.50
1:B:528:SER:O	1:B:532:VAL:HG22	2.12	0.50
1:C:165:VAL:HB	1:C:412:PHE:CD2	2.47	0.50
1:C:498:GLU:HG2	1:C:537:VAL:HG21	1.93	0.50
1:D:554:GLY:HA3	1:D:661:TYR:HE1	1.77	0.50
2:A:701:TPP:HM43	1:B:381:LEU:HD21	1.94	0.50
1:D:532:VAL:HG13	1:D:536:MET:CG	2.42	0.50
1:D:589:ASP:O	1:D:593:LYS:HG3	2.12	0.50
1:A:281:TRP:CE2	1:A:283:TYR:HB2	2.46	0.49
1:B:127:VAL:O	1:B:131:MET:HG3	2.11	0.49
1:D:541:ALA:HB3	1:D:591:PHE:CD1	2.47	0.49
1:C:174:GLY:HA3	1:C:211:TYR:O	2.12	0.49
1:C:191:SER:HB3	1:D:380:ASP:OD2	2.11	0.49
1:B:179:GLY:HA2	1:B:240:LYS:O	2.13	0.49
1:C:38:MET:HA	1:C:227:ILE:HD13	1.94	0.49
1:C:58:ALA:HB1	1:C:148:MET:HE1	1.93	0.49
1:D:475:PRO:O	1:D:476:ILE:HD13	2.12	0.49
1:C:127:VAL:HG13	1:C:173:ALA:HB2	1.94	0.49
1:C:151:TYR:CZ	1:C:235:LYS:HE2	2.47	0.49
1:A:28:HIS:CG	1:A:69:HIS:HB2	2.48	0.49
1:A:155:ILE:HG12	1:A:184:LEU:HB2	1.95	0.49
1:B:494:ALA:HB1	1:B:563:VAL:HG11	1.95	0.49
1:C:7:GLN:HA	1:C:7:GLN:HE21	1.78	0.49
1:A:491:ILE:CD1	1:A:587:SER:HB2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:LEU:HD23	1:D:667:ASN:HB3	1.94	0.49
1:C:103:HIS:ND1	1:C:117:GLY:HA2	2.28	0.49
1:A:653:THR:O	1:A:657:VAL:HG23	2.12	0.48
1:C:193:ASP:OD2	1:D:382:SER:N	2.42	0.48
1:A:33:MET:HE1	1:A:267:LEU:HD21	1.94	0.48
1:A:188:ASN:HB2	1:A:250:ILE:HB	1.96	0.48
1:A:361:LYS:HB2	1:A:386:ASN:HB3	1.95	0.48
1:D:158:ASP:O	1:D:162:MET:HG3	2.13	0.48
1:C:446:ARG:CB	1:C:485:MET:HE1	2.40	0.48
1:C:550:GLU:N	1:C:550:GLU:OE2	2.46	0.48
1:D:357:ARG:HG2	1:D:519:SER:O	2.14	0.48
1:B:361:LYS:HB2	1:B:386:ASN:HB3	1.94	0.48
1:C:6:ASP:HB3	1:C:40:TYR:HE1	1.79	0.48
1:A:182:ILE:HG12	1:A:234:ALA:HB1	1.95	0.48
1:A:573:LEU:HD21	1:A:658:VAL:HG13	1.95	0.48
1:D:127:VAL:O	1:D:131:MET:HG3	2.14	0.48
1:D:412:PHE:CZ	1:D:443:PRO:HB2	2.49	0.48
1:A:161:LEU:N	1:A:161:LEU:HD12	2.29	0.48
1:D:414:MET:O	1:D:418:MET:HG3	2.14	0.48
1:D:570:GLN:NE2	1:D:580:VAL:O	2.46	0.48
1:D:320:LYS:HB2	1:D:320:LYS:HE2	1.68	0.47
1:A:67:ALA:HB1	1:A:69:HIS:CE1	2.49	0.47
1:A:98:SER:O	1:A:108:HIS:NE2	2.48	0.47
1:B:187:SER:HB2	1:B:247:LYS:HD2	1.96	0.47
1:C:84:GLN:OE1	1:C:84:GLN:HA	2.14	0.47
1:C:556:LEU:HD12	1:C:580:VAL:HB	1.95	0.47
1:A:2:PHE:HE2	1:A:228:SER:HG	1.59	0.47
1:A:557:ILE:O	1:A:612:ALA:HA	2.15	0.47
1:A:645:LYS:HB2	1:A:645:LYS:HE2	1.63	0.47
1:C:54:SER:HB3	1:C:110:ASP:OD1	2.15	0.47
1:C:207:ARG:HG3	1:D:207:ARG:HG3	1.96	0.47
1:C:253:GLY:HA3	1:C:278:VAL:HG21	1.95	0.47
1:C:256:LYS:HE3	1:C:256:LYS:HB2	1.68	0.47
1:C:526:LEU:HB2	1:C:529:THR:CG2	2.44	0.47
1:A:608:LYS:HB2	1:A:670:PHE:HE1	1.80	0.47
1:B:591:PHE:CZ	1:B:599:LYS:HA	2.50	0.47
1:C:270:ASP:OD1	1:C:270:ASP:N	2.47	0.47
1:C:365:GLN:NE2	1:C:388:MET:O	2.48	0.47
1:C:457:TYR:HB2	1:C:515:ILE:HA	1.97	0.47
1:C:520:ARG:HG2	1:C:520:ARG:NH1	2.30	0.47
1:D:143:GLU:OE2	1:D:322:TYR:OH	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:MET:HE1	1:A:267:LEU:HD11	1.97	0.47
1:B:433:THR:O	1:B:459:LEU:HA	2.15	0.47
1:D:208:TYR:O	1:D:213:TRP:HB2	2.15	0.47
1:A:326:ALA:O	1:A:330:GLU:HG3	2.15	0.47
1:A:435:PHE:O	1:A:438:VAL:HG12	2.14	0.47
1:B:32:PRO:HA	1:B:73:MET:HE2	1.97	0.47
1:C:18:ILE:HD11	1:C:272:ILE:HG23	1.96	0.47
1:B:359:SER:O	1:B:363:VAL:HG23	2.15	0.47
1:D:382:SER:O	1:D:386:ASN:N	2.45	0.46
1:C:21:VAL:HG22	1:C:27:GLY:HA3	1.98	0.46
1:D:342:ASP:HA	1:D:345:LEU:HG	1.97	0.46
1:D:357:ARG:NH1	1:D:384:SER:O	2.49	0.46
1:D:381:LEU:HD13	1:D:434:PHE:CD1	2.50	0.46
1:D:618:SER:HA	1:D:633:THR:HG21	1.98	0.46
2:B:701:TPP:HN42	2:B:701:TPP:H2	1.80	0.46
1:C:14:ARG:HH12	1:C:252:TYR:HB3	1.81	0.46
1:C:576:LYS:NZ	1:C:662:ASN:OD1	2.47	0.46
1:D:123:ILE:HD12	1:D:166:SER:HB3	1.98	0.46
1:D:254:ALA:O	1:D:257:GLU:HG2	2.16	0.46
1:D:664:LEU:HD23	1:D:667:ASN:CB	2.46	0.46
1:A:608:LYS:HE3	1:A:669:TYR:OH	2.16	0.46
1:B:609:LYS:HA	1:B:609:LYS:HD3	1.73	0.46
1:C:47:LEU:HD23	1:C:49:VAL:HG12	1.98	0.46
1:C:368:SER:HB3	1:C:389:VAL:HG11	1.98	0.46
1:B:268:GLY:O	1:B:272:ILE:HG12	2.15	0.46
2:C:701:TPP:H2	2:C:701:TPP:HN42	1.81	0.46
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.72	0.46
1:D:65:LEU:O	1:D:116:THR:OG1	2.32	0.46
1:B:631:THR:OG1	1:B:633:THR:HG23	2.16	0.46
1:B:188:ASN:HB2	1:B:250:ILE:HB	1.98	0.45
1:C:456:VAL:HG11	1:C:503:TRP:CZ3	2.51	0.45
1:A:361:LYS:O	1:A:365:GLN:HG3	2.16	0.45
1:B:397:PRO:HA	1:B:400:TYR:CZ	2.52	0.45
1:B:632:ILE:HD13	1:B:657:VAL:HG12	1.98	0.45
1:C:94:ARG:HG2	1:C:102:GLY:CA	2.46	0.45
1:D:251:GLY:O	1:D:257:GLU:HB3	2.17	0.45
1:D:429:ILE:CD1	1:D:455:VAL:HG22	2.44	0.45
1:A:33:MET:CE	1:A:267:LEU:HD21	2.47	0.45
1:A:123:ILE:HG13	1:A:124:ALA:N	2.28	0.45
