



# Full wwPDB X-ray Structure Validation Report i

Nov 22, 2023 – 08:55 PM JST

PDB ID : 7BYI  
Title : Structure of SHMT2 in complex with CBX  
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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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

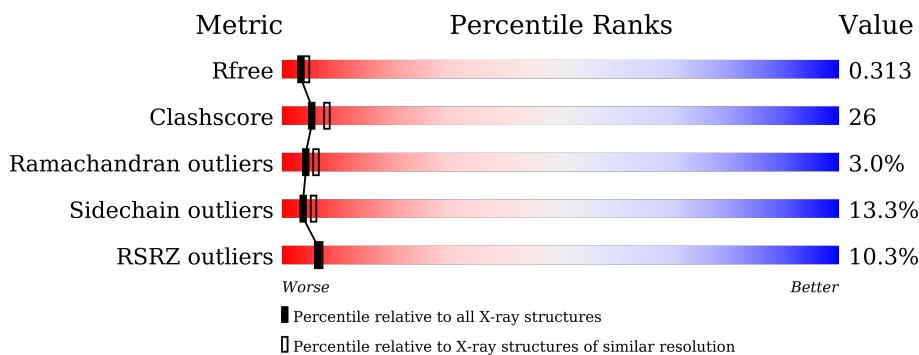
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

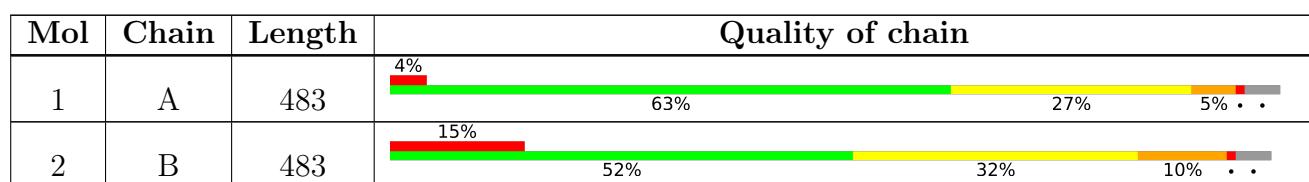
The reported resolution of this entry is 2.76 Å.

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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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



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	-	-	X

## 2 Entry composition (i)

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 3609	N 2273	O 649	S 672	15	0	0

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

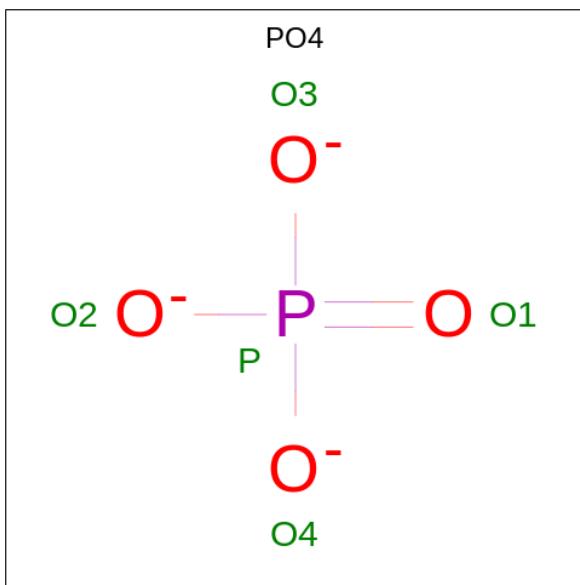
- Molecule 2 is a protein called Serine hydroxymethyltransferase, mitochondrial.

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

There are 7 discrepancies between the modelled and reference sequences:

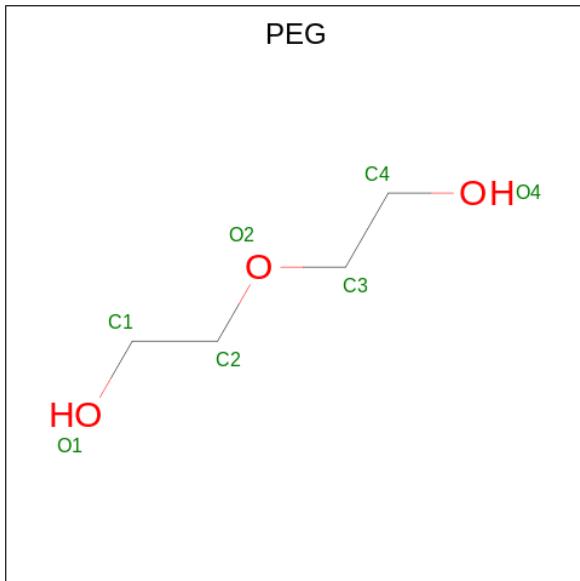
Chain	Residue	Modelled	Actual	Comment	Reference
B	196	GLY	LYS	conflict	UNP P34897
B	198	ALA	ASN	conflict	UNP P34897
B	307	ALA	ILE	conflict	UNP P34897
B	370	GLY	TYR	conflict	UNP P34897
B	371	TYR	SER	conflict	UNP P34897
B	391	GLY	LEU	conflict	UNP P34897
B	392	GLY	ASP	conflict	UNP P34897

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



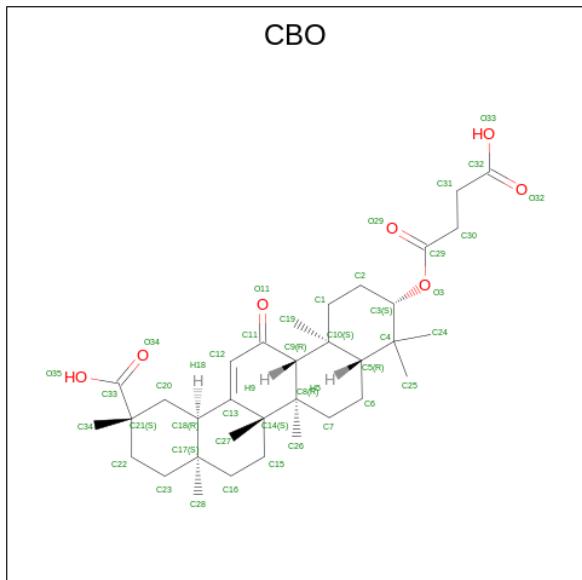
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is CARBENOXOLOLONE (three-letter code: CBO) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



