



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:36 AM UTC

PDB ID : 5XAR / pdb_00005xar
Title : Structural insights into the elevator-like mechanism of the sodium/citrate symporter CitS
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Deposited on : 2017-03-14
Resolution : 3.62 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

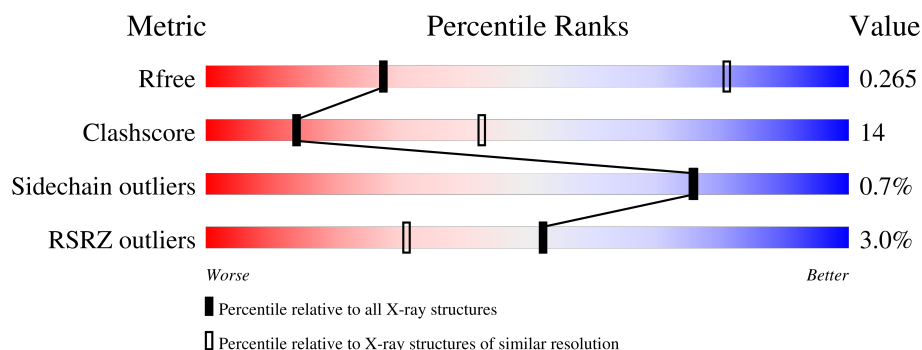
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	438	3% 73% 20% • 5%
1	B	438	3% 71% 21% • 7%
1	C	438	3% 73% 20% • 6%
1	D	438	3% 74% 19% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12403 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 Citrate-sodium symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3124	2076	499	529	20			
1	B	409	Total	C	N	O	S	0	0	0
			3057	2030	487	520	20			
1	C	413	Total	C	N	O	S	0	0	0
			3092	2056	491	525	20			
1	D	411	Total	C	N	O	S	0	0	0
			3078	2047	490	521	20			

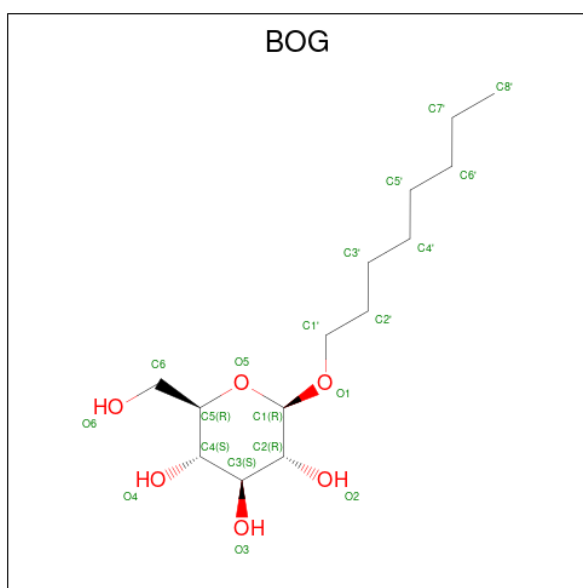
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP P31602
A	12	SER	-	expression tag	UNP P31602
A	447	PRO	-	expression tag	UNP P31602
A	448	ARG	-	expression tag	UNP P31602
B	11	GLY	-	expression tag	UNP P31602
B	12	SER	-	expression tag	UNP P31602
B	447	PRO	-	expression tag	UNP P31602
B	448	ARG	-	expression tag	UNP P31602
C	11	GLY	-	expression tag	UNP P31602
C	12	SER	-	expression tag	UNP P31602
C	447	PRO	-	expression tag	UNP P31602
C	448	ARG	-	expression tag	UNP P31602
D	11	GLY	-	expression tag	UNP P31602
D	12	SER	-	expression tag	UNP P31602
D	447	PRO	-	expression tag	UNP P31602
D	448	ARG	-	expression tag	UNP P31602

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 14 6	0	0
3	B	1	Total C O 20 14 6	0	0

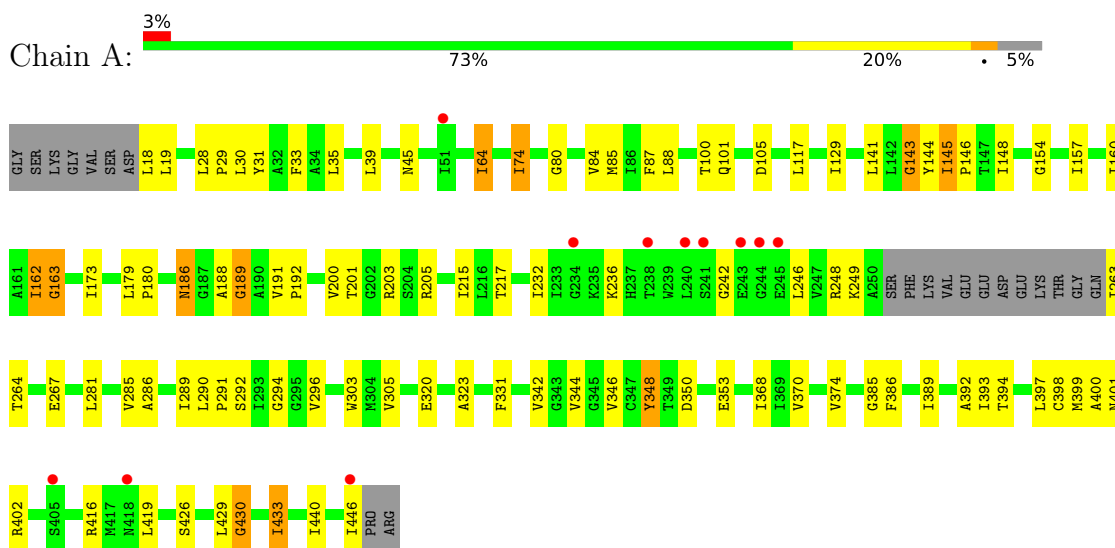
- Molecule 4 is water.