1:A:468:GLU:HB3	1:B:94:ARG:HB3	1.98	0.45
1:B:189:ASP:C	1:B:190:ILE:HD12	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:TYR:O	1:B:213:TRP:HB2	2.17	0.45
1:A:255:PRO:HG3	1:A:274:MET:HG2	1.98	0.45
1:A:380:ASP:OD2	1:A:380:ASP:O	2.35	0.45
1:B:214:GLN:HB3	1:B:242:THR:HG23	1.99	0.45
1:B:616:ALA:O	1:B:633:THR:HB	2.17	0.45
1:C:14:ARG:O	1:C:18:ILE:HG23	2.16	0.45
1:D:357:ARG:HH11	1:D:461:HIS:CE1	2.35	0.45
1:D:562:GLU:HB3	1:D:613:ILE:HG22	1.99	0.45
1:C:357:ARG:NH2	1:C:520:ARG:HG3	2.32	0.45
1:B:169:ALA:HA	1:B:172:MET:HE2	1.99	0.45
1:B:526:LEU:HB3	1:B:544:LEU:HD21	1.99	0.45
1:B:611:VAL:HA	1:B:630:ALA:O	2.17	0.45
1:B:436:VAL:HG11	1:B:473:HIS:HA	1.99	0.45
1:C:19:GLU:OE2	1:C:286:PHE:N	2.48	0.45
1:C:526:LEU:HB3	1:C:544:LEU:HD21	1.99	0.45
1:D:609:LYS:HE3	1:D:665:SER:HB3	1.98	0.45
1:A:237:GLU:CG	1:A:240:LYS:HB2	2.47	0.44
1:C:357:ARG:NE	1:C:520:ARG:HA	2.32	0.44
1:D:131:MET:CE	1:D:421:ILE:HD11	2.47	0.44
1:D:172:MET:HG2	1:D:176:MET:CE	2.48	0.44
1:A:349:GLU:HG2	1:A:530:LYS:NZ	2.31	0.44
1:A:418:MET:HG2	1:A:429:ILE:CG1	2.47	0.44
1:B:435:PHE:HB3	1:B:475:PRO:HG2	2.00	0.44
1:B:519:SER:HB2	1:B:521:GLN:CD	2.38	0.44
1:B:543:VAL:HG23	1:B:543:VAL:O	2.16	0.44
1:C:35:ALA:O	1:C:38:MET:HG2	2.17	0.44
1:C:231:ILE:O	1:C:235:LYS:HG3	2.16	0.44
1:C:530:LYS:H	1:C:530:LYS:HG2	1.61	0.44
1:D:539:LYS:O	1:D:591:PHE:HA	2.17	0.44
1:D:562:GLU:HG2	1:D:652:PHE:CE1	2.52	0.44
1:A:136:LEU:HD21	1:A:427:THR:HG23	1.98	0.44
1:B:161:LEU:HD13	1:B:204:VAL:HG11	1.99	0.44
1:C:78:LEU:CD2	1:C:110:ASP:O	2.65	0.44
1:C:355:ALA:HB3	1:C:358:VAL:HG23	1.99	0.44
1:D:604:PRO:HB2	1:D:607:VAL:HG12	1.98	0.44
1:A:491:ILE:O	1:A:493:PRO:HD3	2.18	0.44
1:B:273:LYS:HE3	1:B:273:LYS:HB3	1.52	0.44
1:C:553:GLU:OE2	1:C:579:ASP:N	2.36	0.44
1:A:19:GLU:HB3	1:A:286:PHE:CE1	2.53	0.44
1:A:533:ALA:O	1:A:537:VAL:HG23	2.18	0.44
1:B:147:VAL:HA	1:B:314:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:SER:O	1:B:386:ASN:N	2.49	0.44
1:C:163:GLU:O	1:C:167:GLN:HG3	2.18	0.44
1:D:146:ASN:ND2	1:D:149:ASP:OD2	2.49	0.44
1:A:208:TYR:O	1:A:213:TRP:HB2	2.17	0.44
1:A:645:LYS:HD2	1:B:96:TRP:HB2	2.00	0.44
1:C:281:TRP:CE2	1:C:283:TYR:HB2	2.53	0.44
1:C:365:GLN:HA	1:C:389:VAL:HG13	2.00	0.44
1:D:438:VAL:HA	1:D:441:LEU:CD2	2.47	0.44
1:A:140:TYR:HD1	1:A:325:LEU:HG	1.83	0.44
1:A:193:ASP:HB3	1:B:406:TRP:CZ3	2.53	0.44
1:B:454:PRO:HG3	1:B:510:THR:O	2.18	0.44
1:C:218:VAL:HG22	1:C:246:VAL:HG13	2.00	0.44
1:D:600:GLU:OE2	1:D:604:PRO:HA	2.17	0.44
1:A:359:SER:O	1:A:363:VAL:HG23	2.18	0.43
1:C:189:ASP:C	1:C:190:ILE:HD12	2.38	0.43
1:C:218:VAL:CG2	1:C:246:VAL:HG13	2.48	0.43
1:D:375:TRP:NE1	1:D:429:ILE:HG23	2.33	0.43
1:D:375:TRP:O	1:D:429:ILE:HA	2.18	0.43
1:D:436:VAL:HB	1:D:475:PRO:HG3	1.98	0.43
1:B:641:ALA:HB3	1:B:646:ILE:HG12	2.00	0.43
1:A:540:GLY:O	1:A:586:PRO:HD2	2.18	0.43
1:B:618:SER:OG	1:B:635:ASP:OD2	2.29	0.43
1:C:300:MET:HE3	1:C:300:MET:HB3	1.77	0.43
1:A:281:TRP:NE1	1:A:283:TYR:HB2	2.33	0.43
1:D:16:LEU:HD11	1:D:288:VAL:HG12	2.01	0.43
1:D:207:ARG:HH21	1:D:208:TYR:HE1	1.66	0.43
1:C:170:SER:HA	1:C:213:TRP:HZ2	1.84	0.43
1:B:272:ILE:HG22	1:B:276:LYS:HE3	2.00	0.43
1:C:71:SER:HB3	1:C:104:PRO:HD3	2.01	0.43
1:D:532:VAL:HG13	1:D:536:MET:HG2	1.99	0.43
1:A:88:ASP:O	1:A:92:GLN:HG2	2.18	0.43
1:A:213:TRP:CD2	1:A:241:PRO:HB2	2.54	0.43
1:A:379:ALA:HB2	1:A:414:MET:CE	2.49	0.43
1:A:415:ALA:HA	1:A:418:MET:HE3	1.99	0.43
1:B:628:GLU:O	1:B:664:LEU:HD11	2.19	0.43
1:C:94:ARG:HE	1:D:468:GLU:HB3	1.83	0.43
1:C:273:LYS:NZ	1:C:276:LYS:HD2	2.34	0.43
1:D:385:ASN:HA	1:D:460:THR:HG21	1.99	0.43
1:A:430:TYR:HA	1:A:456:VAL:O	2.19	0.43
1:A:436:VAL:HB	1:A:475:PRO:HG3	2.01	0.43
1:B:59:ASP:HA	1:B:148:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ALA:O	1:B:141:ASN:HB2	2.19	0.43
1:C:250:ILE:HG12	1:C:262:VAL:HG23	2.01	0.43
1:C:457:TYR:CD2	1:C:515:ILE:HG12	2.54	0.43
1:D:217:LEU:HD12	1:D:245:GLU:HB3	2.01	0.43
1:B:223:ASP:O	1:B:227:ILE:HG13	2.18	0.42
1:B:412:PHE:CZ	1:B:443:PRO:HB2	2.54	0.42
1:B:461:HIS:HB3	1:B:466:VAL:HG21	2.00	0.42
1:C:221:GLY:HA2	1:C:246:VAL:HG12	2.01	0.42
1:D:268:GLY:O	1:D:272:ILE:HG13	2.19	0.42
1:A:247:LYS:HE3	1:A:247:LYS:HB3	1.87	0.42
1:B:289:PRO:HB2	1:B:292:VAL:HG23	2.00	0.42
1:B:429:ILE:O	1:B:429:ILE:HD12	2.20	0.42
1:C:642:PRO:O	1:C:646:ILE:HG13	2.19	0.42
1:D:578:LYS:HD2	1:D:661:TYR:HE2	1.84	0.42
1:D:615:ALA:HA	1:D:652:PHE:CZ	2.54	0.42
1:A:615:ALA:HA	1:A:652:PHE:CZ	2.54	0.42
1:C:31:LEU:HB3	1:C:32:PRO:HD3	2.00	0.42
1:B:630:ALA:HB2	1:B:664:LEU:HD13	2.00	0.42
1:D:494:ALA:HB1	1:D:563:VAL:HG11	2.01	0.42
