



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:34 PM UTC

PDB ID : 7BYI / pdb_00007byi
Title : Structure of SHMT2 in complex with CBX
Authors : Li, L.; Chen, Y.; Lu, D.; Zhang, C.; Su, D.
Deposited on : 2020-04-23
Resolution : 2.76 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

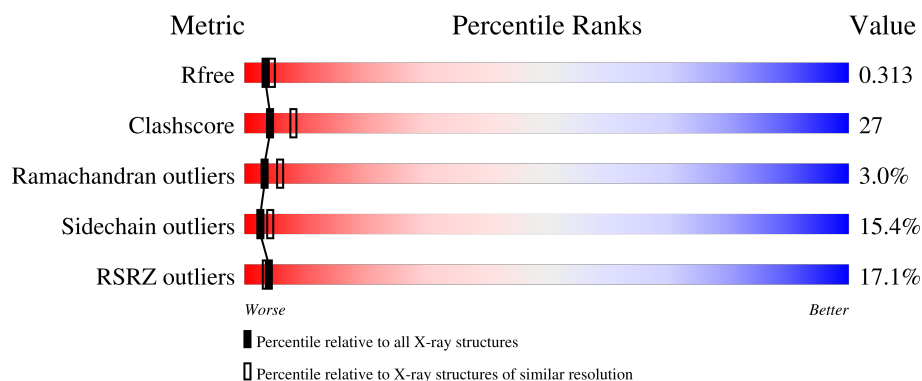
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	
2	B	483	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CBO	B	601	X	-	-	-
5	CBO	B	602	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7363 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3609	2273	649	672	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLY	ALA	conflict	UNP P34897
A	343	ALA	CYS	conflict	UNP P34897

- Molecule 2 is a protein called Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	462	Total	C	N	O	S	0	0	0
			3577	2251	644	666	16			

There are 7 discrepancies between the modelled and reference sequences:

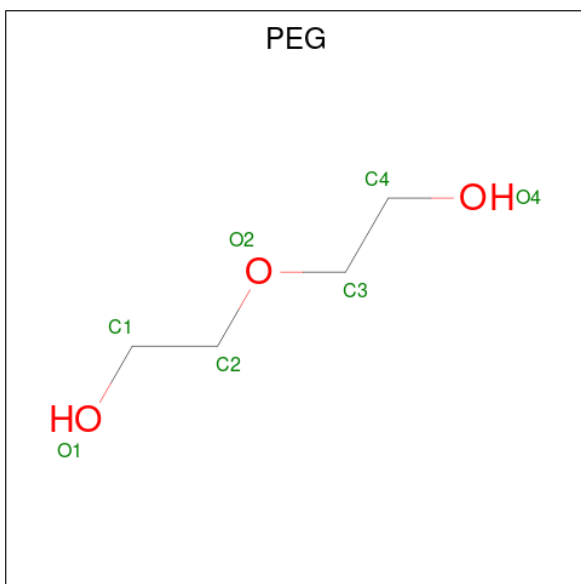
Chain	Residue	Modelled	Actual	Comment	Reference
B	196	GLY	LYS	conflict	UNP P34897
B	198	ALA	ASN	conflict	UNP P34897
B	307	ALA	ILE	conflict	UNP P34897
B	370	GLY	TYR	conflict	UNP P34897
B	371	TYR	SER	conflict	UNP P34897
B	391	GLY	LEU	conflict	UNP P34897
B	392	GLY	ASP	conflict	UNP P34897

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



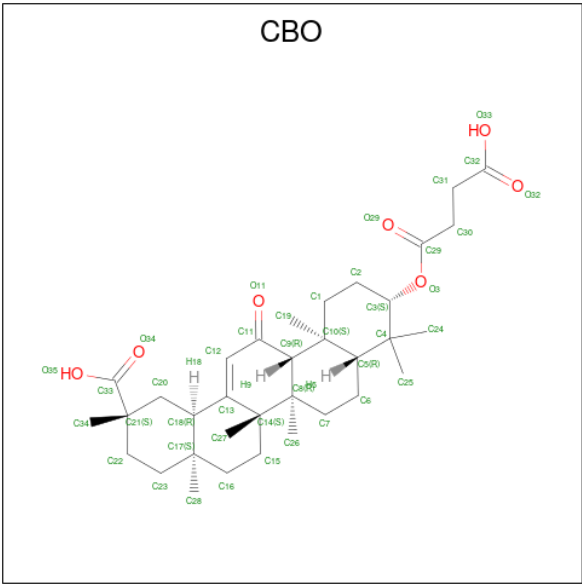
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

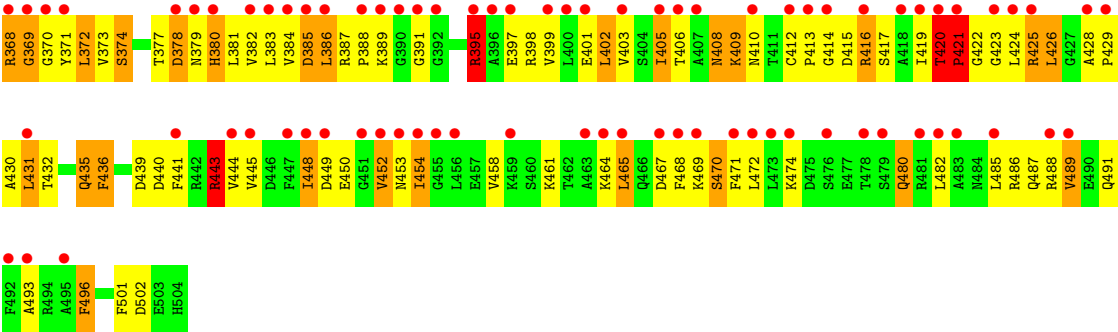
- Molecule 5 is CARBENOXOLONE (CCD ID: CBO) (formula: C₃₄H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			41	34	7		
5	B	1	Total	C	O	0	0
			41	34	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total	O	0	0
			35	35		
6	B	43	Total	O	0	0
			43	43		



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.62Å 158.62Å 209.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.50 – 2.76 34.50 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.50-2.76) 99.8 (34.50-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.242 , 0.311 0.247 , 0.313	Depositor DCC
R_{free} test set	2127 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7363	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CBO, PO4, PEG

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	1.18	4/3682 (0.1%)	1.63	30/4978 (0.6%)
2	B	1.26	3/3650 (0.1%)	1.80	66/4936 (1.3%)
All	All	1.22	7/7332 (0.1%)	1.72	96/9914 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	LEU	C-O	-6.91	1.15	1.23
2	B	385	ASP	C-O	6.13	1.31	1.24
1	A	140	PRO	C-O	-5.99	1.16	1.23
2	B	222	ILE	C-O	5.66	1.30	1.24
1	A	221	ILE	C-O	5.58	1.29	1.24
1	A	163	GLY	C-O	5.44	1.31	1.23
2	B	321	PRO	C-O	-5.17	1.18	1.24

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	341	GLN	N-CA-C	-15.42	86.94	109.15
2	B	419	ILE	CB-CA-C	14.10	129.93	111.88
2	B	194	PRO	N-CA-C	10.62	126.51	111.33
1	A	103	LYS	N-CA-C	-10.09	90.31	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	PRO	CB-CA-C	-9.59	96.64	111.40
1	A	206	TYR	N-CA-C	-9.42	101.21	112.89
2	B	203	LEU	N-CA-C	9.24	123.28	110.35
1	A	301	PRO	N-CA-C	9.04	131.08	112.47
1	A	416	ARG	N-CA-C	-8.38	102.10	111.07
2	B	168	ASP	CA-CB-CG	8.11	120.71	112.60
2	B	194	PRO	CA-C-N	7.86	136.55	121.54
2	B	194	PRO	C-N-CA	7.86	136.55	121.54
2	B	420	THR	N-CA-CB	-7.78	96.53	110.37
2	B	342	ALA	N-CA-C	7.56	126.90	110.80
2	B	206	TYR	N-CA-C	-7.52	104.10	113.28
2	B	421	PRO	CB-CA-C	-7.37	99.41	111.56
1	A	234	TYR	CA-CB-CG	7.34	127.11	113.90
1	A	301	PRO	CB-CA-C	-6.89	100.19	111.56
1	A	234	TYR	CB-CA-C	-6.69	98.94	109.84
2	B	491	GLN	N-CA-C	-6.50	104.83	112.89
2	B	201	THR	N-CA-C	-6.47	97.03	110.80
2	B	420	THR	N-CA-C	6.41	123.98	109.81
2	B	63	GLU	CB-CG-CD	6.34	123.38	112.60
2	B	436	PHE	CA-CB-CG	6.32	120.12	113.80
2	B	202	GLY	N-CA-C	-6.29	105.19	112.73
2	B	322	SER	CA-C-O	-6.16	114.53	121.00
1	A	127	PHE	CA-C-O	-6.14	114.09	121.89
2	B	179	ASP	N-CA-C	-6.00	105.73	113.16
2	B	203	LEU	CB-CA-C	-5.99	100.14	109.61
1	A	446	ASP	N-CA-CB	5.99	119.02	110.16
1	A	270	HIS	CA-CB-CG	-5.99	107.81	113.80
2	B	421	PRO	N-CA-C	5.95	124.72	112.47
2	B	208	GLN	N-CA-C	-5.94	104.93	111.82
2	B	65	ASP	O-C-N	5.86	128.34	122.08
1	A	309	TYR	CA-C-O	-5.83	115.20	121.56
2	B	201	THR	CA-C-N	5.79	126.41	119.98
2	B	201	THR	C-N-CA	5.79	126.41	119.98
2	B	344	THR	CB-CA-C	-5.79	99.90	108.87
2	B	370	GLY	CA-C-O	-5.78	116.92	120.91
2	B	385	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	99	GLY	CA-C-O	-5.73	116.58	122.25
2	B	179	ASP	CB-CA-C	5.70	120.27	110.01
2	B	320	PHE	N-CA-C	5.62	122.23	109.81
2	B	395	ARG	CA-C-N	5.59	128.04	120.38
2	B	395	ARG	C-N-CA	5.59	128.04	120.38
1	A	445	VAL	CA-C-O	-5.55	114.48	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PRO	N-CA-C	5.53	123.85	112.47
2	B	491	GLN	CB-CA-C	5.50	121.48	109.99
2	B	443	ARG	CA-C-O	-5.49	114.15	120.24
1	A	205	ASP	N-CA-C	-5.44	99.22	110.80
2	B	453	ASN	CA-C-O	-5.43	114.67	120.42
2	B	202	GLY	CA-C-N	5.41	129.38	121.31
2	B	202	GLY	C-N-CA	5.41	129.38	121.31
1	A	200	LYS	CA-C-N	5.37	131.80	121.54
1	A	200	LYS	C-N-CA	5.37	131.80	121.54
2	B	470	SER	CA-C-N	5.36	128.00	120.28
2	B	470	SER	C-N-CA	5.36	128.00	120.28
1	A	442	ARG	N-CA-C	-5.35	104.86	111.33
2	B	209	LEU	CA-C-N	5.34	127.70	120.38
2	B	209	LEU	C-N-CA	5.34	127.70	120.38
2	B	496	PHE	CA-CB-CG	5.34	119.14	113.80
2	B	211	LEU	CA-C-N	5.32	128.40	120.31
2	B	211	LEU	C-N-CA	5.32	128.40	120.31
2	B	105	TYR	CB-CA-C	5.29	119.19	109.99
2	B	197	LEU	CA-C-O	-5.27	115.20	121.16
2	B	165	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	373	VAL	CB-CA-C	5.26	119.92	111.29
2	B	68	CYS	CA-C-N	5.26	129.55	121.19
2	B	68	CYS	C-N-CA	5.26	129.55	121.19
1	A	385	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	223	ALA	N-CA-C	-5.25	99.61	110.80
1	A	232	ILE	CA-C-O	-5.25	114.22	120.78
2	B	205	ASP	N-CA-C	-5.25	99.63	110.80
1	A	233	ASP	CA-C-N	5.24	129.00	121.50
1	A	233	ASP	C-N-CA	5.24	129.00	121.50
1	A	501	PHE	CA-C-O	-5.24	115.91	121.94
1	A	128	ASP	CA-C-N	5.23	131.53	121.54
1	A	128	ASP	C-N-CA	5.23	131.53	121.54
2	B	120	GLN	N-CA-C	-5.23	105.27	110.97
2	B	467	ASP	CA-C-N	5.21	127.71	120.63
2	B	467	ASP	C-N-CA	5.21	127.71	120.63
1	A	209	LEU	CA-C-N	5.20	127.20	120.44
1	A	209	LEU	C-N-CA	5.20	127.20	120.44
2	B	195	TYR	CA-C-N	5.20	131.60	121.41
2	B	195	TYR	C-N-CA	5.20	131.60	121.41
2	B	251	ASP	CA-CB-CG	5.16	117.76	112.60
2	B	260	ALA	O-C-N	5.15	127.58	122.12
2	B	358	ALA	CA-C-N	5.12	127.45	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	358	ALA	C-N-CA	5.12	127.45	120.54
2	B	93	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	491	GLN	N-CA-C	-5.06	105.77	111.28
2	B	65	ASP	CA-CB-CG	5.05	117.65	112.60
2	B	65	ASP	CA-C-N	5.04	127.04	120.28
2	B	65	ASP	C-N-CA	5.04	127.04	120.28
1	A	272	ASP	CA-CB-CG	5.02	117.62	112.60
2	B	301	PRO	N-CA-C	5.01	122.78	112.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Peptide
1	A	129	LEU	Peptide