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

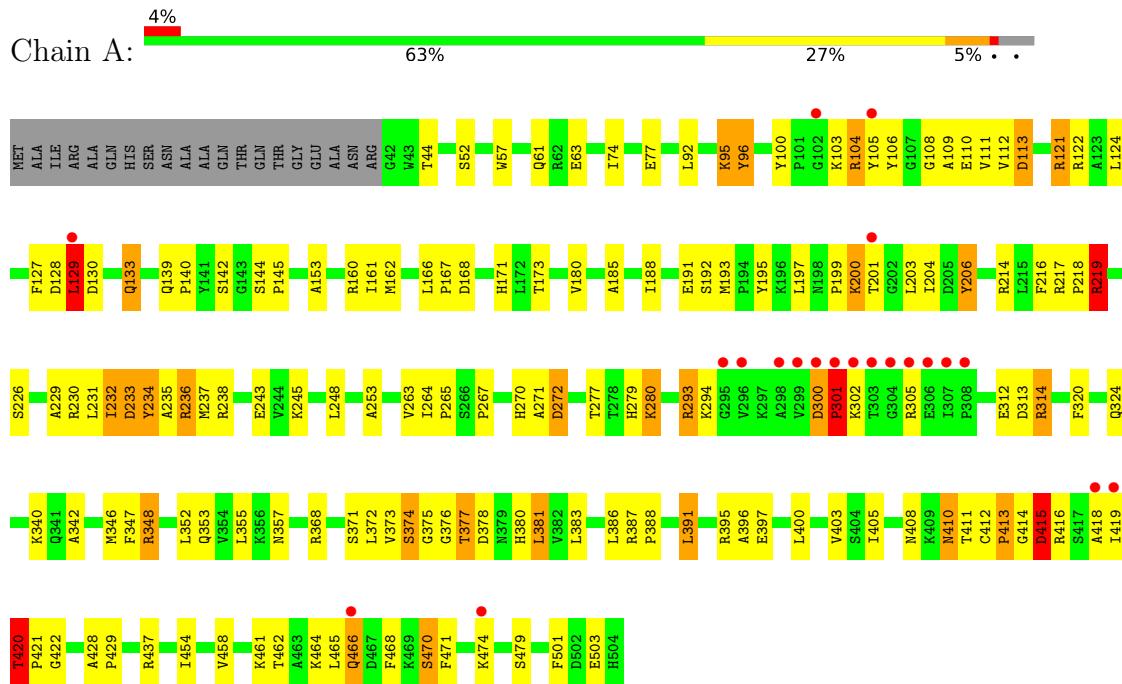
- Molecule 6 is water.

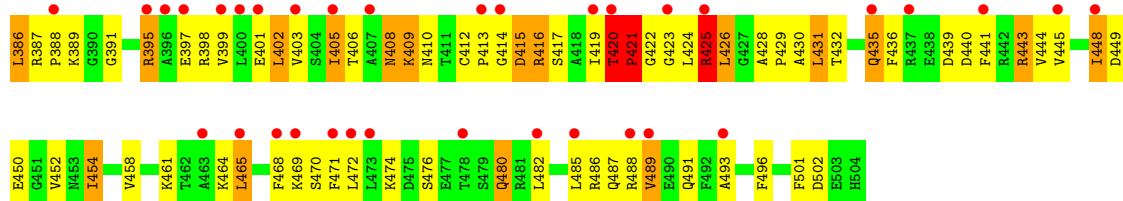
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0
6	B	43	Total O 43 43	0	0

### 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: Serine hydroxymethyltransferase, mitochondrial





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.62Å    158.62Å    209.43Å 90.00°    90.00°    120.00°	Depositor
Resolution (Å)	34.50 – 2.76 34.48 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.50-2.76) 99.9 (34.48-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	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 <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CBO, 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	0.81	0/3682	1.08	7/4978 (0.1%)
2	B	0.85	0/3650	1.14	14/4936 (0.3%)
All	All	0.83	0/7332	1.11	21/9914 (0.2%)

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	234	TYR	CB-CG-CD1	9.42	126.65	121.00
2	B	419	ILE	CB-CA-C	9.16	129.93	111.60
1	A	234	TYR	CB-CG-CD2	-9.12	115.53	121.00
2	B	341	GLN	N-CA-C	-8.91	86.94	111.00
1	A	103	LYS	N-CA-C	-7.66	90.31	111.00
1	A	301	PRO	N-CA-C	7.30	131.08	112.10
2	B	420	THR	N-CA-CB	-7.25	96.53	110.30
1	A	234	TYR	CA-CB-CG	7.22	127.11	113.40
1	A	219	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	B	194	PRO	CB-CA-C	-6.15	96.64	112.00
2	B	194	PRO	C-N-CA	5.94	136.55	121.70
2	B	342	ALA	N-CA-C	5.89	126.90	111.00
2	B	195	TYR	CB-CG-CD1	5.78	124.47	121.00
1	A	234	TYR	CB-CA-C	-5.73	98.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	PRO	N-CA-C	5.54	126.51	112.10
2	B	491	GLN	CB-CA-C	5.54	121.48	110.40
2	B	203	LEU	CB-CA-C	-5.29	100.14	110.20
2	B	201	THR	N-CA-C	-5.17	97.03	111.00
2	B	425	ARG	CG-CD-NE	5.10	122.50	111.80
2	B	223	ALA	CB-CA-C	5.05	117.67	110.10
2	B	421	PRO	CB-CA-C	-5.04	99.41	112.00

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3609	0	3602	138	0
2	B	3577	0	3555	244	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	384	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 26.

All (384) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:193:MET:HE2	2:B:216:PHE:CG	2.13	0.82
2:B:193:MET:HE1	2:B:216:PHE:HB2	1.60	0.81
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: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:193:MET:HE2	2:B:216:PHE:CD1	2.22	0.73
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
2:B:458:VAL:HG13	2:B:471:PHE:CD1	2.26	0.70
2:B:320:PHE:CD1	2:B:320:PHE:C	2.66	0.69
2:B:165:ASP:HB3	2:B:195:TYR:CD2	2.22	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ARG:CB	2:B:469:LYS:HE2	2.27	0.65
2:B:193:MET:HE1	2:B:216:PHE:CB	2.27	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
1:A:320:PHE:CD1	1:A:320:PHE:C	2.69	0.64
1:A:454:ILE:O	1:A:458:VAL:HG13	1.97	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
1:A:419:ILE:C	1:A:420:THR:HG22	2.19	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: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: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:367:GLU:O	2:B:368:ARG:HB2	2.02	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
2:B:205:ASP:CG	2:B:208:GLN:H	2.05	0.60
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
1:A:340:LYS:HE2	2:B:53:ASP:CG	2.23	0.59
2:B:470:SER:O	2:B:474:LYS:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:206:TYR:CD1	1:A:206:TYR:C	2.77	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:233:ASP:O	2:B:237:MET:HG2	2.06	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
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
2:B:193:MET:CE	2:B:216:PHE:CB	2.84	0.55
1:A:96:TYR:OH	2:B:280:LYS:HE3	2.06	0.55
1:A:171:HIS:CE1	1:A:173:THR:HG23	2.41	0.55
2:B:350:TYR:HA	2:B:353:GLN:CD	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:379:ASN:OD1	2:B:379:ASN:C	2.48	0.51
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
1:A:410:ASN:C	1:A:410:ASN:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HD3	1:A:471:PHE:CZ	2.46	0.51
2:B:193:MET:CE	2:B:216:PHE:HB2	2.37	0.51
2:B:431:LEU:HG	2:B:436:PHE:CE2	2.46	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
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
1:A:320:PHE:O	1:A:324:GLN:O	2.31	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: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
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:381:LEU:C	2:B:381:LEU:HD12	2.35	0.47
2:B:450:GLU:O	2:B:454:ILE:CG2	2.62	0.47
2:B:252:MET:HE2	2:B:268:PHE:CE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:77:GLU:O	2:B:78:ASN:HB2	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
1:A:340:LYS:CE	2:B:53:ASP:CG	2.83	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:252:MET:CE	2:B:268:PHE:CE1	2.99	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
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: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:252:MET:HE2	2:B:274:VAL:HG11	1.98	0.45
2:B:398:ARG:O	2:B:402:LEU:HG	2.16	0.45
2:B:320:PHE:HB3	2:B:321:PRO:HD3	1.99	0.45
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:373:VAL:O	1:A:374:SER:C	2.55	0.45
1:A:466:GLN:O	1:A:470:SER:HB2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:230:ARG:C	6:B:709:HOH:O	2.55	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
2:B:165:ASP:CG	2:B:194:PRO:HB3	2.37	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
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:238:ARG:NH1	1:A:270:HIS:O	2.45	0.43
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:111:VAL:HG11	2:B:63:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:454:ILE:O	2:B:454:ILE:HG12	2.19	0.42
1:A:108:GLY:C	1:A:110:GLU:H	2.08	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: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
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: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:113:ASP:C	1:A:113:ASP:OD1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:TYR:O	2:B:354:VAL:HG23	2.20	0.41
1:A:105:TYR:OH	2:B:401:GLU:CD	2.59	0.41
2:B:369:GLY:O	2:B:389:LYS:HD3	2.21	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:377:THR:HG1	2:B:382:VAL:HG22	1.85	0.40
2:B:386:LEU:HD21	2:B:422:GLY:O	2.20	0.40
2:B:415:ASP:CG	2:B:422:GLY:HA2	2.41	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%)	4 6
2	B	460/483 (95%)	389 (85%)	57 (12%)	14 (3%)	4 6
All	All	921/966 (95%)	780 (85%)	113 (12%)	28 (3%)	4 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