1:A:71:SER:HB3	1:A:104:PRO:HD3	2.00	0.42
1:A:161:LEU:HD23	1:A:204:VAL:HG11	2.01	0.42
1:B:28:HIS:HB2	1:B:69:HIS:O	2.20	0.42
1:B:600:GLU:O	1:B:604:PRO:HD3	2.19	0.42
1:D:88:ASP:HA	1:D:91:LYS:HD2	2.01	0.42
1:A:393:LYS:HD2	1:A:393:LYS:HA	1.80	0.42
1:B:43:TRP:HA	1:B:47:LEU:HB3	2.02	0.42
1:B:71:SER:OG	1:B:102:GLY:O	2.28	0.42
1:B:208:TYR:HD2	1:B:213:TRP:CD2	2.37	0.42
1:C:468:GLU:HB3	1:D:94:ARG:HB3	2.02	0.42
1:D:289:PRO:HB2	1:D:292:VAL:HG23	2.02	0.42
1:A:64:VAL:HG13	1:A:116:THR:HG21	2.01	0.42
1:A:415:ALA:HA	1:A:418:MET:CE	2.49	0.42
1:D:32:PRO:O	1:D:36:ALA:HB2	2.20	0.42
1:D:237:GLU:HG3	1:D:240:LYS:H	1.84	0.42
1:A:609:LYS:HZ3	1:A:670:PHE:HB3	1.79	0.42
1:B:49:VAL:HG12	1:B:60:ARG:HB2	2.01	0.42
1:B:188:ASN:HA	1:B:248:THR:O	2.20	0.42
1:B:625:VAL:HG13	1:B:629:GLY:HA3	2.01	0.42
1:D:419:ASN:O	1:D:423:LEU:HG	2.20	0.42
1:D:625:VAL:HG23	1:D:626:GLY:O	2.20	0.42
1:A:408:GLY:HA3	1:B:162:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:HD2	1:B:262:VAL:O	2.20	0.42
1:C:536:MET:HB3	1:C:542:TYR:CG	2.55	0.42
1:C:611:VAL:HA	1:C:630:ALA:O	2.20	0.42
1:C:621:TRP:O	1:C:625:VAL:HG22	2.20	0.42
1:D:127:VAL:HG21	1:D:169:ALA:HB1	2.02	0.42
1:A:15:THR:HG21	1:A:281:TRP:CZ2	2.54	0.42
1:B:490:VAL:HG12	1:B:515:ILE:HB	2.01	0.42
1:C:74:LEU:HG	1:C:78:LEU:CD1	2.39	0.42
1:C:375:TRP:HE1	1:C:427:THR:HB	1.84	0.42
1:D:552:PRO:HB2	1:D:554:GLY:O	2.20	0.42
1:B:250:ILE:HG12	1:B:262:VAL:HG23	2.02	0.41
1:D:4:LYS:H	1:D:4:LYS:HG2	1.61	0.41
1:D:613:ILE:N	1:D:613:ILE:HD12	2.34	0.41
1:A:136:LEU:HD12	1:A:424:HIS:HE1	1.85	0.41
1:C:567:VAL:HA	1:C:582:VAL:HG11	2.02	0.41
1:B:380:ASP:O	1:B:381:LEU:HD23	2.19	0.41
1:B:456:VAL:HG11	1:B:503:TRP:CZ3	2.55	0.41
1:C:64:VAL:O	1:C:154:ALA:HA	2.20	0.41
1:D:368:SER:OG	1:D:389:VAL:HG11	2.20	0.41
1:D:418:MET:SD	1:D:431:GLY:HA3	2.60	0.41
1:A:229:LYS:O	1:A:233:GLU:HG3	2.20	0.41
2:A:701:TPP:HM43	1:B:381:LEU:CD2	2.50	0.41
1:C:136:LEU:HD21	1:C:427:THR:HG23	2.02	0.41
1:C:667:ASN:OD1	1:C:668:LEU:N	2.52	0.41
1:D:526:LEU:HB3	1:D:544:LEU:HD21	2.02	0.41
1:B:64:VAL:O	1:B:154:ALA:HA	2.19	0.41
1:C:8:LEU:O	1:C:12:THR:N	2.46	0.41
1:A:175:HIS:HE1	1:B:197:SER:O	2.03	0.41
1:A:472:THR:HB	1:B:118:PRO:HD3	2.02	0.41
1:B:610:ARG:HD3	1:B:624:TYR:O	2.20	0.41
1:C:46:HIS:HE1	1:C:228:SER:CB	2.31	0.41
1:C:616:ALA:O	1:C:633:THR:HB	2.20	0.41
1:A:547:SER:HB2	1:A:579:ASP:OD2	2.20	0.41
1:B:118:PRO:HG2	1:B:447:LEU:HD21	2.03	0.41
1:B:142:LYS:HG2	1:B:322:TYR:CZ	2.55	0.41
1:B:569:ALA:HB2	1:B:657:VAL:HG21	2.02	0.41
1:C:7:GLN:HA	1:C:7:GLN:NE2	2.35	0.41
1:C:74:LEU:O	1:C:77:LEU:HB2	2.21	0.41
1:C:76:SER:O	1:C:80:LEU:HD12	2.20	0.41
1:C:456:VAL:HG22	1:C:506:ALA:HB1	2.02	0.41
1:C:78:LEU:HD23	1:C:110:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:HD12	1:C:424:HIS:CE1	2.56	0.41
1:A:65:LEU:HD22	1:A:74:LEU:HB2	2.03	0.41
1:A:145:PHE:HD1	1:A:314:MET:HG2	1.86	0.41
1:A:179:GLY:HA2	1:A:240:LYS:O	2.21	0.41
1:A:197:SER:O	1:B:175:HIS:HE1	2.03	0.41
1:A:297:HIS:CD2	1:A:297:HIS:C	2.93	0.41
1:A:611:VAL:HA	1:A:630:ALA:O	2.20	0.41
1:B:489:GLN:HA	1:B:589:ASP:OD2	2.21	0.41
1:C:123:ILE:HD13	1:C:123:ILE:HG21	1.84	0.41
1:C:436:VAL:HG21	1:C:472:THR:O	2.21	0.41
1:D:5:ILE:HB	1:D:295:ARG:HH21	1.86	0.41
1:D:136:LEU:HD12	1:D:136:LEU:HA	1.84	0.41
1:D:491:ILE:HD11	1:D:505:VAL:HG11	2.02	0.41
1:A:409:VAL:N	1:B:162:MET:HE2	2.36	0.41
1:C:541:ALA:HB3	1:C:591:PHE:CD1	2.56	0.41
1:A:196:THR:HB	1:A:200:PHE:HB3	2.03	0.40
1:D:75:TYR:OH	1:D:101:PRO:HD2	2.21	0.40
1:D:387:THR:HB	1:D:430:TYR:HE2	1.86	0.40
1:A:9:GLY:O	1:A:13:ILE:HG13	2.21	0.40
1:A:125:MET:HE3	1:A:447:LEU:HD23	2.03	0.40
1:A:268:GLY:O	1:A:272:ILE:HG13	2.22	0.40
1:D:18:ILE:HD11	1:D:33:MET:HG2	2.03	0.40
1:A:163:GLU:O	1:A:167:GLN:HG3	2.21	0.40
1:A:468:GLU:HG2	1:B:94:ARG:HB3	2.04	0.40
1:B:600:GLU:O	1:B:600:GLU:HG3	2.22	0.40
1:C:58:ALA:O	1:C:62:ARG:NH1	2.54	0.40
1:C:359:SER:O	1:C:363:VAL:HG23	2.21	0.40
1:D:33:MET:SD	1:D:251:GLY:HA2	2.62	0.40
1:D:359:SER:O	1:D:363:VAL:HG23	2.21	0.40
1:D:381:LEU:HD22	1:D:434:PHE:CE1	2.56	0.40
1:A:306:LYS:HB3	1:A:306:LYS:HE3	1.86	0.40
1:D:40:TYR:CZ	1:D:44:THR:HG21	2.57	0.40
1:D:447:LEU:HD23	1:D:447:LEU:HA	1.81	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	670/680 (98%)	653 (98%)	16 (2%)	1 (0%)	51	82
1	B	664/680 (98%)	653 (98%)	10 (2%)	1 (0%)	47	78
1	C	666/680 (98%)	644 (97%)	21 (3%)	1 (0%)	47	78
1	D	666/680 (98%)	649 (97%)	17 (3%)	0	100	100
All	All	2666/2720 (98%)	2599 (98%)	64 (2%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	29	PRO
1	A	409	VAL
1	B	29	PRO