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	3609	0	3602	145	0
2	B	3577	0	3555	250	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	7	0	10	0	0
5	B	82	0	96	17	0
6	A	35	0	0	3	0
6	B	43	0	0	4	0
All	All	7363	0	7263	396	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 27.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:OD2	2:B:208:GLN:HB3	1.31	1.27
2:B:165:ASP:CB	2:B:195:TYR:HD2	1.56	1.16
2:B:165:ASP:HB2	2:B:195:TYR:HD2	1.09	1.14
2:B:165:ASP:HB2	2:B:195:TYR:CD2	1.91	1.05
1:A:420:THR:H	1:A:421:PRO:CD	1.67	1.03
2:B:223:ALA:O	2:B:250:ALA:HA	1.60	1.01
2:B:359:ARG:NH2	2:B:377:THR:O	1.93	1.01
1:A:420:THR:H	1:A:421:PRO:HD3	1.24	1.00
2:B:205:ASP:OD2	2:B:208:GLN:CB	2.11	0.97
2:B:75:ALA:HB1	2:B:380:HIS:NE2	1.78	0.97
5:B:601:CBO:H343	5:B:601:CBO:H161	1.48	0.95
2:B:165:ASP:CB	2:B:195:TYR:CD2	2.47	0.95
2:B:320:PHE:O	2:B:320:PHE:CD1	2.21	0.94
2:B:231:LEU:HD12	6:B:709:HOH:O	1.66	0.94
2:B:193:MET:HE2	2:B:216:PHE:CG	2.03	0.94
1:A:108:GLY:O	1:A:110:GLU:N	2.01	0.94
2:B:174:HIS:HD2	2:B:222:ILE:HG21	1.34	0.92
2:B:174:HIS:CD2	2:B:222:ILE:HG21	2.05	0.91
2:B:193:MET:HE2	2:B:216:PHE:CD1	2.08	0.89
2:B:373:VAL:HG21	2:B:412:CYS:SG	2.14	0.87
2:B:372:LEU:HD11	2:B:382:VAL:CG1	2.05	0.87
2:B:76:SER:OG	2:B:254:HIS:CE1	2.30	0.85
2:B:402:LEU:O	2:B:486:ARG:HD2	1.77	0.85
1:A:197:LEU:HG	1:A:203:LEU:HB3	1.58	0.84
2:B:165:ASP:HB3	2:B:195:TYR:HD2	1.43	0.84
1:A:233:ASP:HB3	1:A:267:PRO:HB3	1.58	0.83
1:A:320:PHE:O	1:A:320:PHE:CD1	2.31	0.83
2:B:452:VAL:HG11	6:B:707:HOH:O	1.80	0.81
2:B:373:VAL:O	2:B:374:SER:OG	1.99	0.81
2:B:377:THR:HG22	2:B:379:ASN:H	1.46	0.80
1:A:420:THR:N	1:A:421:PRO:CD	2.38	0.79
2:B:206:TYR:OH	2:B:233:ASP:N	2.16	0.78
2:B:164:LEU:HA	2:B:195:TYR:HA	1.66	0.78
2:B:341:GLN:O	2:B:342:ALA:HB3	1.82	0.78
1:A:197:LEU:CG	1:A:203:LEU:HB3	2.13	0.77
2:B:205:ASP:OD2	2:B:208:GLN:N	2.17	0.76
2:B:197:LEU:HD21	2:B:202:GLY:O	1.84	0.76
2:B:254:HIS:HB3	2:B:380:HIS:CE1	2.19	0.76
2:B:350:TYR:HA	2:B:353:GLN:NE2	2.01	0.76
1:A:200:LYS:HD3	1:A:374:SER:OG	1.84	0.76
1:A:203:LEU:HD23	1:A:203:LEU:N	2.02	0.75
2:B:353:GLN:HE21	2:B:432:THR:CG2	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:602:CBO:H263	5:B:602:CBO:H191	1.67	0.75
2:B:106:TYR:OH	5:B:601:CBO:O34	2.03	0.75
2:B:402:LEU:HD11	2:B:472:LEU:HD13	1.69	0.75
1:A:415:ASP:OD1	1:A:415:ASP:N	2.17	0.74
2:B:320:PHE:CD1	2:B:320:PHE:C	2.66	0.74
2:B:263:VAL:HG23	2:B:355:LEU:HD11	1.68	0.74
5:B:602:CBO:H271	5:B:602:CBO:H202	1.68	0.74
1:A:124:LEU:O	1:A:127:PHE:O	2.05	0.74
2:B:377:THR:HG21	2:B:379:ASN:O	1.88	0.74
2:B:377:THR:CG2	2:B:379:ASN:O	2.36	0.73
2:B:420:THR:HG23	2:B:421:PRO:HD3	1.70	0.73
2:B:206:TYR:CZ	2:B:233:ASP:HB3	2.23	0.73
2:B:353:GLN:NE2	2:B:432:THR:CG2	2.53	0.72
1:A:204:ILE:HD12	1:A:232:ILE:CG2	2.20	0.71
1:A:214:ARG:NE	1:A:243:GLU:OE1	2.20	0.71
2:B:160:ARG:HB2	2:B:218:PRO:HA	1.72	0.71
2:B:435:GLN:HE21	2:B:435:GLN:HA	1.54	0.71
2:B:165:ASP:OD1	2:B:194:PRO:HG3	1.91	0.70
2:B:441:PHE:HA	2:B:444:VAL:HG22	1.72	0.70
1:A:162:MET:HE3	1:A:193:MET:HE3	1.71	0.70
2:B:458:VAL:HG13	2:B:471:PHE:CD1	2.26	0.70
2:B:252:MET:HE2	2:B:268:PHE:CE1	2.26	0.69
2:B:165:ASP:HB3	2:B:195:TYR:CD2	2.22	0.69
1:A:320:PHE:CD1	1:A:320:PHE:C	2.69	0.69
1:A:168:ASP:HB3	1:A:197:LEU:HB2	1.74	0.68
2:B:341:GLN:O	2:B:342:ALA:CB	2.41	0.68
2:B:353:GLN:HE21	2:B:432:THR:HG21	1.58	0.68
2:B:127:PHE:HB2	2:B:129:LEU:HD12	1.74	0.68
1:A:419:ILE:C	1:A:420:THR:HG22	2.19	0.68
2:B:128:ASP:O	2:B:129:LEU:HG	1.93	0.68
5:B:601:CBO:H191	5:B:601:CBO:H263	1.76	0.67
1:A:162:MET:HE3	1:A:193:MET:CE	2.24	0.67
2:B:377:THR:OG1	2:B:382:VAL:HG22	1.94	0.67
2:B:480:GLN:HE21	2:B:480:GLN:HA	1.58	0.67
2:B:165:ASP:H	2:B:195:TYR:HB3	1.58	0.67
1:A:419:ILE:N	1:A:419:ILE:HD12	2.10	0.66
2:B:231:LEU:CD1	6:B:709:HOH:O	2.31	0.66
2:B:350:TYR:HA	2:B:353:GLN:HE22	1.59	0.66
2:B:198:ALA:O	2:B:201:THR:O	2.13	0.66
2:B:200:LYS:H	2:B:413:PRO:CB	2.09	0.65
2:B:386:LEU:H	2:B:386:LEU:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:ALA:HA	2:B:347:PHE:CB	2.26	0.65
1:A:160:ARG:HG2	1:A:216:PHE:CZ	2.32	0.65
2:B:372:LEU:HD11	2:B:382:VAL:HG13	1.78	0.65
2:B:403:VAL:HG12	2:B:403:VAL:O	1.95	0.65
2:B:398:ARG:CB	2:B:469:LYS:HE2	2.27	0.65
2:B:205:ASP:CG	2:B:208:GLN:H	2.05	0.64
1:A:105:TYR:OH	2:B:401:GLU:OE2	2.14	0.64
1:A:253:ALA:HB1	1:A:280:LYS:HE3	1.79	0.64
2:B:252:MET:HE2	2:B:268:PHE:HE1	1.63	0.64
1:A:454:ILE:O	1:A:458:VAL:HG13	1.97	0.64
1:A:340:LYS:HE2	2:B:53:ASP:CG	2.23	0.64
2:B:126:ALA:O	2:B:260:ALA:HB1	1.97	0.63
1:A:100:TYR:O	1:A:104:ARG:HB3	1.98	0.63
2:B:197:LEU:CD2	2:B:202:GLY:O	2.47	0.63
2:B:386:LEU:HD23	2:B:391:GLY:O	1.97	0.63
2:B:193:MET:CE	2:B:216:PHE:CG	2.81	0.63
2:B:252:MET:SD	2:B:256:SER:HA	2.38	0.63
2:B:415:ASP:OD2	2:B:422:GLY:HA2	1.99	0.62
1:A:133:GLN:O	1:A:133:GLN:HG3	1.97	0.62
1:A:206:TYR:CD1	1:A:206:TYR:C	2.77	0.62
1:A:153:ALA:O	1:A:314:ARG:HG2	2.00	0.62
2:B:450:GLU:O	2:B:454:ILE:HG23	2.00	0.62
5:B:601:CBO:H271	5:B:601:CBO:H202	1.81	0.62
1:A:263:VAL:HG23	1:A:355:LEU:HD11	1.82	0.62
2:B:480:GLN:HA	2:B:480:GLN:NE2	2.14	0.62
2:B:485:LEU:O	2:B:489:VAL:HG13	2.00	0.62
2:B:357:ASN:ND2	2:B:432:THR:OG1	2.33	0.61
1:A:95:LYS:HG2	1:A:112:VAL:HG11	1.83	0.61
1:A:204:ILE:HG22	1:A:204:ILE:O	1.99	0.61
1:A:353:GLN:HE21	1:A:357:ASN:ND2	1.99	0.61
1:A:230:ARG:NH2	1:A:376:GLY:H	1.99	0.61
1:A:419:ILE:O	1:A:420:THR:HG22	2.00	0.61
2:B:350:TYR:O	2:B:353:GLN:NE2	2.33	0.61
2:B:377:THR:CG2	2:B:381:LEU:O	2.48	0.61
1:A:231:LEU:CD1	1:A:378:ASP:HB2	2.30	0.61
2:B:193:MET:HE1	2:B:216:PHE:HB2	1.83	0.60
2:B:196:GLY:HA2	2:B:208:GLN:HE22	1.67	0.60
1:A:166:LEU:HB3	1:A:167:PRO:HD3	1.84	0.60
1:A:232:ILE:HA	1:A:234:TYR:CD1	2.36	0.60
2:B:372:LEU:HD11	2:B:382:VAL:HG12	1.81	0.60
1:A:458:VAL:HG23	1:A:468:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:VAL:HA	2:B:448:ILE:CG2	2.32	0.60
2:B:403:VAL:O	2:B:403:VAL:CG1	2.50	0.59
2:B:350:TYR:HA	2:B:353:GLN:CD	2.27	0.59
2:B:367:GLU:O	2:B:368:ARG:HB2	2.02	0.59
2:B:470:SER:O	2:B:474:LYS:HG2	2.03	0.59
1:A:342:ALA:HA	1:A:347:PHE:CG	2.38	0.59
1:A:380:HIS:CE1	1:A:381:LEU:CD2	2.86	0.59
1:A:419:ILE:O	1:A:419:ILE:HG22	2.02	0.59
2:B:205:ASP:OD2	2:B:208:GLN:CA	2.50	0.59
2:B:398:ARG:HB2	2:B:469:LYS:HE2	1.84	0.58
2:B:350:TYR:CD1	2:B:353:GLN:NE2	2.71	0.58
1:A:428:ALA:H	1:A:429:PRO:HD3	1.67	0.58
2:B:440:ASP:O	2:B:444:VAL:HG13	2.04	0.58
2:B:129:LEU:HD23	2:B:134:TRP:CD1	2.39	0.58
2:B:50:SER:HG	2:B:57:TRP:CD1	2.22	0.57
1:A:234:TYR:HB3	1:A:236:ARG:HG2	1.85	0.57
2:B:444:VAL:O	2:B:448:ILE:HG22	2.04	0.57
1:A:458:VAL:CG2	1:A:468:PHE:CE2	2.87	0.57
2:B:162:MET:HG3	2:B:218:PRO:HG3	1.86	0.57
2:B:166:LEU:HA	2:B:170:GLY:HA2	1.86	0.57
1:A:264:ILE:HB	1:A:265:PRO:HD2	1.87	0.57
1:A:63:GLU:HG2	2:B:92:LEU:HD23	1.85	0.57
1:A:387:ARG:N	1:A:388:PRO:CD	2.68	0.57
2:B:377:THR:HG22	2:B:379:ASN:N	2.18	0.57
2:B:428:ALA:N	2:B:429:PRO:CD	2.67	0.57
1:A:204:ILE:HD12	1:A:232:ILE:HG21	1.85	0.56
1:A:428:ALA:N	1:A:429:PRO:CD	2.68	0.56
2:B:357:ASN:HB3	2:B:441:PHE:CZ	2.40	0.56
2:B:129:LEU:HD22	2:B:134:TRP:CG	2.40	0.56
2:B:379:ASN:OD1	2:B:379:ASN:C	2.48	0.56
2:B:233:ASP:O	2:B:237:MET:HG2	2.06	0.56
2:B:193:MET:CE	2:B:216:PHE:CB	2.84	0.56
2:B:342:ALA:HA	2:B:347:PHE:CG	2.40	0.56
1:A:57:TRP:O	1:A:61:GLN:HG3	2.06	0.56
1:A:410:ASN:C	1:A:410:ASN:HD22	2.13	0.56
2:B:377:THR:CG2	2:B:379:ASN:H	2.16	0.56
2:B:387:ARG:HB3	2:B:388:PRO:HD3	1.88	0.56
2:B:165:ASP:HB2	2:B:194:PRO:HB3	1.88	0.55
1:A:294:LYS:HE2	1:A:312:GLU:OE1	2.06	0.55
2:B:445:VAL:O	2:B:448:ILE:HG23	2.05	0.55
1:A:96:TYR:OH	2:B:280:LYS:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:MET:CE	2:B:216:PHE:HB2	2.37	0.55
1:A:171:HIS:CE1	1:A:173:THR:HG23	2.41	0.55
2:B:493:ALA:O	2:B:496:PHE:N	2.37	0.55
1:A:111:VAL:HG11	2:B:63:GLU:HB2	1.89	0.55
1:A:387:ARG:N	1:A:388:PRO:HD2	2.22	0.55
2:B:350:TYR:CA	2:B:353:GLN:NE2	2.70	0.55
1:A:300:ASP:HB3	1:A:301:PRO:HD2	1.89	0.54
2:B:501:PHE:O	2:B:502:ASP:HB2	2.07	0.54
1:A:185:ALA:HA	1:A:188:ILE:HD12	1.90	0.54
1:A:348:ARG:HH11	1:A:348:ARG:CG	2.19	0.54
2:B:127:PHE:HA	2:B:260:ALA:HA	1.89	0.54
2:B:263:VAL:CG2	2:B:355:LEU:HD11	2.36	0.54
1:A:396:ALA:O	1:A:400:LEU:HG	2.07	0.54
2:B:363:ASP:O	2:B:367:GLU:HG3	2.07	0.53
2:B:416:ARG:O	2:B:421:PRO:HB2	2.08	0.53
1:A:204:ILE:CD1	1:A:232:ILE:HG21	2.37	0.53
2:B:197:LEU:CG	2:B:202:GLY:O	2.56	0.53
5:B:601:CBO:H343	5:B:601:CBO:C16	2.30	0.53
1:A:108:GLY:C	1:A:110:GLU:H	2.08	0.53
2:B:165:ASP:OD1	2:B:194:PRO:CG	2.55	0.53
2:B:166:LEU:HD12	2:B:170:GLY:HA3	1.90	0.53
2:B:264:ILE:HD12	2:B:355:LEU:HD11	1.90	0.53
1:A:139:GLN:N	1:A:140:PRO:CD	2.72	0.53
1:A:203:LEU:HD23	1:A:203:LEU:H	1.72	0.53
1:A:235:ALA:HB2	1:A:270:HIS:CE1	2.44	0.53
1:A:428:ALA:N	1:A:429:PRO:HD3	2.24	0.53
1:A:92:LEU:HD23	2:B:63:GLU:HG2	1.91	0.53
1:A:231:LEU:N	1:A:231:LEU:HD12	2.24	0.53
1:A:380:HIS:CE1	1:A:381:LEU:HD23	2.44	0.53
1:A:277:THR:HB	1:A:279:HIS:CE1	2.44	0.53
2:B:174:HIS:CD2	2:B:222:ILE:CG2	2.88	0.52
2:B:200:LYS:H	2:B:413:PRO:HB3	1.74	0.52
1:A:372:LEU:HB2	1:A:375:GLY:O	2.09	0.52
2:B:299:VAL:HG11	2:B:305:ARG:HA	1.89	0.52
1:A:400:LEU:HB3	1:A:405:ILE:HB	1.91	0.52
2:B:71:LEU:O	2:B:405:ILE:HA	2.09	0.52
2:B:381:LEU:C	2:B:381:LEU:HD12	2.35	0.52
2:B:204:ILE:HD11	2:B:228:TYR:CE2	2.45	0.52