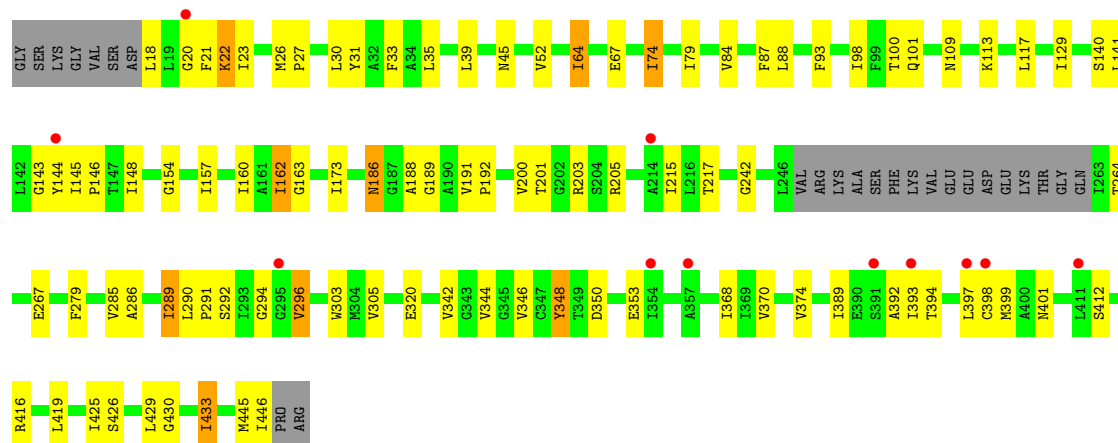
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0

3 Residue-property plots

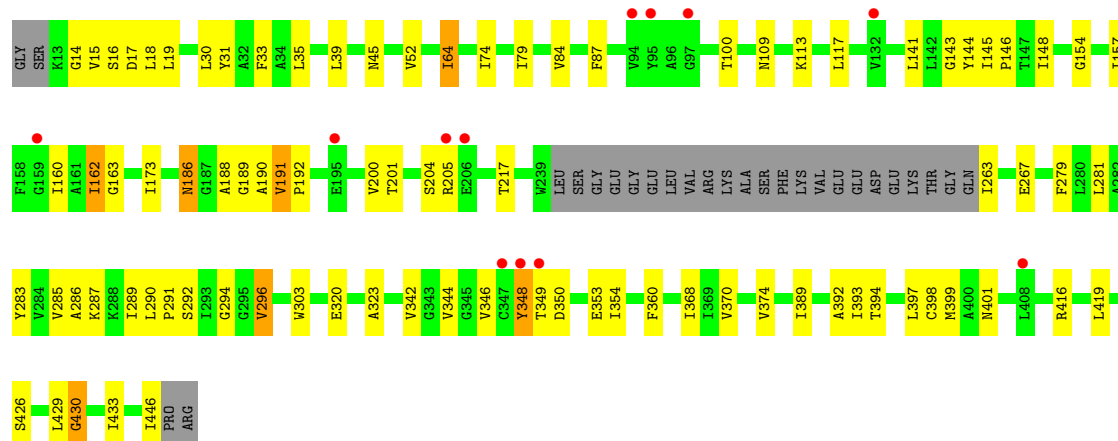
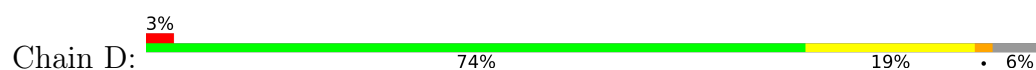
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Citrate-sodium symporter





• Molecule 1: Citrate-sodium symporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.37Å 163.99Å 93.67Å 90.00° 93.50° 90.00°	Depositor
Resolution (Å)	93.49 – 3.62 93.49 – 3.62	Depositor EDS
% Data completeness (in resolution range)	98.5 (93.49-3.62) 98.5 (93.49-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.235 , 0.267 (Not available) , 0.265	Depositor DCC
R_{free} test set	1433 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	164.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 207.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12403	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.19	10/3186 (0.3%)	1.30	8/4323 (0.2%)
1	B	1.18	7/3117 (0.2%)	1.31	12/4230 (0.3%)
1	C	1.20	8/3154 (0.3%)	1.30	9/4281 (0.2%)
1	D	1.19	6/3140 (0.2%)	1.30	8/4262 (0.2%)
All	All	1.19	31/12597 (0.2%)	1.30	37/17096 (0.2%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	ILE	C-O	-7.24	1.16	1.24
1	D	64	ILE	C-O	-6.46	1.16	1.24
1	B	85	MET	C-O	-6.15	1.16	1.24
1	D	348	TYR	C-O	-5.98	1.15	1.23
1	D	79	ILE	C-O	5.88	1.29	1.23
1	D	186	ASN	N-CA	-5.80	1.40	1.47
1	A	145	ILE	CA-CB	-5.79	1.51	1.54
1	B	412	SER	C-O	5.67	1.30	1.24
1	A	64	ILE	C-O	-5.53	1.17	1.24
1	D	430	GLY	C-O	5.52	1.30	1.23
1	C	79	ILE	C-O	5.52	1.29	1.23
1	A	186	ASN	N-CA	-5.42	1.40	1.47
1	B	79	ILE	C-O	5.41	1.29	1.23
1	C	348	TYR	C-O	-5.39	1.16	1.23
1	A	189	GLY	N-CA	5.35	1.53	1.45
1	C	64	ILE	C-O	-5.31	1.18	1.24
1	C	412	SER	C-O	5.26	1.30	1.24
1	B	201	THR	C-O	-5.25	1.17	1.23
1	B	95	TYR	C-O	-5.23	1.18	1.24
1	C	296	VAL	CA-CB	5.22	1.60	1.54
1	A	348	TYR	C-O	-5.19	1.16	1.23
1	C	88	LEU	N-CA	5.19	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	VAL	CA-CB	5.17	1.60	1.54
1	A	88	LEU	N-CA	5.13	1.52	1.46
1	A	143	GLY	N-CA	5.13	1.52	1.45
1	C	186	ASN	N-CA	-5.09	1.41	1.47
1	A	85	MET	C-O	-5.07	1.18	1.24
1	A	430	GLY	C-O	5.05	1.29	1.23
1	C	143	GLY	N-CA	5.02	1.52	1.45
1	B	186	ASN	N-CA	-5.01	1.41	1.47
1	A	163	GLY	N-CA	5.00	1.52	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	74	ILE	CB-CA-C	-8.39	101.23	111.97
1	C	74	ILE	CB-CA-C	-8.05	101.67	111.97
1	B	74	ILE	CB-CA-C	-8.00	101.73	111.97
1	A	242	GLY	N-CA-C	-7.78	99.42	111.64
1	A	74	ILE	CB-CA-C	-7.59	102.26	111.97
1	D	162	ILE	CB-CA-C	-7.49	101.88	112.22
1	C	162	ILE	CB-CA-C	-7.29	102.16	112.22
1	B	360	PHE	N-CA-C	-7.00	103.66	111.71
1	A	162	ILE	CB-CA-C	-6.46	101.79	112.26
1	A	344	VAL	CB-CA-C	-6.27	103.57	112.22
1	D	190	ALA	CA-C-N	6.12	124.09	120.24
1	D	190	ALA	C-N-CA	6.12	124.09	120.24
1	D	344	VAL	CB-CA-C	-6.12	103.78	112.22
1	B	162	ILE	CB-CA-C	-6.10	102.38	112.26
1	B	344	VAL	CB-CA-C	-6.10	103.80	112.22
1	D	191	VAL	CB-CA-C	-5.97	108.02	114.35
1	A	249	LYS	N-CA-C	5.89	118.14	109.24
1	C	344	VAL	CB-CA-C	-5.82	104.19	112.22
1	B	64	ILE	N-CA-CB	5.82	117.36	110.55