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	541/550 (98%)	529 (98%)	12 (2%)	52	81
1	B	537/550 (98%)	523 (97%)	14 (3%)	46	77
1	C	539/550 (98%)	517 (96%)	22 (4%)	30	64
1	D	538/550 (98%)	517 (96%)	21 (4%)	32	66
All	All	2155/2200 (98%)	2086 (97%)	69 (3%)	39	73

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	97	ASP
1	A	123	ILE
1	A	158	ASP
1	A	353	SER
1	A	356	SER
1	A	373	SER
1	A	375	TRP
1	A	378	SER
1	A	392	ASP
1	A	409	VAL
1	A	412	PHE
1	B	187	SER
1	B	336	LYS
1	B	357	ARG
1	B	373	SER
1	B	375	TRP
1	B	382	SER
1	B	388	MET
1	B	412	PHE
1	B	454	PRO
1	B	455	VAL
1	B	589	ASP
1	B	605	LYS
1	B	606	SER
1	B	655	GLU
1	C	45	LYS
1	C	47	LEU
1	C	87	ILE
1	C	218	VAL
1	C	238	THR
1	C	260	SER
1	C	290	GLU
1	C	299	THR
1	C	314	MET
1	C	341	TRP
1	C	375	TRP
1	C	392	ASP
1	C	412	PHE
1	C	472	THR
1	C	511	ASP
1	C	530	LYS
1	C	556	LEU