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Mol	Chain	Res	Type
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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	380/394 (96%)	340 (90%)	40 (10%)	7 11
2	B	373/389 (96%)	313 (84%)	60 (16%)	2 3
All	All	753/783 (96%)	653 (87%)	100 (13%)	4 6

All (100) 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	96	TYR
1	A	106	TYR
1	A	113	ASP
1	A	121	ARG
1	A	128	ASP
1	A	129	LEU
1	A	133	GLN
1	A	142	SER
1	A	206	TYR
1	A	219	ARG
1	A	226	SER
1	A	233	ASP
1	A	236	ARG
1	A	245	LYS
1	A	272	ASP
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	368	ARG
1	A	377	THR
1	A	381	LEU
1	A	391	LEU
1	A	410	ASN
1	A	415	ASP
1	A	416	ARG
1	A	420	THR
1	A	437	ARG
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

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Mol	Chain	Res	Type
2	B	61	GLN
2	B	72	GLU
2	B	96	TYR
2	B	142	SER
2	B	160	ARG
2	B	168	ASP
2	B	180	VAL
2	B	181	LYS
2	B	193	MET
2	B	203	LEU
2	B	208	GLN
2	B	217	ARG
2	B	230	ARG
2	B	252	MET
2	B	264	ILE
2	B	272	ASP
2	B	281	THR
2	B	293	ARG
2	B	294	LYS
2	B	300	ASP
2	B	305	ARG
2	B	353	GLN
2	B	359	ARG
2	B	371	TYR
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	415	ASP
2	B	416	ARG
2	B	417	SER
2	B	420	THR
2	B	421	PRO
2	B	425	ARG
2	B	426	LEU

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Mol	Chain	Res	Type
2	B	431	LEU
2	B	435	GLN
2	B	443	ARG
2	B	448	ILE
2	B	449	ASP
2	B	454	ILE
2	B	461	LYS
2	B	464	LYS
2	B	465	LEU
2	B	476	SER
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	357	ASN
1	A	453	ASN
2	B	61	GLN
2	B	156	GLN
2	B	208	GLN
2	B	254	HIS
2	B	270	HIS
2	B	353	GLN
2	B	357	ASN
2	B	408	ASN
2	B	435	GLN
2	B	480	GLN
2	B	491	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

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

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	0.89	0	6,6,6	0.41	0
5	CBO	B	602	-	45,45,45	2.63	17 (37%)	76,76,76	2.17	25 (32%)
5	CBO	B	601	-	45,45,45	3.16	15 (33%)	76,76,76	2.74	35 (46%)
3	PO4	A	701	-	4,4,4	1.08	0	6,6,6	0.56	0
4	PEG	A	702	-	6,6,6	0.23	0	5,5,5	0.12	0

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	601	-	1/1/15/16	5/15/109/109	0/5/5/5
4	PEG	A	702	-	-	0/4/4/4	-
5	CBO	B	602	-	1/1/15/16	6/15/109/109	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	CBO	C9-C11	-9.34	1.41	1.52
5	B	601	CBO	C10-C9	8.81	1.69	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	CBO	C20-C21	8.16	1.64	1.54
5	B	601	CBO	C14-C13	-7.81	1.40	1.53
5	B	602	CBO	C14-C13	-7.70	1.40	1.53
5	B	601	CBO	C9-C11	-6.39	1.44	1.52
5	B	601	CBO	C10-C5	6.36	1.66	1.56
5	B	601	CBO	C12-C13	5.66	1.41	1.34
5	B	602	CBO	C12-C13	4.80	1.40	1.34
5	B	601	CBO	C20-C18	4.67	1.63	1.54
5	B	602	CBO	C20-C21	4.14	1.59	1.54
5	B	602	CBO	C18-C13	-4.00	1.44	1.52
5	B	602	CBO	C10-C9	3.79	1.62	1.56
5	B	601	CBO	C15-C14	3.65	1.60	1.54
5	B	601	CBO	C23-C17	3.50	1.60	1.54
5	B	601	CBO	C1-C10	3.16	1.59	1.54
5	B	602	CBO	C12-C11	-3.05	1.40	1.46
5	B	601	CBO	C4-C3	-2.69	1.47	1.54
5	B	602	CBO	C8-C14	2.67	1.63	1.58
5	B	601	CBO	C8-C9	-2.59	1.54	1.56
5	B	602	CBO	C20-C18	2.55	1.59	1.54
5	B	601	CBO	C18-C13	-2.52	1.47	1.52
5	B	602	CBO	C1-C10	2.48	1.58	1.54
5	B	601	CBO	C4-C5	2.37	1.60	1.56
5	B	602	CBO	C6-C5	2.35	1.57	1.53
5	B	602	CBO	C21-C33	2.29	1.57	1.53
5	B	602	CBO	O3-C3	2.25	1.50	1.46
5	B	601	CBO	C7-C8	-2.21	1.50	1.54
5	B	602	CBO	C23-C17	2.19	1.57	1.54
5	B	602	CBO	C22-C21	-2.17	1.49	1.54
5	B	602	CBO	C7-C6	-2.06	1.49	1.53
5	B	602	CBO	C15-C14	2.02	1.58	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	CBO	C8-C9-C10	-7.59	112.56	118.10
5	B	602	CBO	C17-C18-C13	-6.92	106.07	112.70
5	B	601	CBO	C17-C18-C13	-6.33	106.63	112.70
5	B	601	CBO	C14-C8-C9	5.80	112.62	107.93
5	B	601	CBO	C9-C11-C12	5.45	122.24	116.81
5	B	601	CBO	C10-C9-C11	5.22	119.99	115.50
5	B	601	CBO	C9-C10-C5	4.98	112.27	106.47
5	B	602	CBO	C8-C9-C10	-4.89	114.53	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	CBO	C9-C11-C12	4.77	121.56	116.81
5	B	602	CBO	C27-C14-C8	-4.75	107.89	112.33
5	B	601	CBO	C19-C10-C5	-4.60	104.40	112.92
5	B	601	CBO	C6-C5-C4	-4.37	108.83	114.11
5	B	601	CBO	C7-C8-C9	-4.36	105.06	109.77
5	B	601	CBO	C1-C10-C9	4.31	112.86	108.19
5	B	602	CBO	C15-C14-C13	-4.28	106.42	111.68
5	B	601	CBO	C23-C17-C18	4.17	114.25	109.02
5	B	601	CBO	C14-C13-C12	-3.93	116.67	120.29
5	B	602	CBO	O3-C3-C4	3.91	114.16	107.72
5	B	602	CBO	C1-C10-C5	3.86	112.75	108.02
5	B	601	CBO	C27-C14-C8	-3.82	108.76	112.33
5	B	602	CBO	C23-C17-C18	3.70	113.66	109.02
5	B	602	CBO	C5-C4-C3	3.45	112.92	106.84
5	B	601	CBO	C20-C18-C13	3.42	117.06	111.33
5	B	601	CBO	O11-C11-C12	-3.35	115.72	121.50
5	B	602	CBO	C2-C1-C10	3.33	118.50	112.78
5	B	601	CBO	C34-C21-C22	3.27	114.83	109.76
5	B	601	CBO	C27-C14-C15	3.25	113.22	107.75
5	B	602	CBO	C6-C5-C10	-3.22	107.59	110.95
5	B	601	CBO	C15-C14-C8	-3.18	106.70	110.51
5	B	601	CBO	C6-C5-C10	3.17	114.27	110.95
5	B	601	CBO	C8-C9-C11	-3.17	105.93	108.81
5	B	602	CBO	C30-C31-C32	-3.14	106.85	113.60
5	B	601	CBO	C2-C3-C4	-3.12	109.81	114.39
5	B	601	CBO	C8-C14-C13	3.10	112.78	108.80
5	B	602	CBO	O3-C3-C2	3.08	113.77	108.48
5	B	601	CBO	C15-C14-C13	-3.08	107.89	111.68
5	B	602	CBO	C34-C21-C20	3.00	114.74	109.56
5	B	602	CBO	C2-C3-C4	-2.97	110.03	114.39
5	B	602	CBO	C8-C14-C13	2.96	112.61	108.80
5	B	601	CBO	C15-C16-C17	2.92	120.39	113.88
5	B	601	CBO	C7-C8-C14	-2.85	107.29	110.26
5	B	602	CBO	O3-C29-C30	2.84	117.61	111.50
5	B	602	CBO	O11-C11-C12	-2.80	116.66	121.50
5	B	602	CBO	C31-C30-C29	-2.73	105.48	113.43
5	B	601	CBO	C3-O3-C29	-2.72	112.80	117.92
5	B	602	CBO	C20-C18-C17	2.67	115.24	113.13
5	B	601	CBO	C26-C8-C7	2.53	112.15	107.84
5	B	601	CBO	C30-C31-C32	-2.51	108.20	113.60
5	B	601	CBO	C6-C7-C8	-2.48	108.57	112.84
5	B	601	CBO	C16-C17-C18	-2.40	106.02	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	CBO	C20-C18-C13	2.35	115.27	111.33
5	B	601	CBO	C34-C21-C20	2.25	113.44	109.56
5	B	601	CBO	C20-C21-C33	2.23	115.74	110.93
5	B	601	CBO	C28-C17-C23	-2.18	105.19	108.94
5	B	602	CBO	C4-C5-C10	-2.17	115.03	117.17
5	B	602	CBO	C1-C2-C3	2.16	114.78	110.63
5	B	602	CBO	C3-O3-C29	2.11	121.89	117.92
5	B	601	CBO	C16-C15-C14	2.11	117.02	113.83
5	B	602	CBO	C19-C10-C5	-2.09	109.05	112.92
5	B	601	CBO	C2-C1-C10	2.04	116.27	112.78