1	C	22	LYS	CD-CE-NZ	5.61	129.85	111.90
1	B	289	ILE	N-CA-C	5.55	115.75	110.42
1	A	433	ILE	N-CA-C	-5.54	105.11	110.42
1	C	217	THR	CB-CA-C	-5.43	101.62	110.85
1	B	145	ILE	N-CA-CB	5.42	114.68	110.45
1	C	242	GLY	N-CA-C	-5.36	102.13	111.62
1	C	79	ILE	N-CA-C	-5.35	106.58	111.67
1	B	217	THR	CB-CA-C	-5.32	101.81	110.85
1	A	440	ILE	CB-CA-C	-5.29	105.10	112.04
1	D	217	THR	CB-CA-C	-5.25	101.92	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	MET	N-CA-CB	-5.22	102.19	110.28
1	B	190	ALA	CA-C-N	5.19	124.48	120.33
1	B	190	ALA	C-N-CA	5.19	124.48	120.33
1	C	289	ILE	N-CA-C	5.19	115.40	110.42
1	A	217	THR	CB-CA-C	-5.17	102.06	110.85
1	B	79	ILE	N-CA-C	-5.13	107.40	111.81
1	C	433	ILE	N-CA-C	-5.13	105.50	110.42
1	D	360	PHE	N-CA-C	-5.03	105.93	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3124	0	3307	85	0
1	B	3057	0	3232	108	0
1	C	3092	0	3267	100	0
1	D	3078	0	3256	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	28	0	0
3	B	20	0	28	5	0
4	A	2	0	0	1	0
4	B	2	0	0	2	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	12403	0	13118	364	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 14.

All (364) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:HD23	1:D:145:ILE:CD1	1.24	1.62
1:C:141:LEU:CA	1:C:145:ILE:HD12	1.50	1.38
1:C:141:LEU:HA	1:C:145:ILE:CD1	1.63	1.28
1:D:141:LEU:CD2	1:D:145:ILE:CD1	2.12	1.28
1:B:263:ILE:CD1	1:B:327:ARG:HH11	1.47	1.26
1:B:31:TYR:OH	1:B:64:ILE:HG23	1.34	1.24
1:C:22:LYS:HE2	1:C:27:PRO:HG3	1.16	1.16
1:B:209:TYR:CE1	1:B:213:ILE:HD11	1.82	1.14
1:D:141:LEU:CD2	1:D:145:ILE:HD12	1.74	1.14
1:D:205:ARG:HD2	1:D:348:TYR:CE1	1.82	1.13
1:C:22:LYS:CE	1:C:27:PRO:HG3	1.81	1.11
1:B:152:ILE:HG12	1:B:182:MET:HE3	1.31	1.10
1:B:205:ARG:HD2	1:B:348:TYR:CE2	1.88	1.09
1:A:205:ARG:HD2	1:A:348:TYR:CE2	1.88	1.09
1:C:205:ARG:HD2	1:C:348:TYR:CE2	1.87	1.08
1:B:263:ILE:HD13	1:B:327:ARG:HH11	0.93	1.08
1:B:359:THR:OG1	1:B:362:ASN:CG	1.96	1.08
1:B:31:TYR:OH	1:B:64:ILE:CG2	2.01	1.07
1:D:141:LEU:HD23	1:D:145:ILE:HD12	1.07	1.03
1:B:263:ILE:CD1	1:B:327:ARG:NH1	2.21	1.03
1:B:331:PHE:CE2	3:B:502:BOG:H4'1	1.93	1.03
1:C:141:LEU:HD23	1:C:145:ILE:HD13	1.37	1.03
1:D:141:LEU:HD23	1:D:145:ILE:HD13	1.02	1.02
1:B:152:ILE:HG23	1:B:182:MET:HE1	1.40	1.02
1:C:141:LEU:HA	1:C:145:ILE:CG1	1.90	1.00
1:B:263:ILE:HD13	1:B:327:ARG:NH1	1.77	1.00
1:C:141:LEU:HD23	1:C:145:ILE:CD1	1.92	0.98
1:D:141:LEU:CD2	1:D:145:ILE:HD13	1.82	0.97
1:D:15:VAL:HA	1:D:18:LEU:HD12	1.46	0.96
1:C:141:LEU:CB	1:C:145:ILE:HD12	1.94	0.96
1:C:144:TYR:CE2	1:C:148:ILE:HD11	2.00	0.96
1:C:141:LEU:HA	1:C:145:ILE:HD12	0.98	0.95
1:D:205:ARG:HD2	1:D:348:TYR:HE1	1.27	0.94
1:C:23:ILE:HG23	1:C:67:GLU:HG3	1.47	0.94
1:B:359:THR:OG1	1:B:362:ASN:ND2	2.00	0.94
1:D:16:SER:HA	1:D:19:LEU:HD12	1.46	0.93
1:D:109:ASN:CG	1:D:113:LYS:HD2	1.94	0.91
1:A:246:LEU:HD21	1:A:386:PHE:CG	2.05	0.90
1:B:31:TYR:CZ	1:B:64:ILE:HG23	2.06	0.90
1:A:263:ILE:HD11	1:A:323:ALA:HB3	1.52	0.90
1:C:22:LYS:HG2	1:C:27:PRO:CA	2.01	0.89
1:C:22:LYS:HE2	1:C:27:PRO:CG	2.00	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HG2	1:C:27:PRO:HA	1.54	0.88
1:D:141:LEU:CG	1:D:145:ILE:HD12	2.02	0.88