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Mol	Chain	Res	Type
1	C	562	GLU
1	C	580	VAL
1	C	605	LYS
1	C	627	THR
1	C	668	LEU
1	D	94	ARG
1	D	97	ASP
1	D	136	LEU
1	D	143	GLU
1	D	147	VAL
1	D	166	SER
1	D	192	LEU
1	D	193	ASP
1	D	196	THR
1	D	375	TRP
1	D	399	HIS
1	D	412	PHE
1	D	427	THR
1	D	547	SER
1	D	571	LYS
1	D	580	VAL
1	D	581	SER
1	D	600	GLU
1	D	657	VAL
1	D	664	LEU
1	D	668	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	297	HIS
1	A	385	ASN
1	A	667	ASN
1	B	107	HIS
1	B	175	HIS
1	B	263	HIS
1	C	7	GLN
1	C	46	HIS
1	C	146	ASN
1	C	215	HIS
1	C	298	GLN

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Mol	Chain	Res	Type
1	C	385	ASN
1	C	386	ASN
1	D	305	GLN
1	D	473	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	701	3	22,27,27	0.49	0	29,40,40	0.75	1 (3%)
2	TPP	C	701	3	22,27,27	0.48	0	29,40,40	0.76	0
2	TPP	D	701	3	22,27,27	0.49	0	29,40,40	0.75	0
2	TPP	B	701	3	22,27,27	0.52	0	29,40,40	0.74	1 (3%)

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	701	3	-	4/16/17/17	0/2/2/2
2	TPP	C	701	3	-	4/16/17/17	0/2/2/2
2	TPP	D	701	3	-	2/16/17/17	0/2/2/2
2	TPP	B	701	3	-	5/16/17/17	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	TPP	C5-C4-N3	2.10	111.78	107.57
2	B	701	TPP	C5-C4-N3	2.02	111.62	107.57

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TPP	C5-C6-C7-O7
2	A	701	TPP	C7-O7-PA-O1A
2	A	701	TPP	C7-O7-PA-O2A
2	B	701	TPP	C5-C6-C7-O7
2	B	701	TPP	C7-O7-PA-O1A
2	C	701	TPP	C5-C6-C7-O7
2	C	701	TPP	C7-O7-PA-O1A
2	D	701	TPP	C5-C6-C7-O7
2	B	701	TPP	C7-O7-PA-O3A
2	C	701	TPP	C7-O7-PA-O3A
2	B	701	TPP	C7-O7-PA-O2A
2	C	701	TPP	C7-O7-PA-O2A
2	B	701	TPP	PB-O3A-PA-O2A
2	A	701	TPP	C7-O7-PA-O3A
2	D	701	TPP	C7-O7-PA-O3A

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	TPP	3	0
2	C	701	TPP	2	0
2	D	701	TPP	1	0
2	B	701	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 701