All (2) chirality outliers are listed below:

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

All (11) 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
5	B	601	CBO	C2-C3-O3-C29

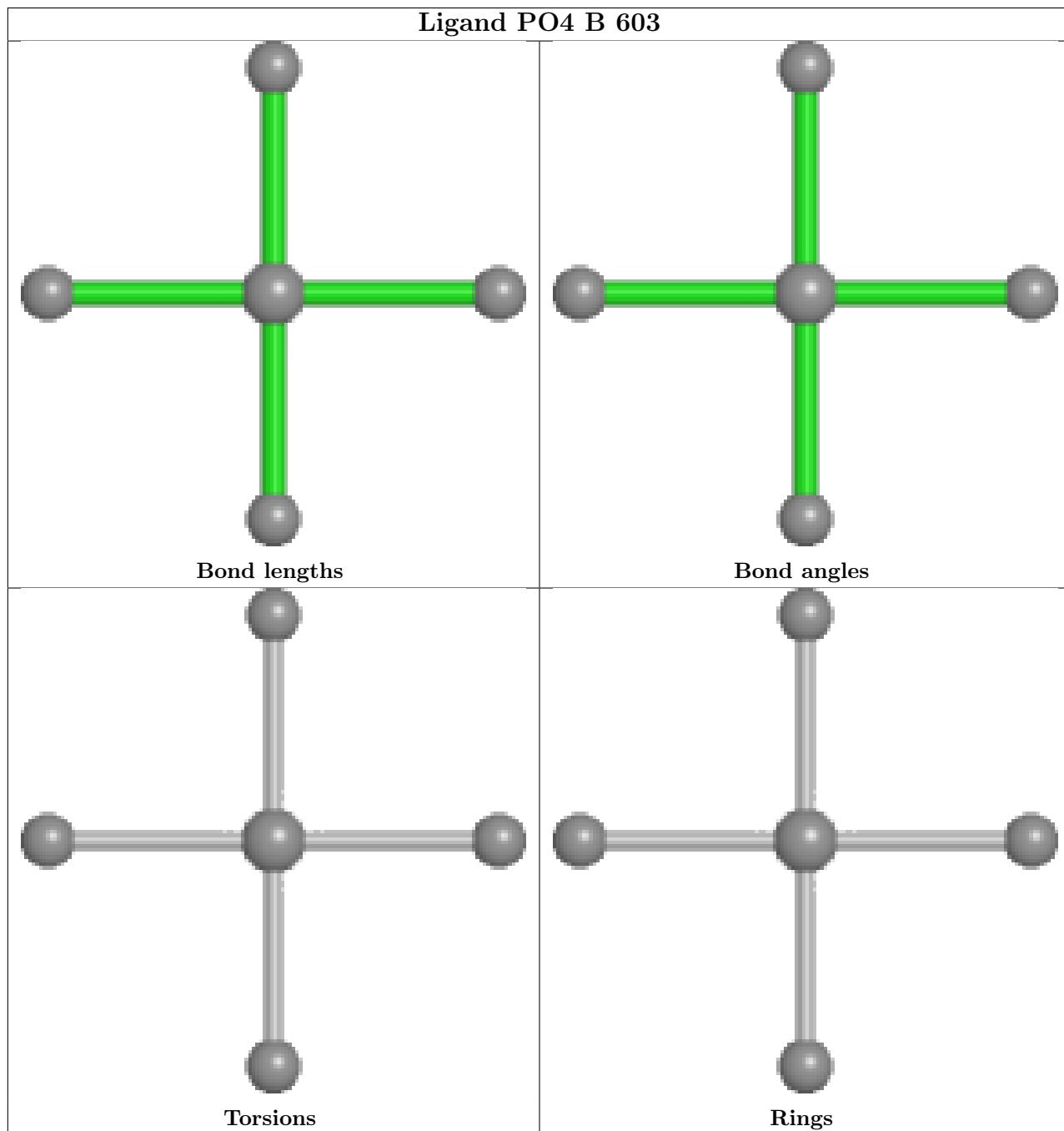
There are no ring outliers.