1:B:31:TYR:CZ	1:B:64:ILE:CG2	2.56	0.88
1:B:264:THR:N	1:B:267:GLU:OE1	2.07	0.88
1:C:141:LEU:CG	1:C:145:ILE:HD12	2.04	0.88
1:B:263:ILE:HD12	1:B:327:ARG:NH1	1.89	0.86
1:B:209:TYR:CZ	1:B:213:ILE:HG13	2.10	0.85
1:A:205:ARG:HD2	1:A:348:TYR:HE2	1.40	0.85
1:A:246:LEU:CD2	1:A:386:PHE:HB3	2.07	0.85
1:C:205:ARG:HD2	1:C:348:TYR:HE2	1.40	0.85
1:B:205:ARG:HD2	1:B:348:TYR:HE2	1.39	0.84
1:B:152:ILE:HG12	1:B:182:MET:CE	2.07	0.84
1:B:18:LEU:O	1:B:21:PHE:HB3	1.76	0.84
1:D:141:LEU:CA	1:D:145:ILE:HD12	2.09	0.83
1:C:22:LYS:CD	1:C:27:PRO:HG3	2.08	0.83
1:B:209:TYR:CE1	1:B:213:ILE:CD1	2.62	0.82
1:C:23:ILE:N	1:C:26:MET:O	2.11	0.82
1:D:263:ILE:HD11	1:D:323:ALA:HB3	1.60	0.82
1:B:152:ILE:CG2	1:B:182:MET:HE1	2.09	0.81
1:D:141:LEU:HA	1:D:145:ILE:HD12	1.61	0.81
1:B:209:TYR:CE2	1:B:213:ILE:HG13	2.16	0.81
1:C:141:LEU:CD2	1:C:145:ILE:CD1	2.59	0.81
1:C:141:LEU:CA	1:C:145:ILE:CD1	2.36	0.80
1:B:359:THR:HG1	1:B:362:ASN:HB2	1.46	0.80
1:C:141:LEU:CD2	1:C:145:ILE:HD13	2.10	0.80
1:B:190:ALA:CB	1:B:213:ILE:HD13	2.13	0.79
1:B:359:THR:HG1	1:B:362:ASN:CB	1.96	0.78
1:B:331:PHE:CD2	3:B:502:BOG:H4'1	2.18	0.78
1:B:152:ILE:HG23	1:B:182:MET:CE	2.14	0.77
1:C:144:TYR:CE2	1:C:425:ILE:HG22	2.20	0.76
1:B:327:ARG:CZ	3:B:502:BOG:O6	2.33	0.76
1:B:359:THR:OG1	1:B:362:ASN:CB	2.33	0.76
1:C:141:LEU:CG	1:C:145:ILE:CD1	2.63	0.75
1:A:246:LEU:CD2	1:A:386:PHE:CG	2.70	0.75
1:B:190:ALA:HB1	1:B:213:ILE:HD13	1.68	0.74
1:B:18:LEU:O	1:B:21:PHE:CB	2.35	0.74
1:A:232:ILE:CG2	1:A:236:LYS:HE3	2.17	0.74
1:D:283:TYR:CE1	1:D:287:LYS:HE2	2.22	0.73
1:A:148:ILE:HG23	1:A:399:MET:HE3	1.70	0.73
1:D:144:TYR:CE2	1:D:148:ILE:HD11	2.24	0.73
1:B:190:ALA:HB1	1:B:213:ILE:CD1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLY:O	1:D:18:LEU:HG	1.87	0.73
1:D:15:VAL:HA	1:D:18:LEU:CD1	2.19	0.73
1:A:263:ILE:CD1	1:A:323:ALA:HB3	2.18	0.72
1:D:141:LEU:O	1:D:146:PRO:HD3	1.89	0.72
1:C:148:ILE:HG23	1:C:399:MET:HE3	1.71	0.72
1:B:184:GLY:HA2	4:B:601:HOH:O	1.88	0.72
1:B:190:ALA:CB	1:B:213:ILE:CD1	2.67	0.71
1:B:148:ILE:HG23	1:B:399:MET:HE3	1.73	0.71
1:D:148:ILE:HG23	1:D:399:MET:HE3	1.72	0.71
1:D:141:LEU:HA	1:D:145:ILE:HB	1.72	0.70
1:A:263:ILE:HG23	1:A:267:GLU:HB2	1.74	0.69
1:D:109:ASN:ND2	1:D:113:LYS:HD2	2.07	0.69
1:A:141:LEU:HA	1:A:145:ILE:HD12	1.75	0.68
1:A:246:LEU:HD23	1:A:386:PHE:HB3	1.76	0.68
1:C:141:LEU:O	1:C:146:PRO:HD3	1.92	0.68
1:C:144:TYR:OH	1:C:426:SER:N	2.27	0.68
1:D:15:VAL:O	1:D:19:LEU:HG	1.95	0.67
1:B:141:LEU:O	1:B:146:PRO:HD3	1.95	0.67
1:A:398:CYS:HA	1:A:401:ASN:ND2	2.10	0.66
1:C:141:LEU:HG	1:C:145:ILE:CD1	2.26	0.66
1:D:141:LEU:HA	1:D:145:ILE:CD1	2.25	0.66
1:B:152:ILE:CG1	1:B:182:MET:HE3	2.19	0.65
1:A:246:LEU:CD2	1:A:386:PHE:CD1	2.79	0.65
1:A:292:SER:HB3	1:A:294:GLY:O	1.96	0.65
1:A:400:ALA:O	4:A:601:HOH:O	2.14	0.65
1:B:178:VAL:HG12	1:B:182:MET:SD	2.38	0.64
1:A:141:LEU:O	1:A:146:PRO:HD3	1.97	0.64
1:B:141:LEU:HA	1:B:145:ILE:HD12	1.77	0.64
1:C:141:LEU:HD23	1:C:145:ILE:HD12	1.80	0.64
1:C:22:LYS:HB3	1:C:26:MET:C	2.23	0.63
1:D:263:ILE:HG23	1:D:267:GLU:HB2	1.80	0.63
1:D:141:LEU:HA	1:D:145:ILE:CG1	2.28	0.63