Bond lengths — Bond angles — Torsions — Rings

Ligand TPP C 701

Bond lengths — Bond angles — Torsions — Rings

Ligand TPP D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP B 701

Bond lengths

Bond angles

Torsions

Rings
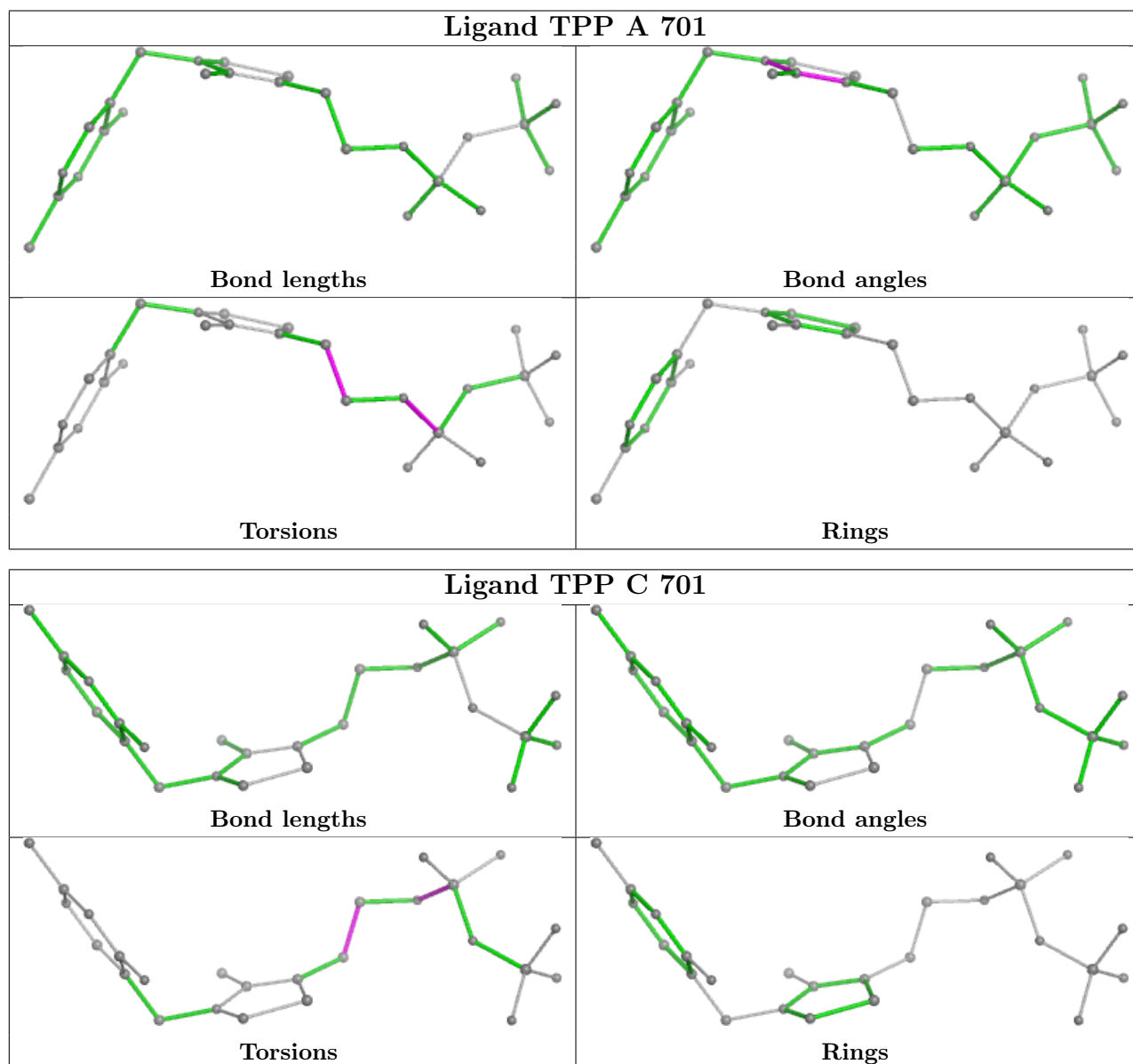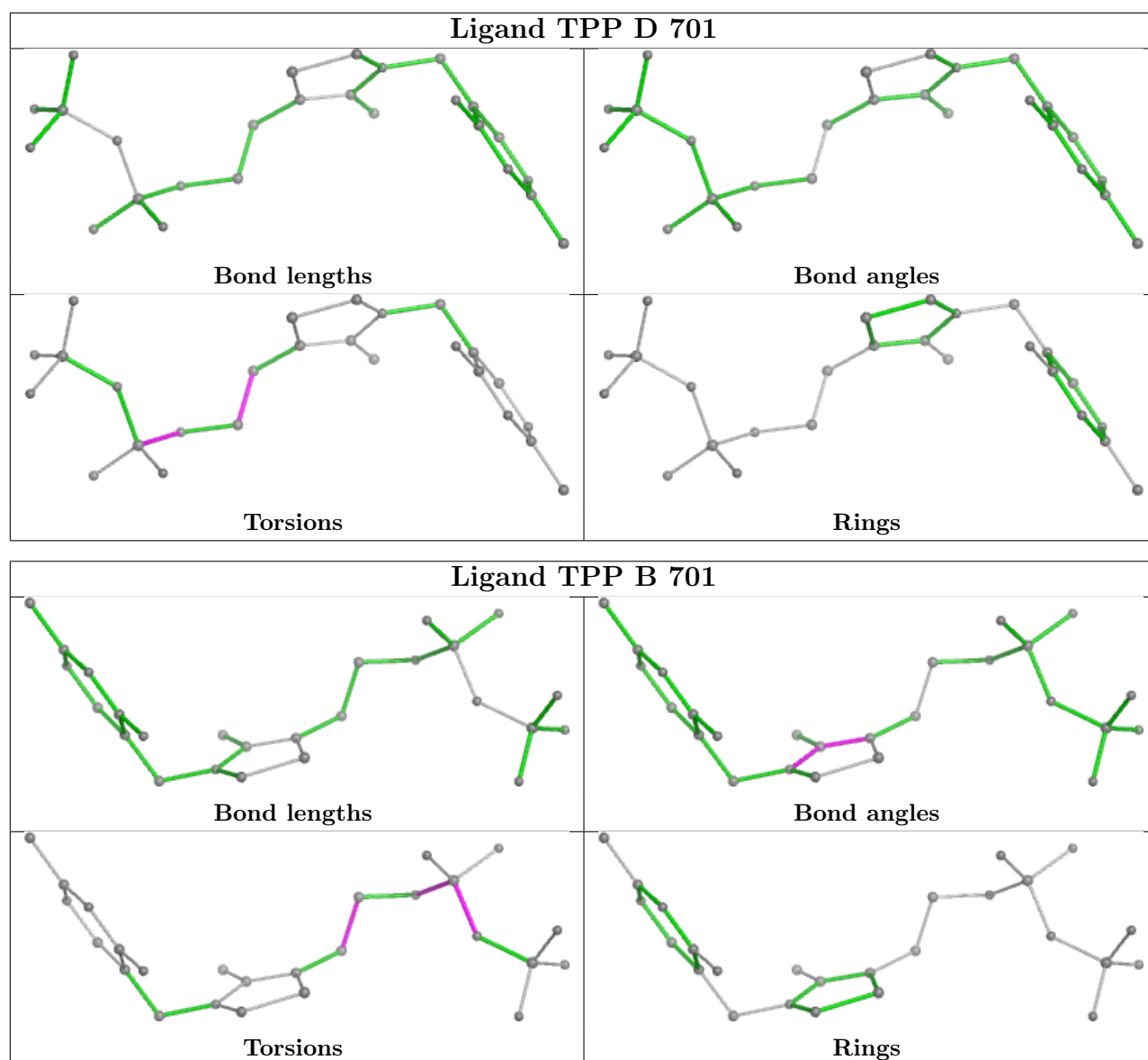
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	672/680 (98%)	0.05	5 (0%)	87	87	44, 64, 80, 102	0
1	B	666/680 (97%)	-0.05	5 (0%)	86	86	40, 54, 75, 96	0
1	C	668/680 (98%)	0.33	20 (2%)	50	45	54, 76, 92, 102	0
1	D	668/680 (98%)	0.01	9 (1%)	77	77	46, 60, 77, 98	0
All	All	2674/2720 (98%)	0.08	39 (1%)	73	73	40, 63, 86, 102	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	665	SER	4.2
1	D	578	LYS	3.9
1	C	256	LYS	3.7
1	D	666	GLU	3.5
1	C	286	PHE	3.2
1	C	258	GLY	3.0
1	C	191	SER	3.0
1	C	259	THR	2.9