1:A:197:LEU:CD1	1:A:203:LEU:HB3	2.40	0.52
1:A:293:ARG:NH1	6:A:801:HOH:O	2.40	0.52
1:A:386:LEU:HB3	1:A:391:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:HIS:CE1	1:A:381:LEU:HD22	2.45	0.51
5:B:602:CBO:H192	5:B:602:CBO:C29	2.39	0.51
5:B:602:CBO:H192	5:B:602:CBO:O29	2.11	0.51
1:A:234:TYR:HB3	1:A:236:ARG:CZ	2.41	0.51
1:A:74:ILE:HB	1:A:77:GLU:HG3	1.92	0.51
2:B:162:MET:SD	2:B:218:PRO:HG3	2.51	0.51
2:B:232:ILE:HB	2:B:234:TYR:CZ	2.46	0.51
1:A:461:LYS:HD3	1:A:471:PHE:CZ	2.46	0.51
2:B:431:LEU:HG	2:B:436:PHE:CE2	2.46	0.51
1:A:340:LYS:CE	2:B:53:ASP:CG	2.83	0.51
2:B:350:TYR:CA	2:B:353:GLN:HE22	2.24	0.51
2:B:397:GLU:OE1	2:B:409:LYS:HG2	2.10	0.51
1:A:234:TYR:HB2	1:A:237:MET:HG2	1.92	0.50
1:A:420:THR:N	1:A:421:PRO:HD2	2.21	0.50
2:B:95:LYS:HE2	2:B:108:GLY:O	2.12	0.50
1:A:204:ILE:CG2	1:A:234:TYR:OH	2.60	0.50
1:A:373:VAL:HB	1:A:383:LEU:HB2	1.93	0.50
5:B:602:CBO:H191	5:B:602:CBO:C26	2.39	0.50
2:B:445:VAL:HA	2:B:448:ILE:HG23	1.94	0.50
1:A:234:TYR:CD2	1:A:236:ARG:HG2	2.47	0.50
2:B:238:ARG:NH2	2:B:270:HIS:O	2.45	0.50
2:B:232:ILE:HB	2:B:234:TYR:CE1	2.46	0.49
1:A:373:VAL:O	1:A:374:SER:C	2.55	0.49
2:B:364:ALA:O	2:B:445:VAL:HG11	2.12	0.49
2:B:75:ALA:HB1	2:B:380:HIS:CD2	2.46	0.49
2:B:166:LEU:N	2:B:167:PRO:HD2	2.28	0.49
2:B:196:GLY:O	2:B:205:ASP:N	2.46	0.49
2:B:277:THR:HB	2:B:279:HIS:CE1	2.48	0.49
2:B:72:GLU:O	2:B:430:ALA:HB3	2.13	0.48
2:B:164:LEU:HG	2:B:168:ASP:O	2.13	0.48
2:B:230:ARG:C	6:B:709:HOH:O	2.55	0.48
1:A:320:PHE:O	1:A:324:GLN:O	2.31	0.48
2:B:165:ASP:CG	2:B:194:PRO:HB3	2.37	0.48
5:B:601:CBO:C29	5:B:601:CBO:H253	2.43	0.48
1:A:234:TYR:HB2	1:A:237:MET:H	1.79	0.48
1:A:200:LYS:HA	1:A:374:SER:OG	2.14	0.48
1:A:340:LYS:HZ2	1:A:340:LYS:HB3	1.78	0.48
1:A:403:VAL:HG23	1:A:405:ILE:HG13	1.96	0.48
2:B:395:ARG:HB3	2:B:468:PHE:CZ	2.49	0.48
1:A:458:VAL:O	1:A:462:THR:HG23	2.14	0.47
1:A:204:ILE:HD12	1:A:232:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:HB3	1:A:267:PRO:CB	2.37	0.47
1:A:348:ARG:HH11	1:A:348:ARG:HG3	1.79	0.47
2:B:129:LEU:CD2	2:B:134:TRP:CG	2.97	0.47
2:B:162:MET:HG3	2:B:218:PRO:CB	2.43	0.47
2:B:193:MET:HE2	2:B:216:PHE:CB	2.44	0.47
2:B:450:GLU:O	2:B:454:ILE:CG2	2.62	0.47
2:B:318:ALA:HA	2:B:322:SER:HB2	1.96	0.47
2:B:377:THR:HG23	2:B:381:LEU:O	2.15	0.47
2:B:408:ASN:HB2	2:B:425:ARG:HD2	1.97	0.47
1:A:419:ILE:N	1:A:419:ILE:CD1	2.77	0.47
2:B:166:LEU:HD21	5:B:602:CBO:C27	2.45	0.47
1:A:200:LYS:HD3	1:A:200:LYS:HA	1.81	0.47
1:A:340:LYS:HE2	2:B:53:ASP:OD1	2.15	0.47
2:B:160:ARG:HB3	2:B:216:PHE:CE2	2.50	0.46
2:B:235:ALA:HB2	2:B:270:HIS:CE1	2.51	0.46
1:A:248:LEU:HD23	1:A:271:ALA:HA	1.96	0.46
2:B:420:THR:HG23	2:B:421:PRO:CD	2.43	0.46
2:B:480:GLN:NE2	2:B:480:GLN:CA	2.78	0.46
5:B:602:CBO:H273	5:B:602:CBO:H71	1.76	0.46
1:A:420:THR:O	1:A:420:THR:OG1	2.30	0.46
2:B:151:TYR:HE2	2:B:186:THR:CG2	2.28	0.46
2:B:227:ALA:HB2	2:B:425:ARG:NH2	2.31	0.46
2:B:377:THR:HG21	2:B:381:LEU:O	2.15	0.46
2:B:217:ARG:HA	2:B:217:ARG:HD2	1.57	0.46
2:B:193:MET:HE1	2:B:216:PHE:CB	2.45	0.46
2:B:261:ALA:CB	2:B:351:SER:OG	2.63	0.46
1:A:232:ILE:HA	1:A:234:TYR:CE1	2.51	0.46
2:B:151:TYR:HE2	2:B:186:THR:HG21	1.81	0.46
1:A:113:ASP:C	1:A:113:ASP:OD1	2.58	0.46
2:B:231:LEU:HD13	2:B:378:ASP:HB3	1.97	0.46
2:B:263:VAL:HG23	2:B:264:ILE:HD12	1.98	0.46
1:A:105:TYR:OH	2:B:401:GLU:CD	2.59	0.45
1:A:272:ASP:OD1	1:A:272:ASP:N	2.49	0.45
1:A:229:ALA:HB1	1:A:377:THR:HB	1.98	0.45
1:A:234:TYR:CB	1:A:236:ARG:HG2	2.46	0.45
1:A:395:ARG:HD3	1:A:468:PHE:CD2	2.51	0.45
2:B:350:TYR:CE1	2:B:432:THR:HG22	2.52	0.45
1:A:122:ARG:CZ	1:A:340:LYS:HE3	2.46	0.45
2:B:398:ARG:O	2:B:402:LEU:HG	2.16	0.45
2:B:415:ASP:CG	2:B:422:GLY:HA2	2.41	0.45
2:B:320:PHE:HB3	2:B:321:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:LEU:HD21	2:B:382:VAL:HG11	1.98	0.45
2:B:373:VAL:O	2:B:374:SER:CB	2.65	0.45
1:A:464:LYS:HG2	1:A:465:LEU:HD12	1.98	0.45
2:B:200:LYS:N	2:B:413:PRO:CB	2.79	0.45
1:A:466:GLN:O	1:A:470:SER:HB2	2.17	0.45
2:B:77:GLU:O	2:B:78:ASN:HB2	2.15	0.45
2:B:350:TYR:HA	2:B:353:GLN:OE1	2.16	0.45
1:A:139:GLN:N	1:A:140:PRO:HD3	2.32	0.45
2:B:225:THR:HG23	2:B:232:ILE:HD11	1.99	0.45
2:B:367:GLU:O	2:B:368:ARG:CB	2.65	0.45
2:B:162:MET:CG	2:B:218:PRO:HG3	2.48	0.44
2:B:200:LYS:H	2:B:413:PRO:CG	2.30	0.44
2:B:386:LEU:CD2	2:B:422:GLY:O	2.65	0.44
2:B:439:ASP:O	2:B:443:ARG:HD3	2.16	0.44
5:B:602:CBO:H192	5:B:602:CBO:O3	2.17	0.44
2:B:129:LEU:CD2	2:B:134:TRP:CD1	3.00	0.44
2:B:458:VAL:HG22	2:B:471:PHE:HE1	1.81	0.44
2:B:53:ASP:OD2	2:B:56:MET:HB2	2.17	0.44
2:B:127:PHE:C	2:B:128:ASP:O	2.58	0.44
2:B:395:ARG:NH1	2:B:465:LEU:HD22	2.31	0.44
2:B:299:VAL:CG1	2:B:305:ARG:HA	2.48	0.44
2:B:353:GLN:NE2	2:B:432:THR:HG22	2.32	0.44
2:B:165:ASP:CB	2:B:194:PRO:HB3	2.48	0.44
2:B:170:GLY:O	2:B:174:HIS:ND1	2.51	0.44
2:B:197:LEU:HG	2:B:202:GLY:O	2.16	0.44
1:A:387:ARG:HD3	1:A:422:GLY:HA3	1.99	0.44
2:B:458:VAL:HG21	2:B:472:LEU:CD2	2.48	0.44
1:A:217:ARG:N	1:A:218:PRO:CD	2.81	0.44
1:A:314:ARG:NH1	6:A:802:HOH:O	2.50	0.44
1:A:397:GLU:OE1	1:A:408:ASN:HA	2.17	0.44
1:A:162:MET:SD	1:A:218:PRO:HG3	2.57	0.43
1:A:294:LYS:CE	1:A:312:GLU:OE1	2.66	0.43
1:A:501:PHE:HE2	2:B:89:GLY:O	2.01	0.43
2:B:420:THR:HG21	2:B:465:LEU:HD23	2.00	0.43
2:B:161:ILE:O	2:B:192:SER:HA	2.19	0.43
2:B:142:SER:C	2:B:145:PRO:HD2	2.43	0.43
5:B:601:CBO:C29	5:B:601:CBO:C25	2.96	0.43
1:A:197:LEU:HD11	1:A:203:LEU:HB3	2.01	0.43
2:B:264:ILE:CD1	2:B:355:LEU:HD11	2.48	0.43
1:A:372:LEU:O	1:A:373:VAL:C	2.61	0.43
1:A:238:ARG:NH1	1:A:270:HIS:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LEU:HD23	2:B:271:ALA:HA	2.01	0.43
2:B:276:THR:OG1	2:B:277:THR:O	2.31	0.43
2:B:397:GLU:OE1	2:B:409:LYS:HE3	2.18	0.43
1:A:101:PRO:O	1:A:102:GLY:C	2.62	0.43
1:A:111:VAL:HG11	2:B:63:GLU:HA	2.01	0.43
1:A:43:TRP:HB3	2:B:346:MET:HE3	2.01	0.43
2:B:74:ILE:HG13	2:B:406:THR:O	2.19	0.43
2:B:204:ILE:CD1	2:B:228:TYR:OH	2.66	0.43
2:B:213:ALA:O	2:B:244:VAL:CG2	2.67	0.43
1:A:162:MET:HA	1:A:193:MET:O	2.18	0.43
2:B:182:ARG:HD3	2:B:187:SER:O	2.18	0.43
2:B:272:ASP:OD1	2:B:272:ASP:N	2.52	0.43
2:B:387:ARG:HD3	2:B:414:GLY:O	2.18	0.43
1:A:203:LEU:HD21	1:A:374:SER:OG	2.19	0.42
1:A:248:LEU:O	1:A:272:ASP:OD1	2.37	0.42
1:A:418:ALA:O	1:A:420:THR:HG22	2.19	0.42
2:B:252:MET:CE	2:B:268:PHE:CZ	3.02	0.42
1:A:161:ILE:O	1:A:192:SER:HA	2.19	0.42
1:A:199:PRO:HG3	1:A:413:PRO:HB3	2.01	0.42
2:B:254:HIS:C	2:B:281:THR:HG21	2.44	0.42
1:A:108:GLY:C	1:A:110:GLU:N	2.71	0.42
1:A:160:ARG:HA	1:A:191:GLU:O	2.19	0.42
1:A:206:TYR:CE2	1:A:236:ARG:HB2	2.54	0.42
1:A:219:ARG:H	1:A:219:ARG:HG2	1.70	0.42
2:B:60:LEU:HD23	2:B:60:LEU:HA	1.86	0.42
2:B:371:TYR:CE2	2:B:385:ASP:OD2	2.72	0.42
2:B:458:VAL:HG22	2:B:471:PHE:CE1	2.54	0.42
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.54	0.42
1:A:195:TYR:CD1	1:A:195:TYR:O	2.72	0.42
1:A:121:ARG:HB2	1:A:121:ARG:NH1	2.35	0.42
2:B:165:ASP:H	2:B:195:TYR:CB	2.30	0.42
2:B:252:MET:CE	2:B:268:PHE:CE1	2.99	0.42
2:B:458:VAL:HG13	2:B:471:PHE:HD1	1.81	0.42
1:A:144:SER:N	1:A:145:PRO:CD	2.83	0.42
2:B:381:LEU:HB2	2:B:426:LEU:O	2.19	0.42
2:B:223:ALA:HB1	2:B:232:ILE:HG21	2.02	0.42
5:B:602:CBO:H202	5:B:602:CBO:H151	2.01	0.42
1:A:346:MET:HG3	2:B:43:TRP:HB2	2.02	0.41
2:B:166:LEU:HD21	5:B:602:CBO:H271	2.01	0.41
1:A:180:VAL:HG22	1:A:180:VAL:O	2.21	0.41
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:TYR:O	2:B:385:ASP:N	2.47	0.41
2:B:441:PHE:HA	2:B:444:VAL:CG2	2.45	0.41
2:B:76:SER:HA	2:B:280:LYS:HG2	2.01	0.41
2:B:139:GLN:O	2:B:140:PRO:C	2.60	0.41
2:B:431:LEU:HD12	2:B:431:LEU:HA	1.92	0.41
1:A:167:PRO:HB3	1:A:411:THR:HG21	2.02	0.41
2:B:162:MET:HG3	2:B:218:PRO:CG	2.48	0.41
2:B:162:MET:HG3	2:B:218:PRO:HB3	2.02	0.41
2:B:397:GLU:OE1	2:B:409:LYS:CE	2.68	0.41
2:B:410:ASN:O	2:B:423:GLY:N	2.48	0.41
2:B:127:PHE:HB2	2:B:129:LEU:CD1	2.47	0.41
1:A:412:CYS:HB2	6:A:803:HOH:O	2.20	0.41
1:A:122:ARG:NH1	1:A:340:LYS:HE3	2.36	0.41
2:B:162:MET:O	2:B:221:ILE:HA	2.21	0.41
2:B:350:TYR:O	2:B:354:VAL:HG23	2.20	0.41
2:B:369:GLY:O	2:B:389:LYS:HD3	2.21	0.41
2:B:372:LEU:O	2:B:373:VAL:C	2.64	0.41
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.93	0.41
2:B:342:ALA:HA	2:B:347:PHE:HB3	2.01	0.41
2:B:127:PHE:HE1	2:B:256:SER:O	2.04	0.40
2:B:386:LEU:HD21	2:B:422:GLY:O	2.20	0.40
2:B:377:THR:HG22	2:B:378:ASP:N	2.36	0.40
2:B:436:PHE:CD2	2:B:440:ASP:HB3	2.56	0.40
2:B:171:HIS:HB3	2:B:174:HIS:HD1	1.87	0.40
2:B:386:LEU:CD1	2:B:424:LEU:HB2	2.52	0.40
2:B:403:VAL:HG12	2:B:405:ILE:HG22	2.04	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	461/483 (95%)	391 (85%)	56 (12%)	14 (3%)	3	6
2	B	460/483 (95%)	389 (85%)	57 (12%)	14 (3%)	3	6
All	All	921/966 (95%)	780 (85%)	113 (12%)	28 (3%)	3	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ALA
1	A	129	LEU
1	A	201	THR
1	A	302	LYS
1	A	415	ASP
1	A	420	THR
2	B	195	TYR
2	B	215	LEU
2	B	305	ARG
2	B	368	ARG
1	A	232	ILE
1	A	371	SER
1	A	374	SER
2	B	128	ASP
2	B	216	PHE
2	B	342	ALA
1	A	280	LYS
1	A	413	PRO
2	B	77	GLU
2	B	171	HIS
1	A	414	GLY
2	B	196	GLY
2	B	200	LYS
1	A	130	ASP
2	B	380	HIS
1	A	200	LYS
2	B	374	SER
2	B	369	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/394 (96%)	335 (88%)	45 (12%)	5	9
2	B	373/389 (96%)	302 (81%)	71 (19%)	1	2
All	All	753/783 (96%)	637 (85%)	116 (15%)	2	4