1:D:263:ILE:CD1	1:D:323:ALA:HB3	2.29	0.63
1:A:203:ARG:NH1	1:D:204:SER:OG	2.32	0.63
1:A:246:LEU:CD2	1:A:386:PHE:CB	2.76	0.63
1:A:232:ILE:O	1:A:236:LYS:HG3	1.98	0.62
1:C:141:LEU:CD2	1:C:145:ILE:HD12	2.28	0.62
1:D:141:LEU:CB	1:D:145:ILE:HD12	2.29	0.62
1:A:246:LEU:HD21	1:A:386:PHE:CB	2.30	0.62
1:D:144:TYR:OH	1:D:426:SER:OG	2.15	0.60
1:A:248:ARG:HB3	1:A:385:GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:TYR:HE2	1:C:425:ILE:HG22	1.64	0.60
1:C:22:LYS:HG2	1:C:27:PRO:CB	2.31	0.60
1:C:84:VAL:HA	1:C:87:PHE:CE2	2.38	0.59
1:A:163:GLY:HA3	1:A:173:ILE:HD11	1.84	0.59
1:A:144:TYR:CE2	1:A:148:ILE:HD11	2.36	0.58
1:C:188:ALA:O	1:C:192:PRO:HG3	2.03	0.58
1:B:209:TYR:CZ	1:B:213:ILE:CG1	2.84	0.58
1:D:84:VAL:HA	1:D:87:PHE:CE2	2.39	0.58
1:C:320:GLU:CD	1:C:320:GLU:H	2.11	0.58
1:D:163:GLY:HA3	1:D:173:ILE:HD11	1.86	0.58
1:B:184:GLY:CA	4:B:601:HOH:O	2.50	0.58
1:B:31:TYR:OH	1:B:64:ILE:HG21	2.00	0.58
1:B:320:GLU:H	1:B:320:GLU:CD	2.12	0.58
1:D:141:LEU:HA	1:D:145:ILE:CB	2.33	0.57
1:A:320:GLU:CD	1:A:320:GLU:H	2.12	0.57
1:B:268:THR:OG1	3:B:502:BOG:H62	2.04	0.57
1:C:141:LEU:HA	1:C:145:ILE:CB	2.33	0.57
1:B:163:GLY:HA3	1:B:173:ILE:HD11	1.85	0.57
1:B:144:TYR:CE2	1:B:148:ILE:HD11	2.39	0.57
1:C:163:GLY:HA3	1:C:173:ILE:HD11	1.85	0.57
1:C:141:LEU:N	1:C:145:ILE:CD1	2.67	0.57
1:A:399:MET:HE1	1:A:430:GLY:HA3	1.87	0.57
1:B:399:MET:HE1	1:B:430:GLY:HA3	1.87	0.57
1:A:416:ARG:HB3	1:A:419:LEU:HD13	1.87	0.57
1:B:152:ILE:CG1	1:B:182:MET:CE	2.81	0.57
1:B:84:VAL:HA	1:B:87:PHE:CE2	2.40	0.56
1:A:19:LEU:HD22	1:A:29:PRO:HG3	1.87	0.56
1:B:188:ALA:O	1:B:192:PRO:HG3	2.05	0.56
1:A:188:ALA:O	1:A:192:PRO:HG3	2.05	0.56
1:B:31:TYR:CE2	1:B:64:ILE:CG2	2.88	0.56
1:C:141:LEU:N	1:C:145:ILE:HD12	2.16	0.56
1:C:416:ARG:HB3	1:C:419:LEU:HD13	1.87	0.56
1:B:264:THR:HG23	1:B:267:GLU:OE1	2.05	0.56
1:C:160:ILE:HA	1:C:173:ILE:HD13	1.87	0.56
1:A:350:ASP:OD2	1:A:353:GLU:HG2	2.06	0.56
1:D:399:MET:HE1	1:D:430:GLY:HA3	1.87	0.56
1:D:188:ALA:O	1:D:192:PRO:HG3	2.04	0.56
1:B:72:LEU:HD12	1:B:85:MET:CE	2.36	0.56
1:C:22:LYS:HA	1:C:27:PRO:HA	1.86	0.56
1:B:416:ARG:HB3	1:B:419:LEU:HD13	1.87	0.55
1:D:283:TYR:CE1	1:D:287:LYS:CE	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASN:O	1:B:191:VAL:HG23	2.06	0.55
1:C:399:MET:HE1	1:C:430:GLY:HA3	1.88	0.55
1:A:232:ILE:HG23	1:A:236:LYS:HE3	1.89	0.54
1:B:178:VAL:CG1	1:B:182:MET:SD	2.95	0.54
1:C:148:ILE:CG2	1:C:399:MET:HE3	2.37	0.54
1:A:160:ILE:HA	1:A:173:ILE:HD13	1.89	0.54
1:C:186:ASN:O	1:C:191:VAL:HG23	2.07	0.54
1:D:350:ASP:OD2	1:D:353:GLU:HG2	2.07	0.54
1:C:144:TYR:CE2	1:C:425:ILE:CG2	2.89	0.54
1:A:84:VAL:HA	1:A:87:PHE:CE2	2.42	0.54
1:C:23:ILE:HG23	1:C:67:GLU:CG	2.30	0.54
1:D:186:ASN:O	1:D:191:VAL:HG23	2.08	0.54
1:D:416:ARG:HB3	1:D:419:LEU:HD13	1.89	0.54
1:B:160:ILE:HA	1:B:173:ILE:HD13	1.90	0.54
1:C:350:ASP:OD2	1:C:353:GLU:HG2	2.08	0.54
1:D:148:ILE:CG2	1:D:399:MET:HE3	2.38	0.54
1:B:350:ASP:OD2	1:B:353:GLU:HG2	2.07	0.53
1:D:320:GLU:H	1:D:320:GLU:CD	2.16	0.53
1:A:148:ILE:CG2	1:A:399:MET:HE3	2.38	0.53
1:C:154:GLY:HA2	1:C:157:ILE:HG22	1.90	0.53
1:D:160:ILE:HA	1:D:173:ILE:HD13	1.89	0.53
1:A:186:ASN:O	1:A:191:VAL:HG23	2.09	0.53