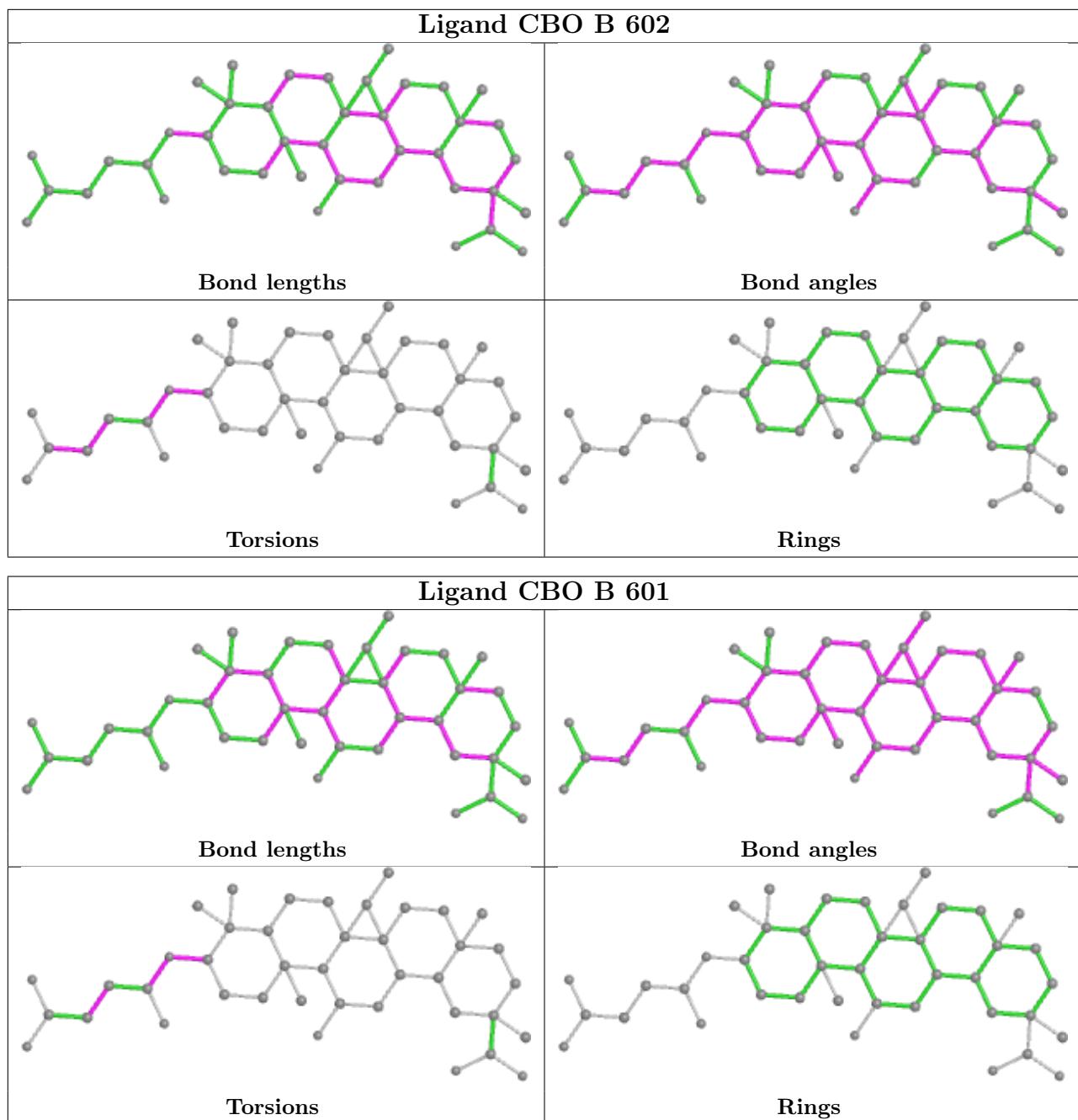
2 monomers are involved in 17 short contacts:

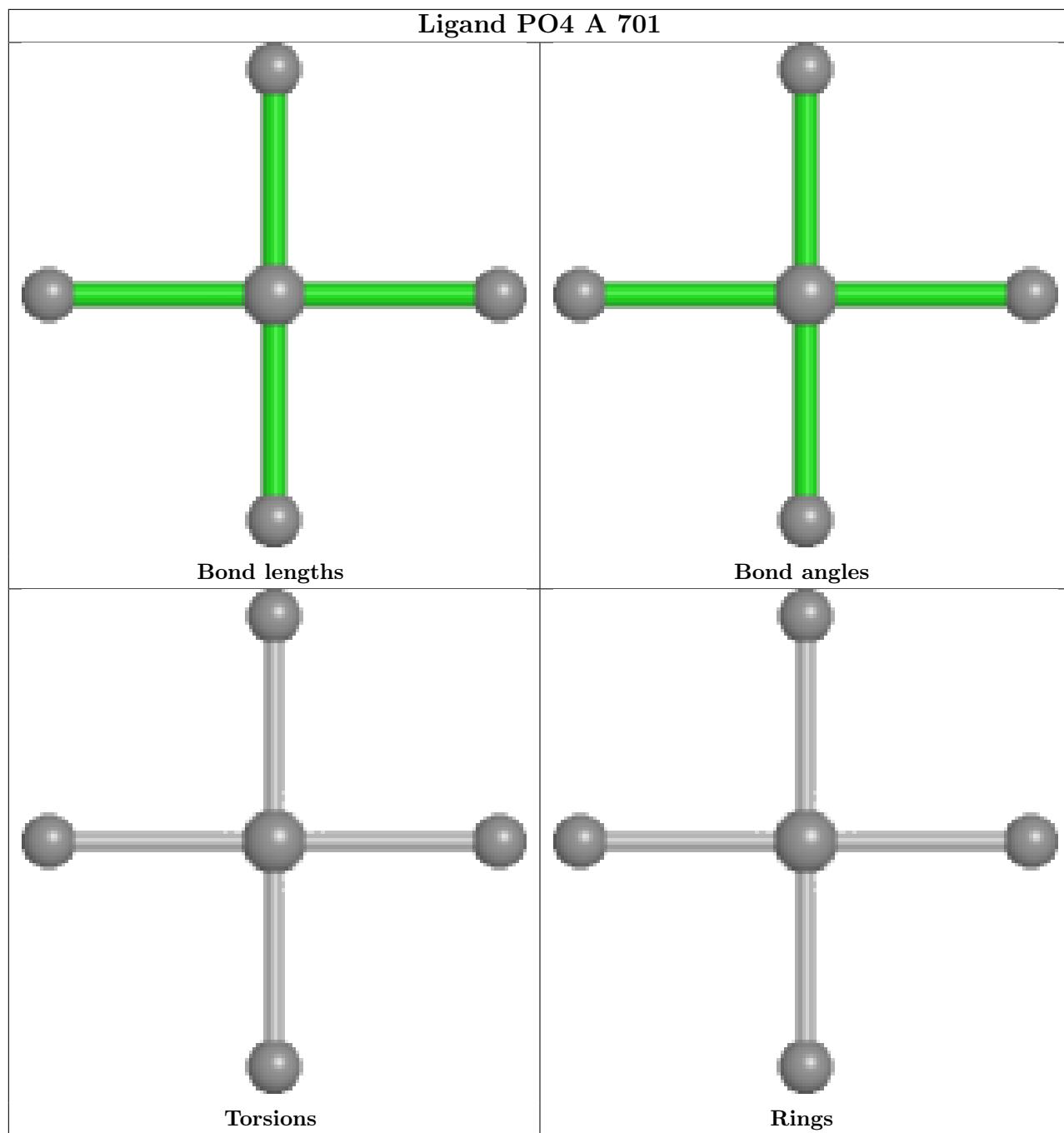
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	CBO	10	0
5	B	601	CBO	7	0