1	C	144	ASN	2.8
1	C	325	LEU	2.8
1	C	287	THR	2.7
1	D	662	ASN	2.7
1	C	444	ALA	2.6
1	D	440	TYR	2.5
1	B	577	GLY	2.5
1	C	578	LYS	2.5
1	A	552	PRO	2.5
1	C	1	MET	2.4
1	B	575	GLU	2.4
1	C	141	ASN	2.4
1	D	439	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	137	ALA	2.3
1	B	144	ASN	2.3
1	A	195	PRO	2.3
1	A	577	GLY	2.3
1	D	392	ASP	2.3
1	C	613	ILE	2.3
1	D	661	TYR	2.2
1	C	254	ALA	2.2
1	D	577	GLY	2.2
1	B	315	PHE	2.2
1	C	255	PRO	2.1
1	C	54	SER	2.1
1	C	298	GLN	2.1
1	C	318	TYR	2.1
1	B	578	LYS	2.1
1	A	322	TYR	2.1
1	C	443	PRO	2.0
1	A	255	PRO	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	702	1/1	0.81	0.08	96,96,96,96	0
3	MG	D	702	1/1	0.88	0.11	64,64,64,64	0
3	MG	B	702	1/1	0.94	0.09	47,47,47,47	0
3	MG	C	702	1/1	0.94	0.15	74,74,74,74	0
2	TPP	C	701	26/26	0.94	0.19	63,77,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TPP	A	701	26/26	0.95	0.16	55,68,78,84	0