1:B:178:VAL:O	1:B:182:MET:HG3	2.09	0.53
1:D:286:ALA:O	1:D:291:PRO:HA	2.10	0.52
1:B:331:PHE:CD2	3:B:502:BOG:C4'	2.91	0.52
1:C:286:ALA:O	1:C:291:PRO:HA	2.09	0.52
1:D:154:GLY:HA2	1:D:157:ILE:HG22	1.92	0.52
1:A:154:GLY:HA2	1:A:157:ILE:HG22	1.92	0.52
1:A:232:ILE:HG22	1:A:236:LYS:CE	2.39	0.52
1:D:109:ASN:CG	1:D:113:LYS:CD	2.78	0.52
1:A:45:ASN:HB2	1:C:101:GLN:NE2	2.26	0.51
1:B:286:ALA:O	1:B:291:PRO:HA	2.09	0.51
1:B:209:TYR:CD1	1:B:213:ILE:HD11	2.40	0.51
1:A:286:ALA:O	1:A:291:PRO:HA	2.10	0.51
1:A:144:TYR:OH	1:A:426:SER:OG	2.18	0.51
1:A:232:ILE:CG2	1:A:236:LYS:CE	2.87	0.51
1:A:232:ILE:HG22	1:A:236:LYS:HE3	1.92	0.51
1:C:144:TYR:CE2	1:C:148:ILE:CD1	2.83	0.51
1:A:80:GLY:HA3	1:A:402:ARG:NH1	2.26	0.51
1:A:246:LEU:HD23	1:A:386:PHE:CD1	2.46	0.51
1:A:331:PHE:CD1	1:B:265:HIS:HD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLY:HA2	1:B:157:ILE:HG22	1.92	0.51
1:B:263:ILE:HD13	1:B:327:ARG:HG3	1.93	0.50
1:A:105:ASP:OD2	1:C:113:LYS:HE2	2.12	0.50
1:B:186:ASN:OD1	1:B:213:ILE:HD12	2.11	0.50
1:B:163:GLY:HA3	1:B:173:ILE:CD1	2.42	0.50
1:C:264:THR:OG1	1:C:267:GLU:HG2	2.11	0.50
1:B:148:ILE:CG2	1:B:399:MET:HE3	2.40	0.50
1:C:163:GLY:HA3	1:C:173:ILE:CD1	2.42	0.49
1:A:141:LEU:CA	1:A:145:ILE:HD12	2.42	0.49
1:C:140:SER:C	1:C:145:ILE:HG13	2.37	0.49
1:A:246:LEU:HD23	1:A:246:LEU:C	2.37	0.49
1:B:209:TYR:CE1	1:B:213:ILE:CG1	2.95	0.49
1:C:23:ILE:O	1:C:26:MET:N	2.45	0.49
1:C:141:LEU:HA	1:C:145:ILE:HB	1.94	0.49
1:C:22:LYS:HD3	1:C:27:PRO:HG3	1.93	0.49
1:B:18:LEU:O	1:B:21:PHE:N	2.40	0.49
1:C:22:LYS:CG	1:C:27:PRO:HA	2.34	0.49
1:D:163:GLY:HA3	1:D:173:ILE:CD1	2.42	0.49
1:A:429:LEU:O	1:A:433:ILE:HG12	2.12	0.49
1:C:141:LEU:O	1:C:145:ILE:HB	2.12	0.49
1:A:163:GLY:HA3	1:A:173:ILE:CD1	2.42	0.48
1:D:109:ASN:OD1	1:D:113:LYS:CE	2.61	0.48
1:C:292:SER:HB3	1:C:294:GLY:O	2.14	0.48
1:D:283:TYR:CE1	1:D:287:LYS:NZ	2.79	0.48
1:C:342:VAL:O	1:C:346:VAL:HG23	2.13	0.48
1:D:35:LEU:O	1:D:39:LEU:HG	2.14	0.48
1:B:342:VAL:O	1:B:346:VAL:HG23	2.14	0.48
1:D:14:GLY:HA2	1:D:17:ASP:OD2	2.14	0.48
1:D:109:ASN:OD1	1:D:113:LYS:HE3	2.13	0.48
1:A:18:LEU:O	1:A:28:LEU:HD12	2.13	0.47
1:B:30:LEU:O	1:B:33:PHE:HB3	2.14	0.47
1:C:52:VAL:HG11	1:D:279:PHE:CD1	2.49	0.47
1:B:35:LEU:O	1:B:39:LEU:HG	2.14	0.47
1:C:31:TYR:OH	1:C:64:ILE:HB	2.15	0.47
1:A:263:ILE:HG23	1:A:267:GLU:CB	2.42	0.47
1:C:35:LEU:O	1:C:39:LEU:HG	2.15	0.47
1:D:292:SER:HB3	1:D:294:GLY:O	2.15	0.47
1:B:203:ARG:NH2	1:C:445:MET:O	2.43	0.47
1:C:429:LEU:O	1:C:433:ILE:HG12	2.14	0.47
1:A:342:VAL:O	1:A:346:VAL:HG23	2.14	0.47
1:D:342:VAL:O	1:D:346:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:LEU:O	1:D:433:ILE:HG12	2.15	0.47
1:B:429:LEU:O	1:B:433:ILE:HG12	2.14	0.47
1:B:190:ALA:HB1	1:B:213:ILE:HD11	1.93	0.47
1:C:398:CYS:HA	1:C:401:ASN:ND2	2.29	0.47
1:D:205:ARG:CD	1:D:348:TYR:HE1	2.14	0.47
1:A:246:LEU:HD21	1:A:386:PHE:HB3	1.87	0.46
1:D:143:GLY:C	1:D:146:PRO:HD2	2.40	0.46
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.78	0.46
1:A:141:LEU:HA	1:A:145:ILE:HB	1.97	0.46
1:C:18:LEU:CA	1:C:21:PHE:HD2	2.29	0.46
1:B:292:SER:HB3	1:B:294:GLY:O	2.15	0.45