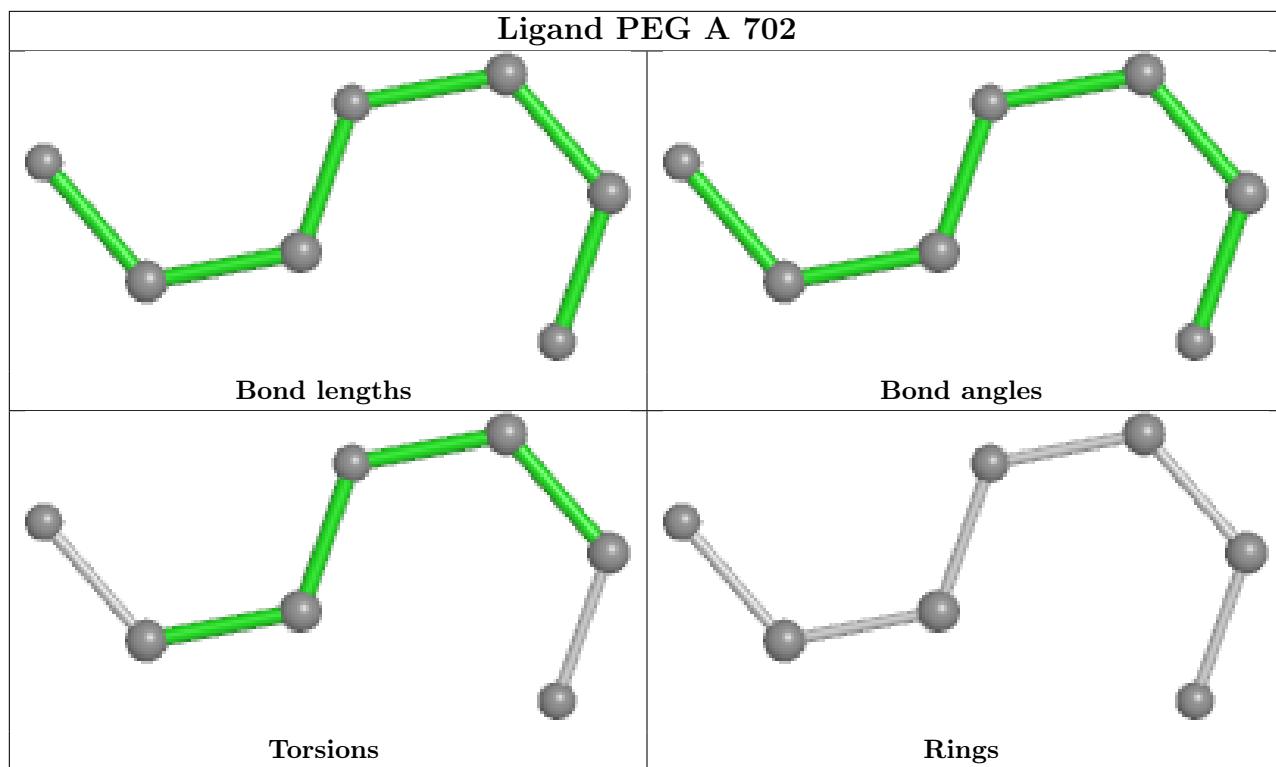
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	463/483 (95%)	0.08	21 (4%) 33 39	25, 60, 106, 174	0
2	B	462/483 (95%)	0.78	74 (16%) 1 2	38, 77, 120, 183	0
All	All	925/966 (95%)	0.43	95 (10%) 6 7	25, 68, 115, 183	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	489	VAL	7.0
1	A	299	VAL	6.9
1	A	419	ILE	6.5
2	B	396	ALA	6.4
2	B	472	LEU	6.2
1	A	303	THR	5.5
1	A	305	ARG	5.4
2	B	482	LEU	5.0
2	B	301	PRO	5.0
2	B	465	LEU	4.9
1	A	298	ALA	4.5
2	B	300	ASP	4.4
1	A	306	GLU	4.3
1	A	418	ALA	4.3
1	A	301	PRO	4.2
2	B	419	ILE	4.2
2	B	71	LEU	4.2
2	B	207	ASN	4.1
2	B	400	LEU	4.1
2	B	352	LEU	4.0
2	B	399	VAL	4.0
2	B	413	PRO	4.0
2	B	305	ARG	3.9
2	B	279	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	302	LYS	3.8
2	B	405	ILE	3.7
1	A	296	VAL	3.7
2	B	371	TYR	3.6
1	A	304	GLY	3.5
2	B	441	PHE	3.4
2	B	471	PHE	3.4
2	B	445	VAL	3.4
2	B	308	PRO	3.4
1	A	307	ILE	3.3
2	B	68	CYS	3.3
2	B	473	LEU	3.3
2	B	414	GLY	3.3
2	B	351	SER	3.2
2	B	201	THR	3.2
2	B	469	LYS	3.2
2	B	298	ALA	3.2
2	B	448	ILE	3.2
1	A	302	LYS	3.2
2	B	253	ALA	3.1
1	A	102	GLY	3.1
2	B	437	ARG	3.1
2	B	304	GLY	3.1
2	B	306	GLU	3.1
2	B	70	GLY	3.1
2	B	196	GLY	3.1
2	B	299	VAL	3.0
2	B	397	GLU	2.9
2	B	488	ARG	2.8
2	B	425	ARG	2.8
2	B	388	PRO	2.8
2	B	206	TYR	2.8
1	A	295	GLY	2.8
2	B	403	VAL	2.7
2	B	278	THR	2.7
2	B	423	GLY	2.7
2	B	277	THR	2.7
2	B	463	ALA	2.7
2	B	286	ARG	2.7
2	B	407	ALA	2.6
2	B	296	VAL	2.6
2	B	468	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	310	THR	2.5
2	B	280	LYS	2.5
2	B	420	THR	2.5
2	B	478	THR	2.4
1	A	129	LEU	2.4
1	A	300	ASP	2.4
2	B	395	ARG	2.3
2	B	254	HIS	2.3
2	B	368	ARG	2.2
1	A	201	THR	2.2
2	B	401	GLU	2.2
2	B	210	ALA	2.2
2	B	74	ILE	2.2
2	B	143	GLY	2.2
2	B	270	HIS	2.1
2	B	142	SER	2.1
2	B	375	GLY	2.1
2	B	307	ALA	2.1
1	A	466	GLN	2.1
1	A	308	PRO	2.1
2	B	493	ALA	2.1
2	B	435	GLN	2.1
2	B	203	LEU	2.1
2	B	287	SER	2.1
1	A	105	TYR	2.1
2	B	239	GLU	2.1
2	B	245	LYS	2.0
2	B	485	LEU	2.0
1	A	474	LYS	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 [\(i\)](#)