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	52	SER
1	A	95	LYS
1	A	113	ASP
1	A	129	LEU
1	A	133	GLN
1	A	142	SER
1	A	161	ILE
1	A	193	MET
1	A	201	THR
1	A	203	LEU
1	A	206	TYR
1	A	219	ARG
1	A	226	SER
1	A	232	ILE
1	A	236	ARG
1	A	245	LYS
1	A	272	ASP
1	A	274	VAL
1	A	293	ARG
1	A	300	ASP
1	A	301	PRO
1	A	305	ARG
1	A	313	ASP
1	A	314	ARG
1	A	348	ARG
1	A	352	LEU
1	A	356	LYS
1	A	377	THR
1	A	381	LEU
1	A	391	LEU
1	A	399	VAL
1	A	410	ASN

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Mol	Chain	Res	Type
1	A	415	ASP
1	A	416	ARG
1	A	419	ILE
1	A	420	THR
1	A	437	ARG
1	A	442	ARG
1	A	458	VAL
1	A	466	GLN
1	A	470	SER
1	A	474	LYS
1	A	479	SER
1	A	503	GLU
2	B	50	SER
2	B	51	ASP
2	B	52	SER
2	B	61	GLN
2	B	69	ARG
2	B	72	GLU
2	B	77	GLU
2	B	103	LYS
2	B	129	LEU
2	B	142	SER
2	B	160	ARG
2	B	166	LEU
2	B	177	MET
2	B	180	VAL
2	B	181	LYS
2	B	193	MET
2	B	197	LEU
2	B	203	LEU
2	B	208	GLN
2	B	209	LEU
2	B	211	LEU
2	B	214	ARG
2	B	217	ARG
2	B	221	ILE
2	B	230	ARG
2	B	252	MET
2	B	256	SER
2	B	263	VAL
2	B	264	ILE
2	B	272	ASP