2	TPP	B	701	26/26	0.96	0.16	42,56,61,62	0
2	TPP	D	701	26/26	0.96	0.17	59,74,79,83	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.
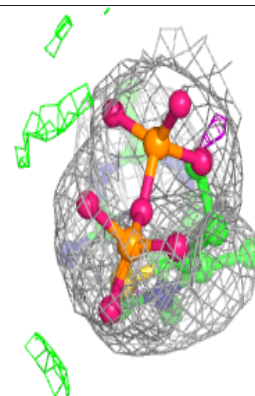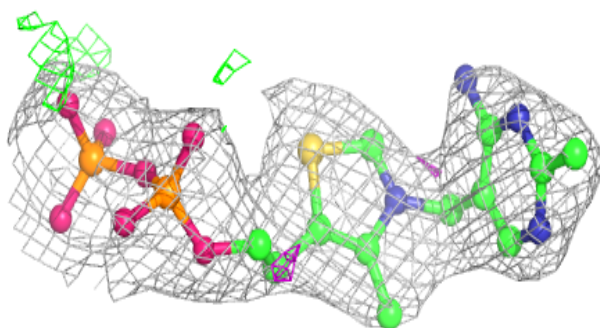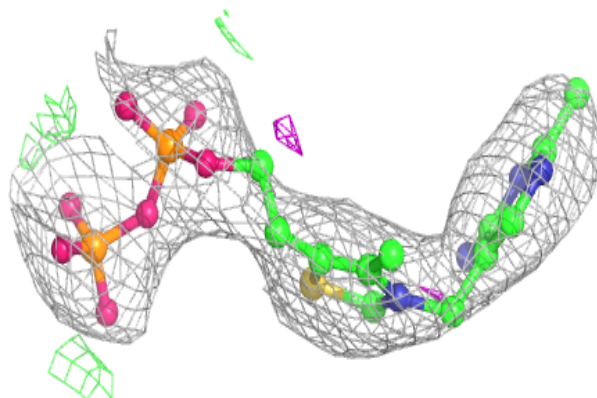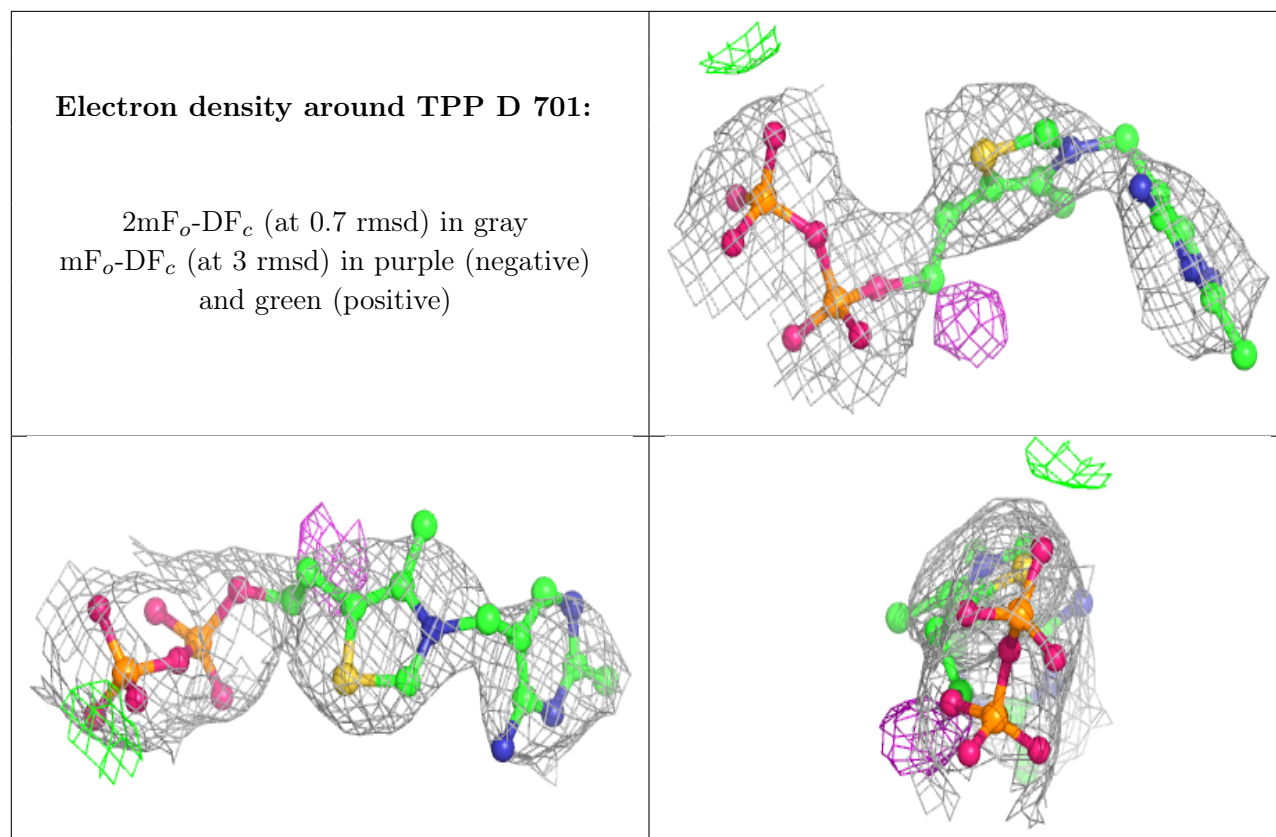
Electron density around TPP C 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
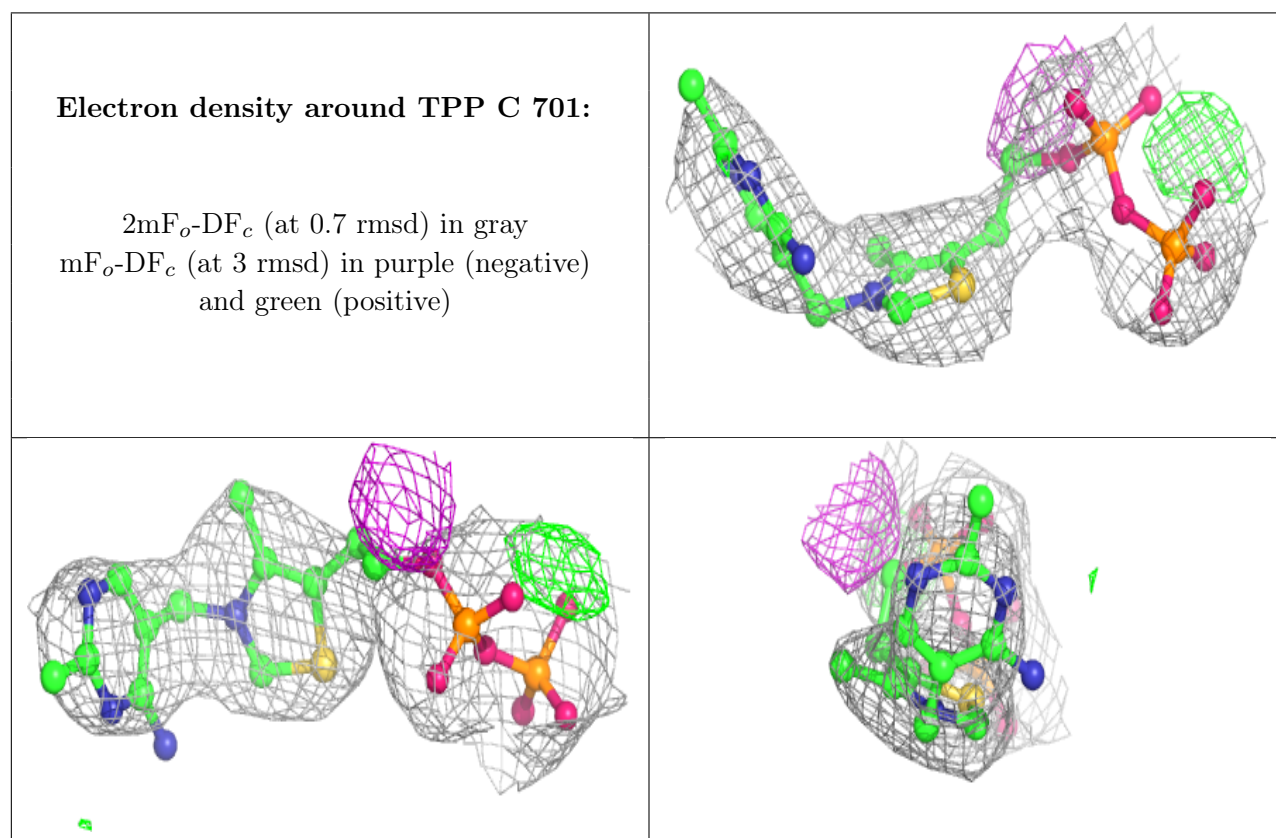
Electron density around TPP A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
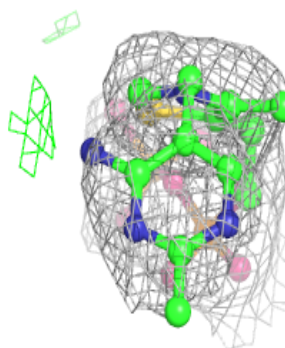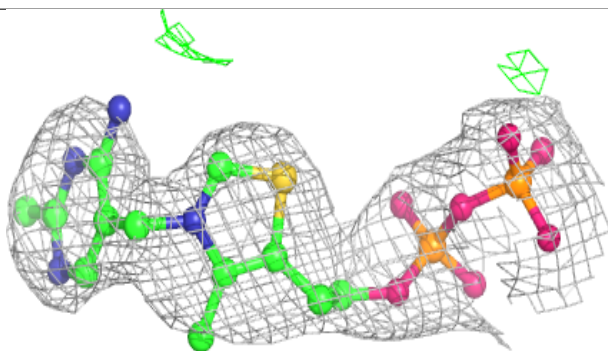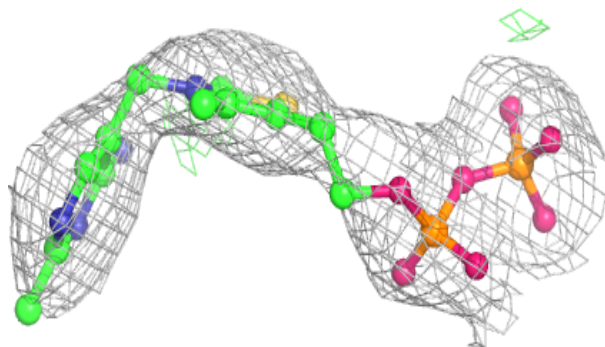
Electron density around TPP B 701:

$2mF_o$-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 701:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.