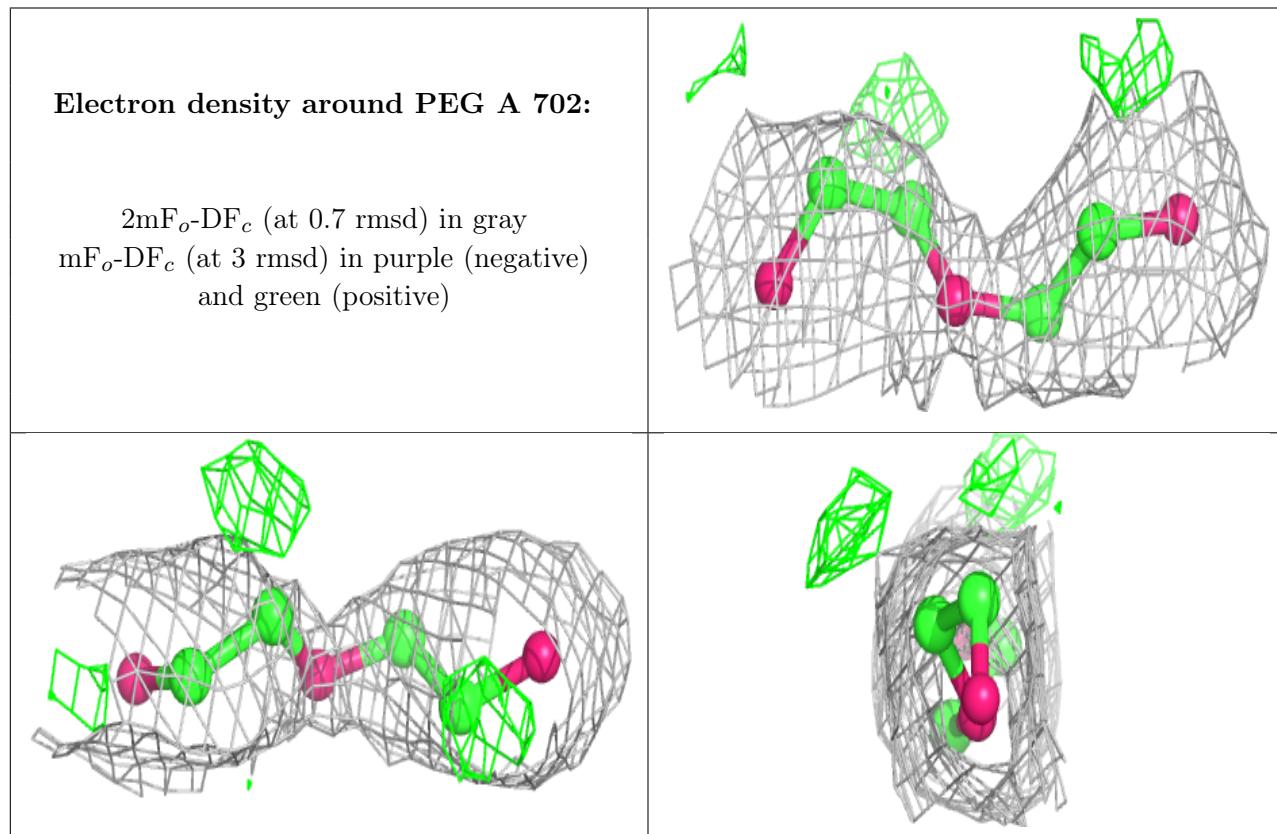
There are no monosaccharides in this entry.

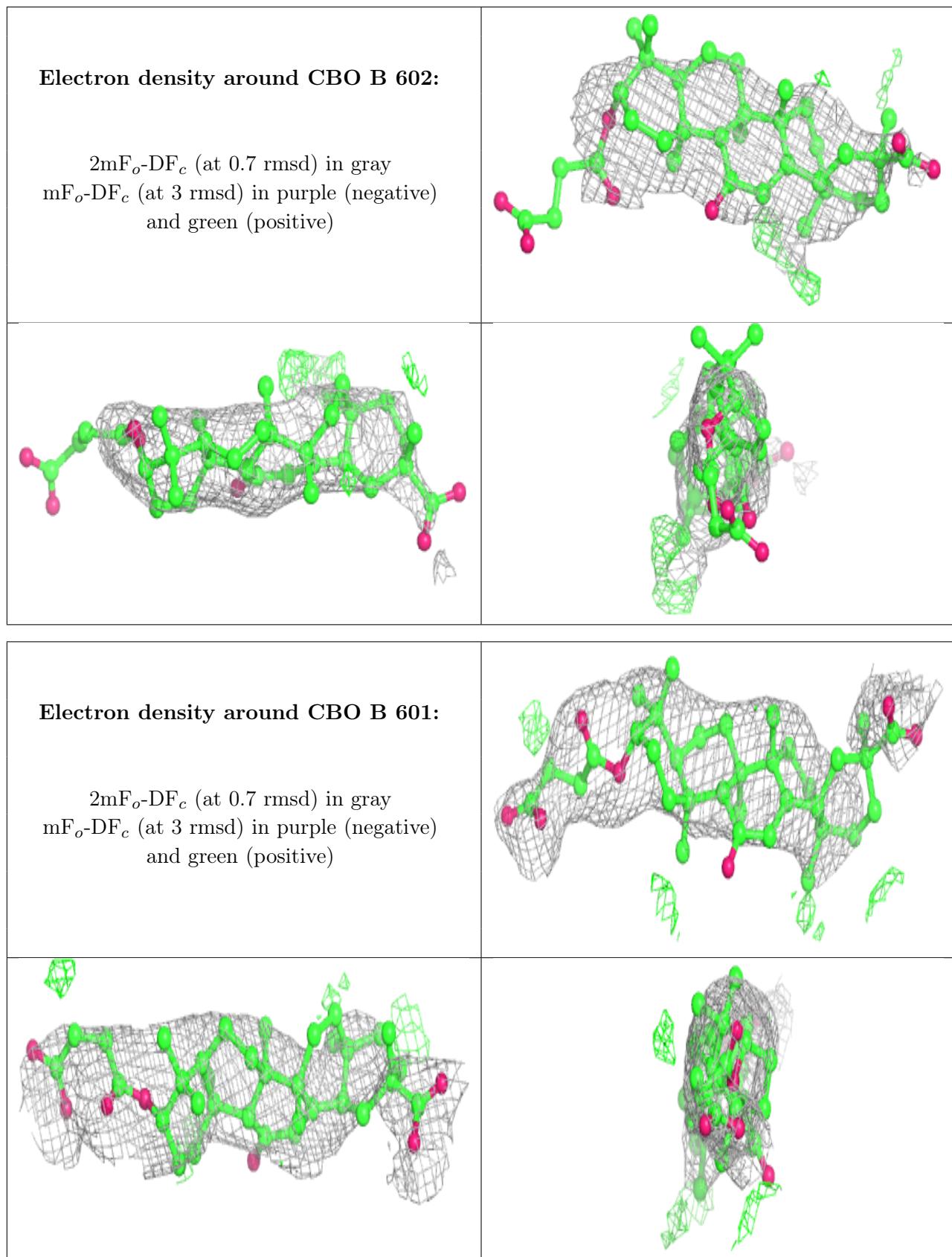
## 6.4 Ligands [\(i\)](#)