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Mol	Chain	Res	Type
2	B	281	THR
2	B	293	ARG
2	B	294	LYS
2	B	300	ASP
2	B	305	ARG
2	B	315	ILE
2	B	340	LYS
2	B	353	GLN
2	B	359	ARG
2	B	372	LEU
2	B	378	ASP
2	B	383	LEU
2	B	384	VAL
2	B	386	LEU
2	B	395	ARG
2	B	399	VAL
2	B	402	LEU
2	B	405	ILE
2	B	408	ASN
2	B	409	LYS
2	B	416	ARG
2	B	417	SER
2	B	420	THR
2	B	421	PRO
2	B	425	ARG
2	B	426	LEU
2	B	431	LEU
2	B	435	GLN
2	B	443	ARG
2	B	448	ILE
2	B	449	ASP
2	B	452	VAL
2	B	454	ILE
2	B	461	LYS
2	B	464	LYS
2	B	465	LEU
2	B	480	GLN
2	B	482	LEU
2	B	487	GLN
2	B	488	ARG
2	B	489	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	357	ASN
1	A	453	ASN
1	A	504	HIS
2	B	156	GLN
2	B	207	ASN
2	B	208	GLN
2	B	254	HIS
2	B	270	HIS
2	B	329	ASN
2	B	353	GLN
2	B	357	ASN
2	B	408	ASN
2	B	435	GLN
2	B	480	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	603	-	4,4,4	0.94	0	6,6,6	0.44	0
5	CBO	B	602	-	45,45,45	2.80	18 (40%)	76,76,76	2.25	26 (34%)
3	PO4	A	701	-	4,4,4	1.13	0	6,6,6	0.59	0
4	PEG	A	702	-	6,6,6	0.23	0	5,5,5	0.12	0
5	CBO	B	601	-	45,45,45	3.33	16 (35%)	76,76,76	2.86	36 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CBO	B	602	-	1/1/15/16	6/15/109/109	0/5/5/5
4	PEG	A	702	-	-	0/4/4/4	-
5	CBO	B	601	-	1/1/15/16	4/15/109/109	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	CBO	C9-C11	-10.13	1.41	1.52
5	B	601	CBO	C10-C9	9.26	1.69	1.57
5	B	601	CBO	C14-C13	-8.50	1.40	1.53
5	B	602	CBO	C14-C13	-8.38	1.40	1.53
5	B	601	CBO	C20-C21	8.33	1.64	1.54
5	B	601	CBO	C9-C11	-6.92	1.44	1.52
5	B	601	CBO	C10-C5	6.68	1.66	1.56
5	B	601	CBO	C12-C13	5.89	1.41	1.34
5	B	601	CBO	C20-C18	5.01	1.63	1.54
5	B	602	CBO	C12-C13	5.00	1.40	1.34
5	B	602	CBO	C18-C13	-4.28	1.44	1.52
5	B	602	CBO	C20-C21	4.23	1.59	1.54
5	B	602	CBO	C10-C9	3.96	1.62	1.57
5	B	601	CBO	C23-C17	3.68	1.60	1.54
5	B	601	CBO	C15-C14	3.68	1.60	1.54
5	B	601	CBO	C1-C10	3.26	1.59	1.54
5	B	602	CBO	C12-C11	-3.25	1.40	1.46
5	B	601	CBO	C4-C3	-3.03	1.47	1.54
5	B	601	CBO	C8-C9	-2.92	1.54	1.56
5	B	602	CBO	C8-C14	2.75	1.63	1.59
5	B	602	CBO	C20-C18	2.74	1.59	1.54
5	B	601	CBO	C18-C13	-2.72	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	CBO	C4-C5	2.61	1.60	1.56
5	B	602	CBO	C1-C10	2.56	1.58	1.54
5	B	602	CBO	C6-C5	2.47	1.57	1.53
5	B	602	CBO	O3-C3	2.37	1.50	1.46
5	B	602	CBO	C21-C33	2.36	1.57	1.53
5	B	601	CBO	C7-C8	-2.34	1.50	1.54
5	B	602	CBO	C23-C17	2.30	1.57	1.54
5	B	602	CBO	C22-C21	-2.28	1.49	1.54
5	B	602	CBO	C7-C6	-2.20	1.49	1.53
5	B	602	CBO	C10-C5	2.04	1.59	1.56
5	B	601	CBO	C7-C6	-2.02	1.49	1.53
5	B	602	CBO	C15-C14	2.02	1.58	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	CBO	C8-C9-C10	-7.96	112.56	118.01
5	B	602	CBO	C17-C18-C13	-7.23	106.07	112.70
5	B	601	CBO	C17-C18-C13	-6.61	106.63	112.70
5	B	601	CBO	C14-C8-C9	6.37	112.62	107.93
5	B	601	CBO	C9-C11-C12	5.90	122.24	116.79
5	B	601	CBO	C9-C10-C5	5.48	112.27	106.36
5	B	601	CBO	C10-C9-C11	5.45	119.99	115.61
5	B	602	CBO	C9-C11-C12	5.16	121.56	116.79
5	B	602	CBO	C8-C9-C10	-5.08	114.53	118.01
5	B	602	CBO	C27-C14-C8	-4.96	107.89	112.31
5	B	601	CBO	C1-C10-C9	4.80	112.86	108.19
5	B	601	CBO	C7-C8-C9	-4.67	105.06	109.88
5	B	601	CBO	C19-C10-C5	-4.62	104.40	112.94
5	B	601	CBO	C6-C5-C4	-4.52	108.83	114.11
5	B	601	CBO	C23-C17-C18	4.31	114.25	108.98
5	B	601	CBO	C14-C13-C12	-4.25	116.67	120.27
5	B	602	CBO	O3-C3-C4	4.15	114.16	107.74
5	B	602	CBO	C15-C14-C13	-4.14	106.42	111.65
5	B	602	CBO	C1-C10-C5	4.00	112.75	108.02
5	B	601	CBO	C27-C14-C8	-3.98	108.76	112.31
5	B	602	CBO	C23-C17-C18	3.83	113.66	108.98
5	B	602	CBO	C5-C4-C3	3.77	112.92	106.81
5	B	601	CBO	C20-C18-C13	3.67	117.06	111.27
5	B	601	CBO	O11-C11-C12	-3.46	115.72	121.46
5	B	602	CBO	C2-C1-C10	3.41	118.50	112.74
5	B	601	CBO	C34-C21-C22	3.35	114.83	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	CBO	C27-C14-C15	3.35	113.22	107.78
5	B	601	CBO	C2-C3-C4	-3.34	109.81	114.32
5	B	601	CBO	C8-C14-C13	3.33	112.78	108.82
5	B	601	CBO	C15-C14-C8	-3.30	106.70	110.40
5	B	601	CBO	C6-C5-C10	3.24	114.27	110.92
5	B	602	CBO	C6-C5-C10	-3.22	107.59	110.92
5	B	602	CBO	C8-C14-C13	3.19	112.61	108.82
5	B	602	CBO	C2-C3-C4	-3.17	110.03	114.32
5	B	602	CBO	O3-C3-C2	3.14	113.77	108.53
5	B	601	CBO	C8-C9-C11	-3.08	105.93	108.66
5	B	602	CBO	C34-C21-C20	3.06	114.74	109.59
5	B	601	CBO	C7-C8-C14	-3.04	107.29	110.22
5	B	601	CBO	C15-C14-C13	-2.98	107.89	111.65
5	B	601	CBO	C15-C16-C17	2.97	120.39	113.88
5	B	602	CBO	O11-C11-C12	-2.89	116.66	121.46
5	B	601	CBO	C3-O3-C29	-2.87	112.80	118.03
5	B	602	CBO	O3-C29-C30	2.83	117.61	111.48
5	B	602	CBO	C20-C18-C17	2.76	115.24	113.11
5	B	602	CBO	C31-C30-C29	-2.68	105.48	113.44
5	B	601	CBO	C26-C8-C7	2.63	112.15	107.83
5	B	602	CBO	C30-C31-C32	-2.57	106.85	113.67
5	B	602	CBO	C20-C18-C13	2.54	115.27	111.27
5	B	601	CBO	C6-C7-C8	-2.48	108.57	112.85
5	B	601	CBO	C16-C17-C18	-2.42	106.02	108.98
5	B	602	CBO	C4-C5-C10	-2.37	115.03	117.18
5	B	601	CBO	C34-C21-C20	2.29	113.44	109.59
5	B	601	CBO	C28-C17-C23	-2.25	105.19	108.99
5	B	602	CBO	C15-C14-C8	2.20	112.87	110.40
5	B	601	CBO	C20-C21-C33	2.19	115.74	110.90
5	B	602	CBO	C1-C2-C3	2.18	114.78	110.66
5	B	601	CBO	C16-C15-C14	2.14	117.02	113.92
5	B	602	CBO	C3-O3-C29	2.11	121.89	118.03
5	B	602	CBO	C19-C10-C5	-2.10	109.05	112.94
5	B	601	CBO	C2-C1-C10	2.09	116.27	112.74
5	B	601	CBO	C30-C31-C32	-2.06	108.20	113.67
5	B	601	CBO	C1-C10-C5	2.06	110.45	108.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	601	CBO	C5
5	B	602	CBO	C5