1:C:141:LEU:CA	1:C:145:ILE:CG1	2.80	0.45
1:C:290:LEU:HD23	1:C:303:TRP:CZ2	2.50	0.45
1:C:145:ILE:HB	1:C:146:PRO:HD3	1.98	0.45
1:B:144:TYR:OH	1:B:426:SER:OG	2.20	0.45
1:B:209:TYR:CZ	1:B:213:ILE:CD1	2.98	0.45
1:D:30:LEU:O	1:D:33:PHE:HB3	2.17	0.45
1:D:117:LEU:HD22	1:D:348:TYR:OH	2.16	0.45
1:B:290:LEU:HD23	1:B:303:TRP:CZ2	2.52	0.45
1:C:30:LEU:O	1:C:33:PHE:HB3	2.17	0.45
1:D:290:LEU:HD23	1:D:303:TRP:CZ2	2.52	0.45
1:A:290:LEU:HD23	1:A:303:TRP:CZ2	2.52	0.45
1:B:141:LEU:CA	1:B:145:ILE:HD12	2.45	0.45
1:A:30:LEU:O	1:A:33:PHE:HB3	2.17	0.45
1:A:35:LEU:O	1:A:39:LEU:HG	2.16	0.45
1:B:141:LEU:HA	1:B:145:ILE:HB	1.97	0.45
1:C:18:LEU:HA	1:C:21:PHE:HD2	1.80	0.45
1:D:398:CYS:HA	1:D:401:ASN:ND2	2.32	0.45
1:C:18:LEU:HA	1:C:21:PHE:CD2	2.52	0.44
1:D:162:ILE:CG1	1:D:368:ILE:HG21	2.48	0.44
1:B:190:ALA:CB	1:B:213:ILE:HD11	2.45	0.44
1:C:264:THR:HG1	1:C:267:GLU:HG2	1.83	0.44
1:B:402:ARG:O	1:B:405:SER:OG	2.35	0.44
1:C:144:TYR:CZ	1:C:148:ILE:HD11	2.50	0.44
1:A:31:TYR:OH	1:A:64:ILE:HB	2.18	0.44
1:A:143:GLY:C	1:A:146:PRO:HD2	2.43	0.44
1:B:290:LEU:HA	1:B:290:LEU:HD12	1.79	0.43
1:C:285:VAL:HA	1:C:289:ILE:HB	2.00	0.43
1:D:285:VAL:HA	1:D:289:ILE:HB	1.98	0.43
1:B:200:VAL:HG12	1:B:446:ILE:HD13	2.00	0.43
1:C:45:ASN:OD1	1:C:100:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:CB	1:C:101:GLN:NE2	2.82	0.43
1:A:101:GLN:HG3	1:C:109:ASN:HD21	1.83	0.43
1:B:162:ILE:CG1	1:B:368:ILE:HG21	2.49	0.43
1:B:64:ILE:HG13	1:B:65:PHE:N	2.33	0.43
1:D:31:TYR:OH	1:D:64:ILE:HB	2.18	0.43
1:D:200:VAL:HG12	1:D:446:ILE:HD13	2.00	0.43
1:A:19:LEU:HD22	1:A:29:PRO:CG	2.47	0.43
1:A:200:VAL:HG12	1:A:446:ILE:HD13	2.00	0.43
1:B:45:ASN:OD1	1:B:100:THR:HG21	2.18	0.43
1:A:331:PHE:HD1	1:B:265:HIS:HD2	1.67	0.43
1:B:374:VAL:HG22	1:B:397:LEU:CD1	2.48	0.43
1:C:162:ILE:CG1	1:C:368:ILE:HG21	2.49	0.43
1:D:389:ILE:O	1:D:393:ILE:HG12	2.19	0.43
1:D:394:THR:O	1:D:398:CYS:HB2	2.19	0.43
1:C:189:GLY:C	1:C:192:PRO:HD2	2.44	0.43
1:D:45:ASN:OD1	1:D:100:THR:HG21	2.18	0.43
1:A:45:ASN:OD1	1:A:100:THR:HG21	2.19	0.42
1:D:283:TYR:CZ	1:D:287:LYS:HE2	2.54	0.42
1:A:201:THR:HG22	1:A:446:ILE:HD11	2.01	0.42
1:A:374:VAL:HG22	1:A:397:LEU:CD1	2.48	0.42
1:D:370:VAL:O	1:D:374:VAL:HG23	2.19	0.42
1:B:285:VAL:HA	1:B:289:ILE:HB	2.02	0.42
1:C:374:VAL:HG13	1:C:392:ALA:HB1	2.02	0.42
1:D:201:THR:HG22	1:D:446:ILE:HD11	2.01	0.42
1:A:162:ILE:CG1	1:A:368:ILE:HG21	2.49	0.42
1:B:389:ILE:O	1:B:393:ILE:HG12	2.20	0.42
1:D:290:LEU:HD12	1:D:290:LEU:HA	1.79	0.42
1:A:246:LEU:HD23	1:A:386:PHE:CB	2.43	0.42
1:A:263:ILE:HG22	1:A:264:THR:N	2.34	0.42
1:B:370:VAL:O	1:B:374:VAL:HG23	2.19	0.42
1:D:189:GLY:C	1:D:192:PRO:HD2	2.44	0.42
1:C:389:ILE:O	1:C:393:ILE:HG12	2.20	0.42
1:A:370:VAL:O	1:A:374:VAL:HG23	2.20	0.42
1:B:197:TYR:CE1	1:B:201:THR:HG21	2.55	0.42
1:B:87:PHE:CZ	1:B:213:ILE:HG21	2.55	0.42
1:C:200:VAL:HG12	1:C:446:ILE:HD13	2.01	0.42
1:C:279:PHE:CD1	1:D:52:VAL:HG11	2.55	0.42
1:D:374:VAL:HG22	1:D:397:LEU:CD1	2.50	0.42
1:A:129:ILE:HD11	1:A:305:VAL:HG13	2.02	0.42
1:A:285:VAL:HA	1:A:289:ILE:HB	2.01	0.42
1:A:389:ILE:O	1:A:393:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:HG22	1:C:446:ILE:HD11	2.02	0.42