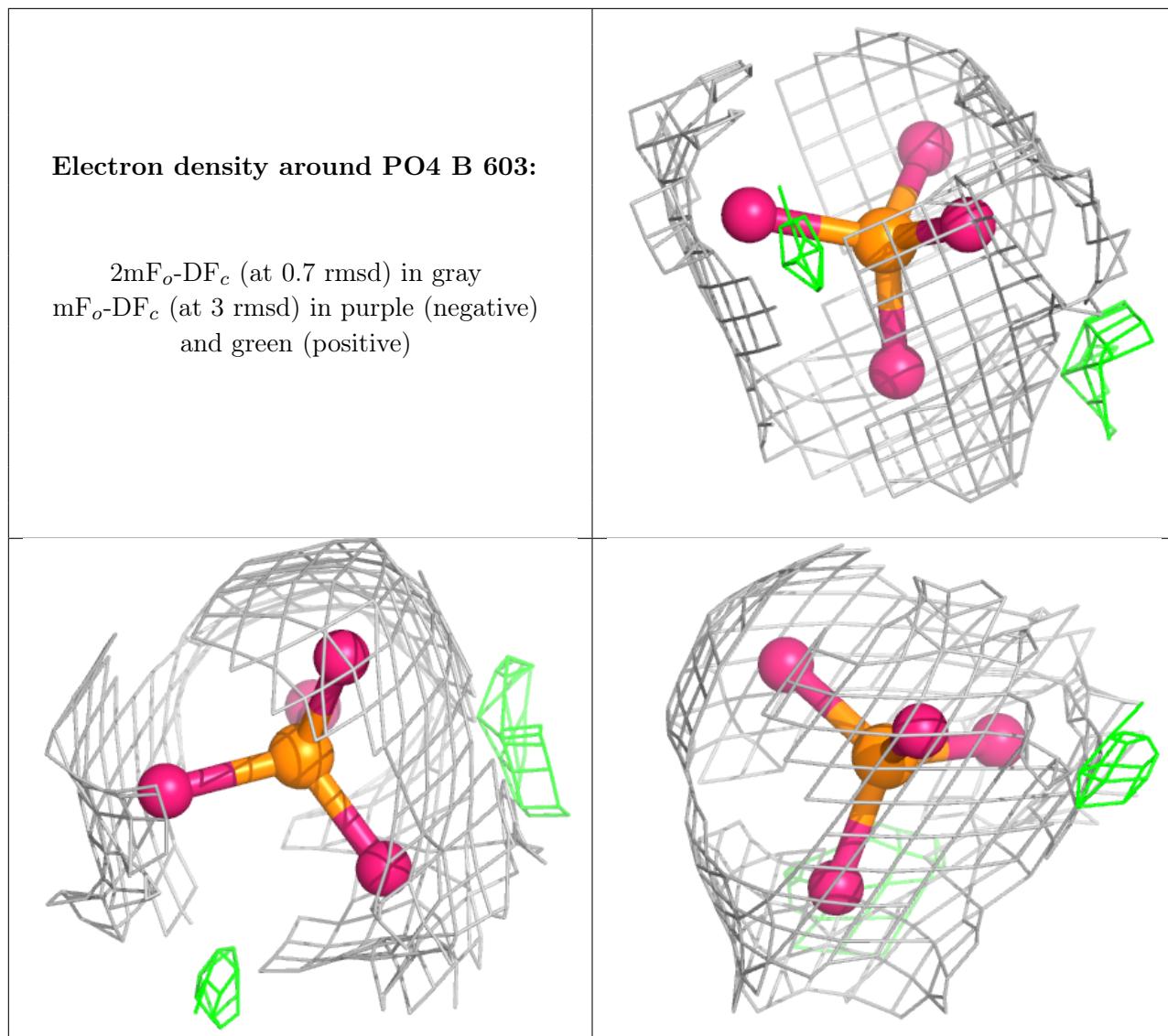
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

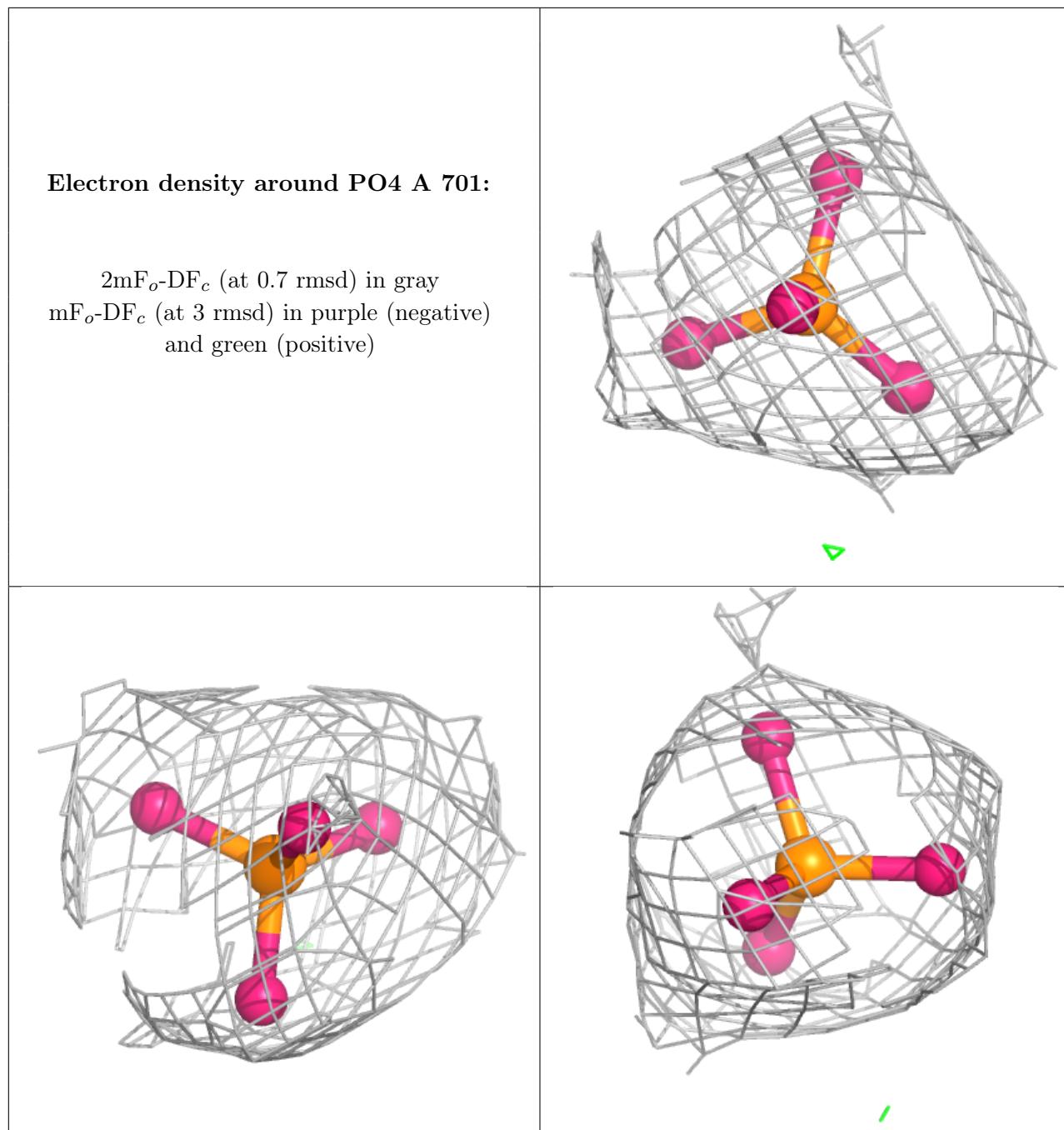
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PEG	A	702	7/7	0.68	0.26	75,90,98,100	0
5	CBO	B	602	41/41	0.73	0.41	120,140,149,153	0
5	CBO	B	601	41/41	0.79	0.30	80,140,156,162	0
3	PO4	B	603	5/5	0.97	0.48	63,74,81,90	0
3	PO4	A	701	5/5	0.98	0.25	49,50,64,68	0

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.









## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.