All (10) torsion outliers are listed below:

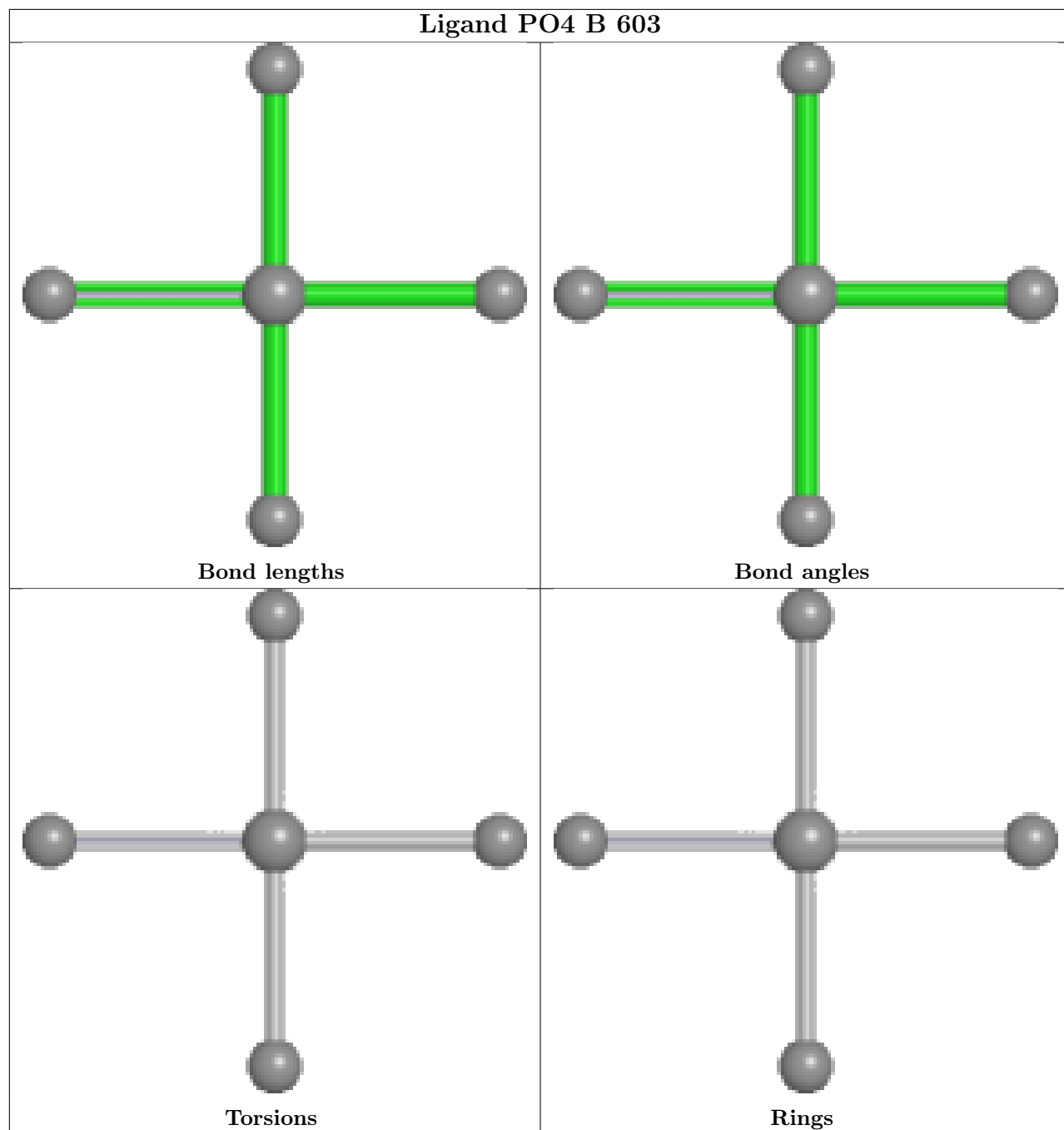
Mol	Chain	Res	Type	Atoms
5	B	602	CBO	C2-C3-O3-C29
5	B	602	CBO	C30-C29-O3-C3
5	B	602	CBO	O29-C29-O3-C3
5	B	602	CBO	C29-C30-C31-C32
5	B	601	CBO	C30-C29-O3-C3
5	B	601	CBO	C29-C30-C31-C32
5	B	601	CBO	O29-C29-O3-C3
5	B	601	CBO	C4-C3-O3-C29
5	B	602	CBO	C30-C31-C32-O32
5	B	602	CBO	C30-C31-C32-O33

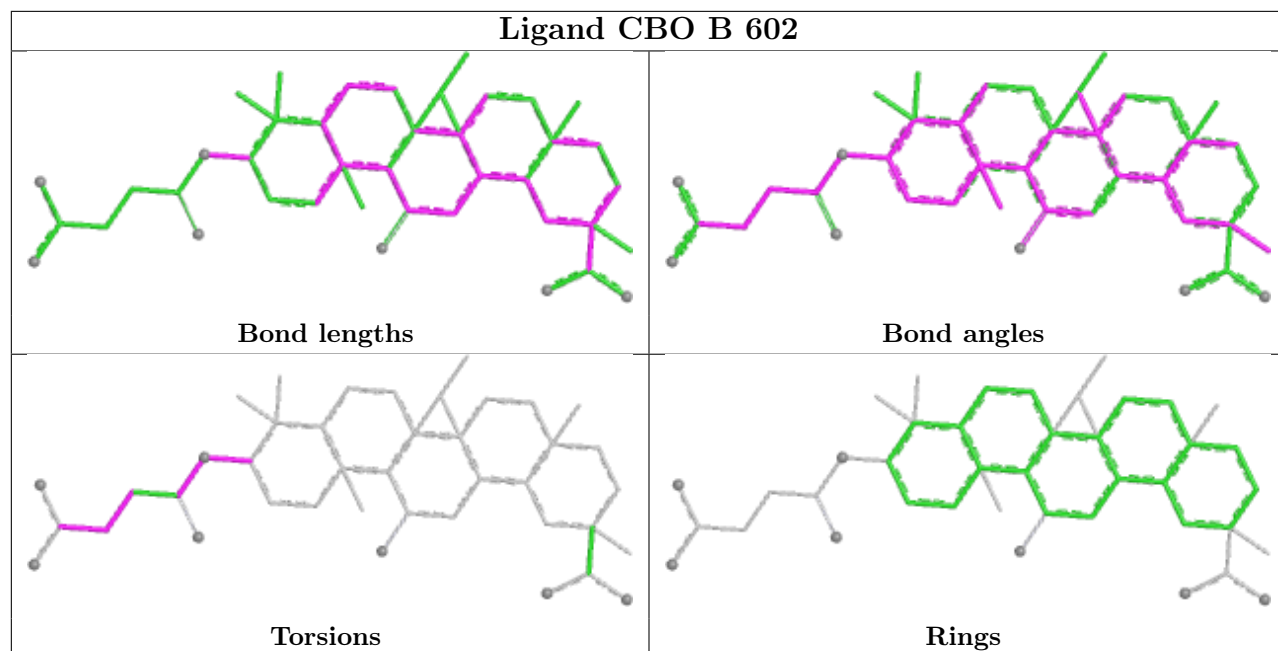
There are no ring outliers.

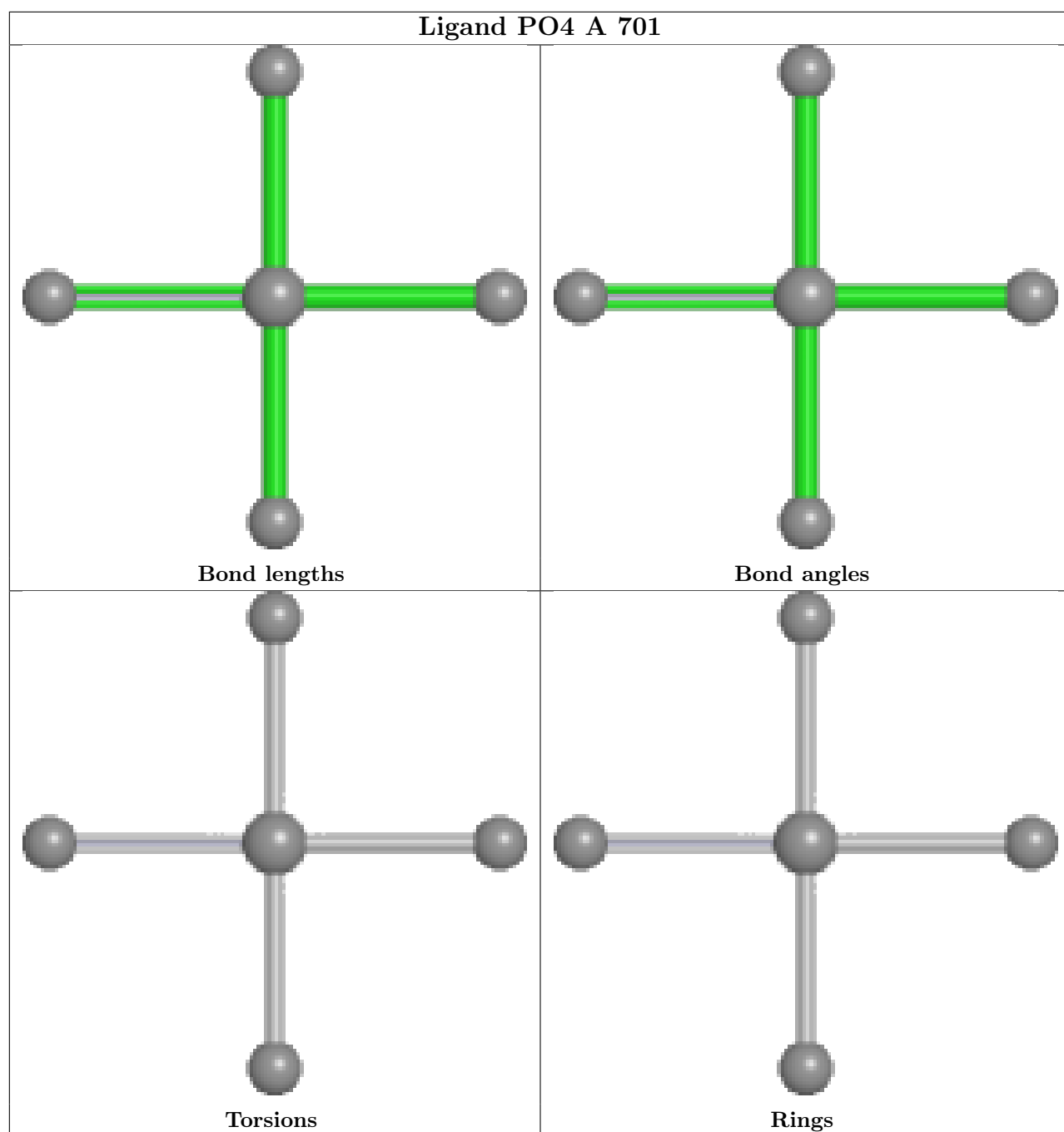
2 monomers are involved in 17 short contacts:

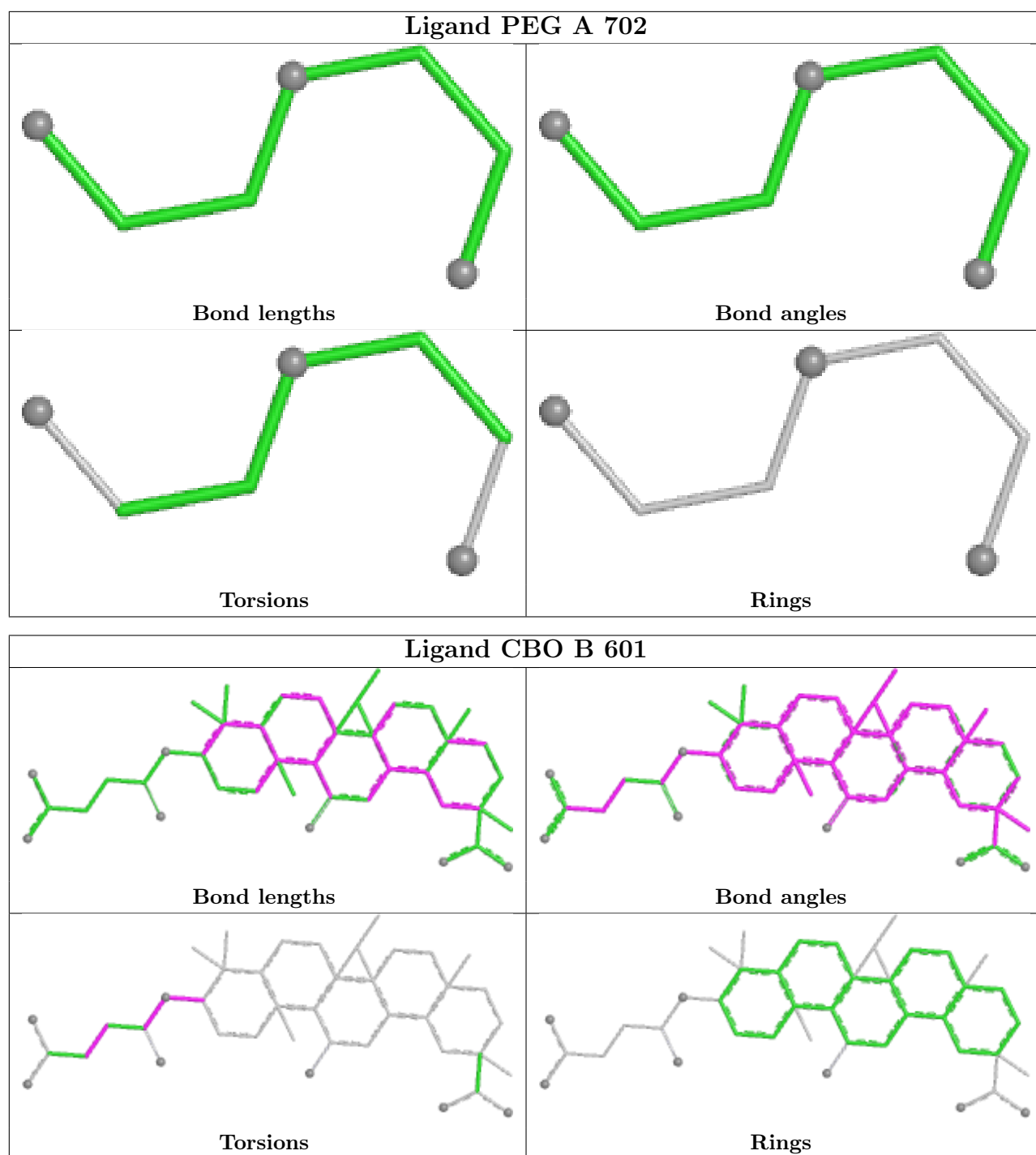
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	CBO	10	0
5	B	601	CBO	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	463/483 (95%)	0.34	29 (6%)	26 26	25, 60, 106, 174	0
2	B	462/483 (95%)	1.33	129 (27%)	1 1	38, 77, 120, 183	0
All	All	925/966 (95%)	0.83	158 (17%)	4 3	25, 68, 115, 183	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	396	ALA	9.8
1	A	419	ILE	8.5
2	B	445	VAL	8.1
2	B	489	VAL	7.0
2	B	400	LEU	6.4
2	B	399	VAL	6.3
2	B	407	ALA	5.9
2	B	71	LEU	5.4
2	B	70	GLY	5.3
2	B	448	ILE	5.2
1	A	418	ALA	5.1
2	B	456	LEU	5.1
2	B	441	PHE	5.0
1	A	129	LEU	5.0
2	B	352	LEU	4.8
2	B	472	LEU	4.7
1	A	299	VAL	4.5
2	B	68	CYS	4.5
2	B	454	ILE	4.5
2	B	405	ILE	4.5
2	B	420	THR	4.5
2	B	389	LYS	4.4
1	A	206	TYR	4.3
2	B	482	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	351	SER	4.3
2	B	413	PRO	4.3
2	B	485	LEU	4.2
2	B	371	TYR	4.2
2	B	478	THR	4.1
2	B	397	GLU	4.1
2	B	380	HIS	4.0
2	B	196	GLY	3.9
2	B	403	VAL	3.8
2	B	388	PRO	3.8
1	A	233	ASP	3.8
2	B	368	ARG	3.7
2	B	444	VAL	3.7
1	A	202	GLY	3.6
2	B	73	LEU	3.5
2	B	234	TYR	3.4
2	B	395	ARG	3.4
2	B	419	ILE	3.4
2	B	428	ALA	3.4
2	B	493	ALA	3.4
2	B	447	PHE	3.4
2	B	266	SER	3.3
1	A	108	GLY	3.3
2	B	209	LEU	3.3
2	B	298	ALA	3.3
2	B	483	ALA	3.3
2	B	206	TYR	3.3
1	A	417	SER	3.3
2	B	401	GLU	3.3
2	B	449	ASP	3.3
2	B	468	PHE	3.3
2	B	414	GLY	3.2
2	B	195	TYR	3.2
2	B	425	ARG	3.2
1	A	320	PHE	3.2
2	B	197	LEU	3.1
2	B	465	LEU	3.1
2	B	301	PRO	3.1
2	B	423	GLY	3.1
1	A	301	PRO	3.1
2	B	74	ILE	3.1
2	B	223	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	106	TYR	3.1
2	B	201	THR	3.1
2	B	229	ALA	3.0
2	B	492	PHE	3.0
2	B	379	ASN	3.0
2	B	385	ASP	3.0
2	B	452	VAL	3.0
2	B	474	LYS	2.9
2	B	106	TYR	2.9
2	B	369	GLY	2.9
2	B	392	GLY	2.9
1	A	416	ARG	2.9
2	B	459	LYS	2.9
2	B	262	LYS	2.8
2	B	356	LYS	2.8
2	B	406	THR	2.8
2	B	200	LYS	2.8
2	B	355	LEU	2.8
2	B	463	ALA	2.8
2	B	198	ALA	2.8
1	A	105	TYR	2.8
2	B	424	LEU	2.7
1	A	303	THR	2.7
1	A	374	SER	2.7
2	B	455	GLY	2.7
2	B	228	TYR	2.7
1	A	232	ILE	2.7
1	A	42	GLY	2.7
2	B	488	ARG	2.7
2	B	370	GLY	2.6
2	B	391	GLY	2.6
2	B	261	ALA	2.6
2	B	263	VAL	2.6
2	B	307	ALA	2.6
1	A	180	VAL	2.6
1	A	201	THR	2.6
2	B	264	ILE	2.5
2	B	270	HIS	2.5
2	B	421	PRO	2.5
1	A	102	GLY	2.5
2	B	211	LEU	2.5
2	B	296	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	366	LEU	2.4
1	A	343	ALA	2.4
2	B	431	LEU	2.4
1	A	302	LYS	2.4
2	B	232	ILE	2.4
2	B	473	LEU	2.4
2	B	162	MET	2.4
2	B	469	LYS	2.4
2	B	416	ARG	2.4
2	B	303	THR	2.4
2	B	168	ASP	2.4
2	B	451	GLY	2.4
2	B	253	ALA	2.4
2	B	383	LEU	2.3
2	B	412	CYS	2.3
2	B	471	PHE	2.3
1	A	113	ASP	2.3
2	B	299	VAL	2.3
2	B	410	ASN	2.3
2	B	199	PRO	2.3
2	B	84	ALA	2.2
2	B	453	ASN	2.2
2	B	476	SER	2.2
2	B	163	GLY	2.2
2	B	481	ARG	2.2
1	A	203	LEU	2.2
2	B	203	LEU	2.2
2	B	378	ASP	2.2
2	B	386	LEU	2.2
2	B	268	PHE	2.2
2	B	320	PHE	2.2
2	B	464	LYS	2.2
2	B	75	ALA	2.1
2	B	169	GLY	2.1
1	A	270	HIS	2.1
2	B	384	VAL	2.1
2	B	429	PRO	2.1
1	A	465	LEU	2.1
2	B	271	ALA	2.1
2	B	382	VAL	2.1
2	B	479	SER	2.1
2	B	164	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	390	GLY	2.1
1	A	111	VAL	2.1
1	A	296	VAL	2.1
2	B	418	ALA	2.0
2	B	66	ARG	2.0
2	B	467	ASP	2.0
2	B	495	ALA	2.0
2	B	134	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

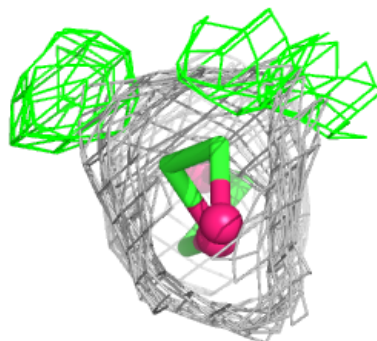
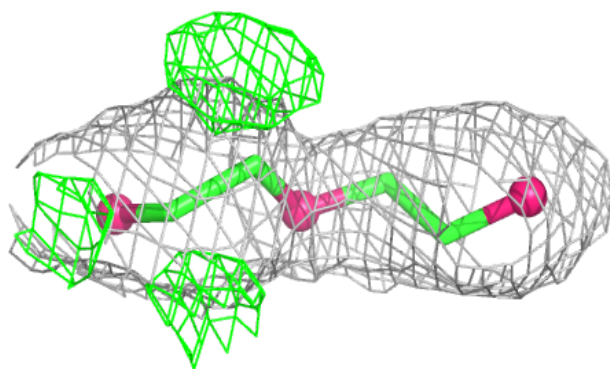
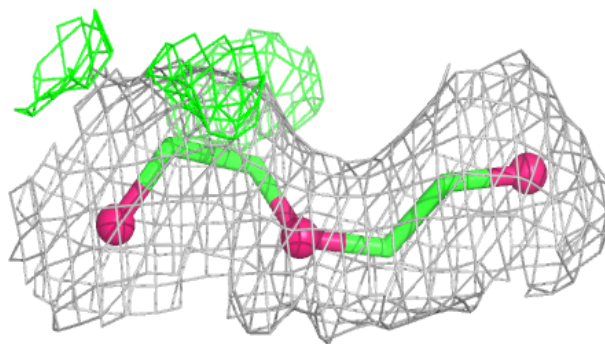
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	A	702	7/7	0.75	0.19	75,90,98,100	0
5	CBO	B	601	41/41	0.79	0.26	80,140,156,162	0
5	CBO	B	602	41/41	0.80	0.21	120,140,149,153	0
3	PO4	B	603	5/5	0.91	0.12	63,74,81,90	0
3	PO4	A	701	5/5	0.96	0.08	49,50,64,68	0

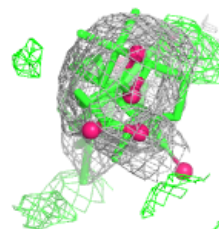
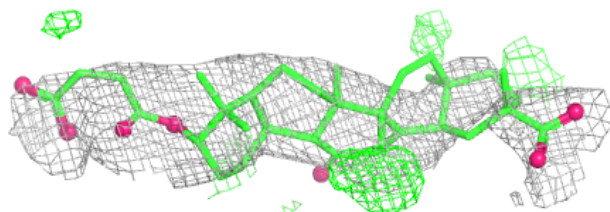
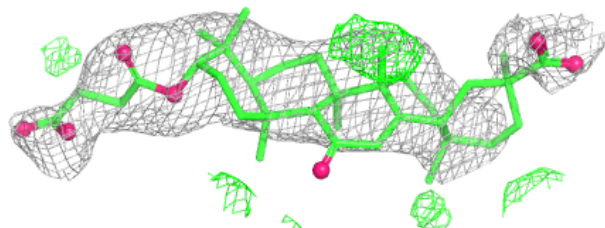
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEG A 702:

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

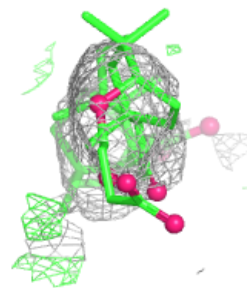
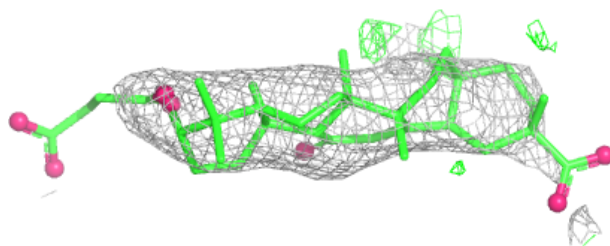
**Electron density around CBO B 601:**

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



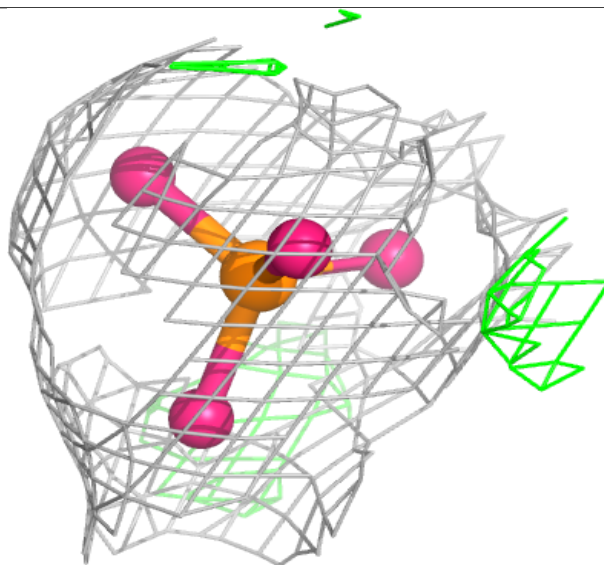
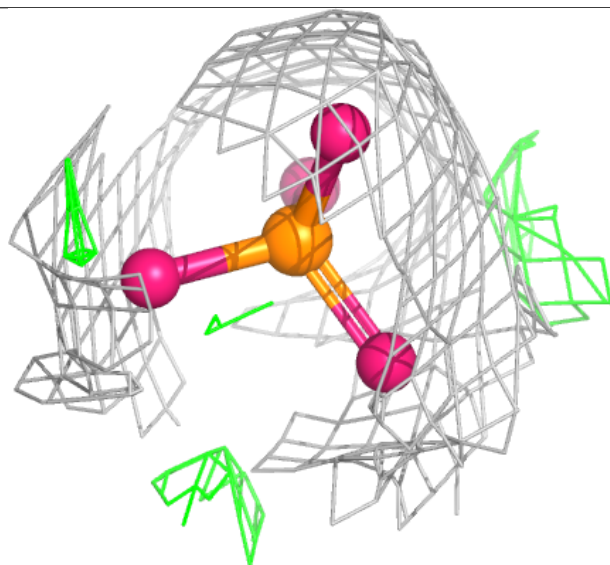
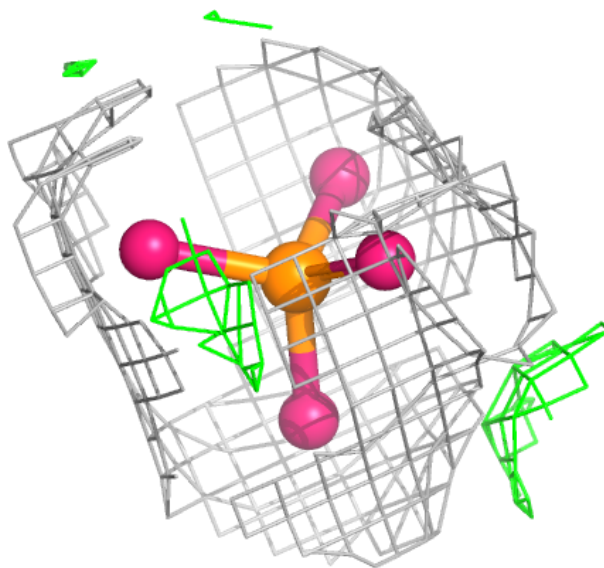
Electron density around CBO B 602:

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



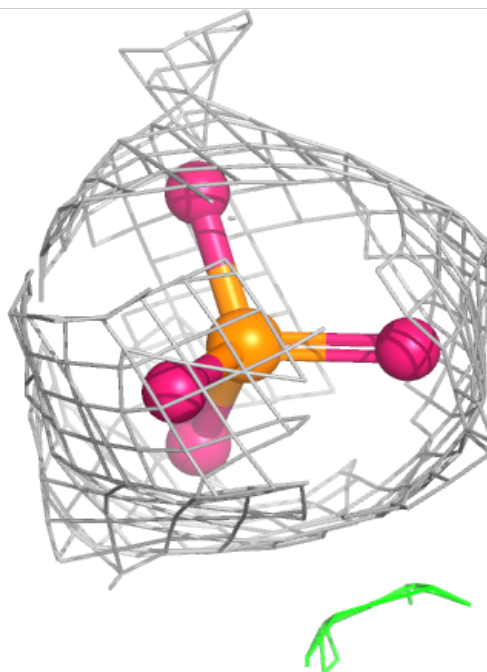
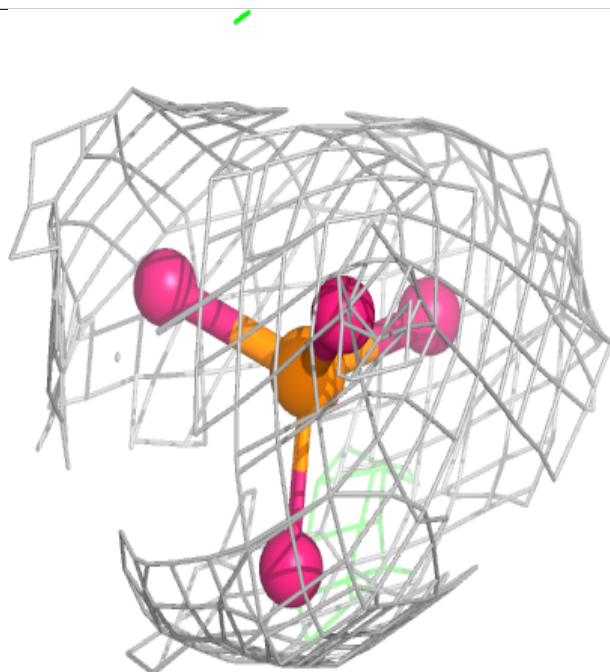
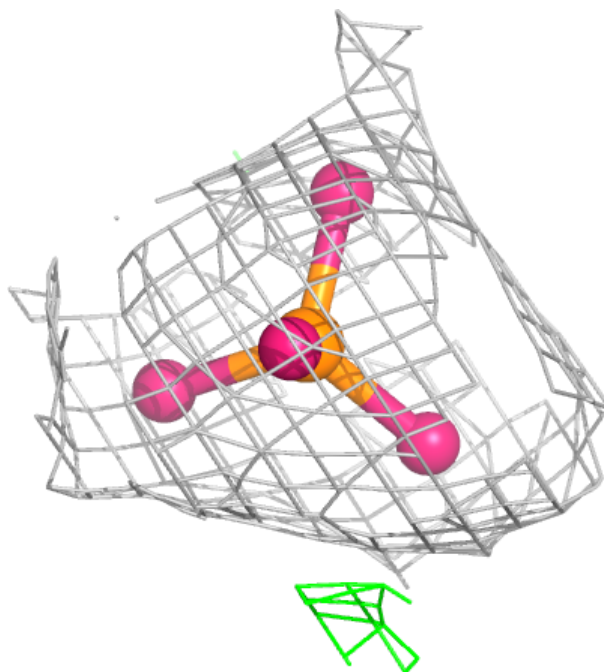
Electron density around PO4 B 603:

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



Electron density around PO4 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.