1:B:201:THR:HG22	1:B:446:ILE:HD11	2.02	0.41
1:B:374:VAL:HG13	1:B:392:ALA:HB1	2.02	0.41
1:B:394:THR:O	1:B:398:CYS:HB2	2.20	0.41
1:C:129:ILE:HD11	1:C:305:VAL:HG13	2.02	0.41
1:D:263:ILE:HG23	1:D:267:GLU:CB	2.49	0.41
1:B:357:ALA:C	1:B:359:THR:H	2.28	0.41
1:C:23:ILE:O	1:C:26:MET:HB2	2.20	0.41
1:C:370:VAL:O	1:C:374:VAL:HG23	2.21	0.41
1:D:374:VAL:HG13	1:D:392:ALA:HB1	2.02	0.41
1:B:87:PHE:CD1	1:B:87:PHE:C	2.98	0.41
1:A:263:ILE:HG12	1:A:267:GLU:HG2	2.02	0.41
1:B:19:LEU:HD22	1:B:29:PRO:HG3	2.02	0.41
1:B:281:LEU:O	1:B:285:VAL:HG23	2.21	0.41
1:C:394:THR:O	1:C:398:CYS:HB2	2.21	0.41
1:A:398:CYS:O	1:A:401:ASN:OD1	2.39	0.41
1:B:117:LEU:HD22	1:B:348:TYR:OH	2.20	0.41
1:A:189:GLY:C	1:A:192:PRO:HD2	2.45	0.41
1:C:374:VAL:HG22	1:C:397:LEU:CD1	2.50	0.41
1:D:349:THR:HG23	1:D:354:ILE:HD11	2.02	0.41
1:A:394:THR:O	1:A:398:CYS:HB2	2.20	0.41
1:D:281:LEU:O	1:D:285:VAL:HG23	2.21	0.41
1:A:117:LEU:HD22	1:A:348:TYR:OH	2.21	0.40
1:A:374:VAL:HG13	1:A:392:ALA:HB1	2.02	0.40
1:D:144:TYR:HE2	1:D:148:ILE:HD11	1.83	0.40
1:B:152:ILE:CG2	1:B:182:MET:CE	2.87	0.40
1:A:263:ILE:CG2	1:A:264:THR:N	2.84	0.40
1:C:117:LEU:HD22	1:C:348:TYR:OH	2.20	0.40
1:B:129:ILE:HD11	1:B:305:VAL:HG13	2.03	0.40
1:C:20:GLY:O	1:C:22:LYS:HG3	2.21	0.40
1:C:93:PHE:HA	1:C:98:ILE:HD12	2.04	0.40
1:A:179:LEU:N	1:A:180:PRO:HD2	2.37	0.40
1:A:281:LEU:O	1:A:285:VAL:HG23	2.22	0.40
1:C:87:PHE:CD1	1:C:87:PHE:C	2.99	0.40
1:C:419:LEU:N	1:C:419:LEU:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	325/343 (95%)	322 (99%)	3 (1%)	70	73
1	B	319/343 (93%)	318 (100%)	1 (0%)	86	81
1	C	322/343 (94%)	318 (99%)	4 (1%)	63	70
1	D	321/343 (94%)	320 (100%)	1 (0%)	86	81
All	All	1287/1372 (94%)	1278 (99%)	9 (1%)	76	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	215	ILE
1	A	296	VAL
1	B	296	VAL
1	C	74	ILE
1	C	203	ARG
1	C	215	ILE
1	C	296	VAL
1	D	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	B	101	GLN
1	B	220	ASN
1	B	265	HIS

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Mol	Chain	Res	Type
1	B	352	GLN
1	B	362	ASN
1	C	101	GLN
1	C	220	ASN
1	D	101	GLN
1	D	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BOG	A	502	-	20,20,20	0.53	0	25,25,25	0.99	1 (4%)
3	BOG	B	502	-	20,20,20	0.62	1 (5%)	25,25,25	0.91	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
3	BOG	A	502	-	-	6/11/31/31	0/1/1/1
3	BOG	B	502	-	-	3/11/31/31	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	BOG	O1-C1	2.22	1.43	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	BOG	C6-C5-C4	-2.13	107.78	113.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	BOG	C4-C5-C6-O6
3	B	502	BOG	O5-C5-C6-O6
3	B	502	BOG	C4-C5-C6-O6
3	A	502	BOG	O1-C1'-C2'-C3'
3	B	502	BOG	O1-C1'-C2'-C3'
3	A	502	BOG	C3'-C4'-C5'-C6'
3	A	502	BOG	O5-C1-O1-C1'
3	A	502	BOG	C5'-C6'-C7'-C8'
3	A	502	BOG	O5-C5-C6-O6

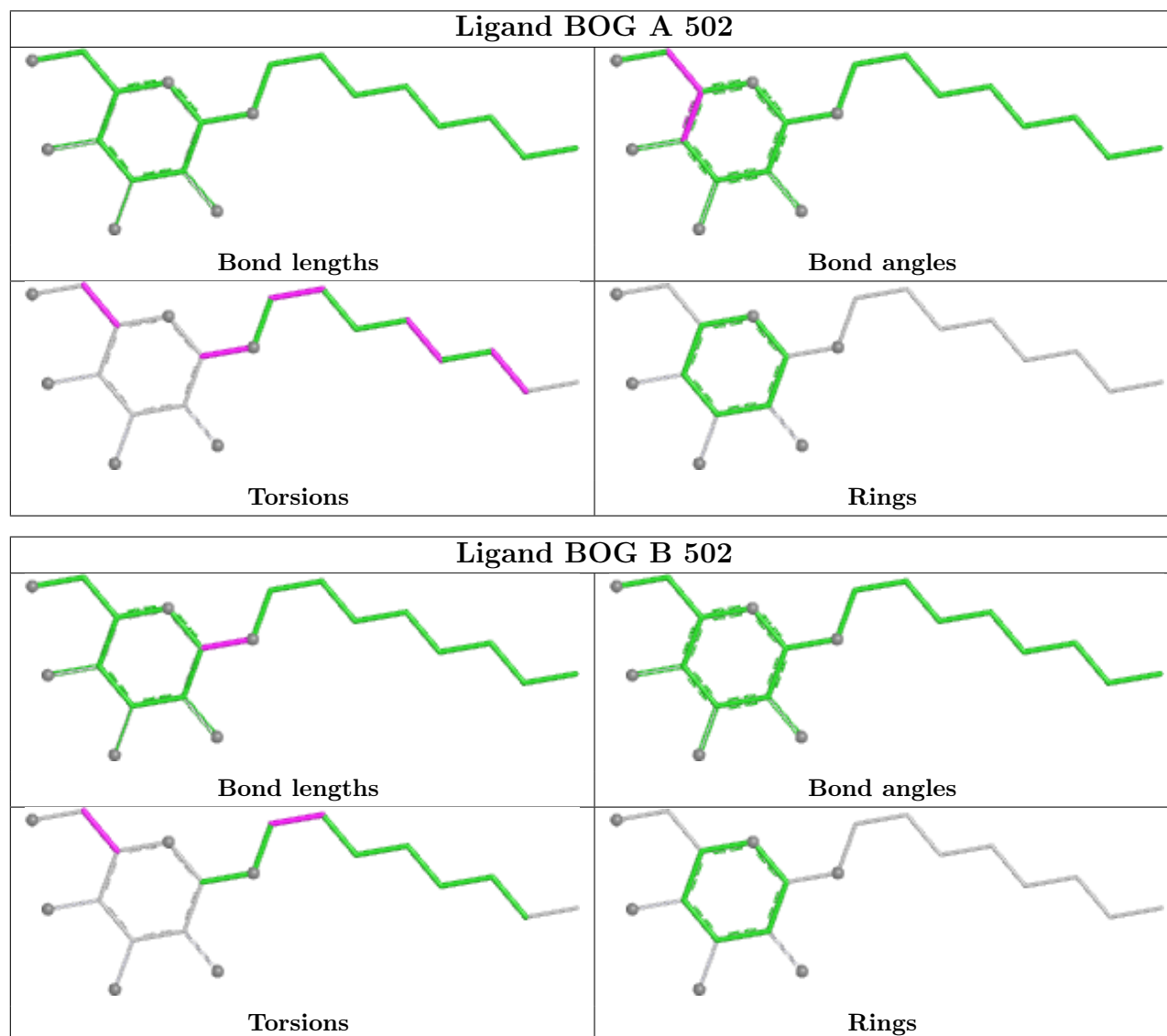
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	BOG	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/438 (95%)	-0.02	11 (2%) 57 35	117, 176, 227, 272	0
1	B	409/438 (93%)	-0.11	15 (3%) 45 27	131, 187, 243, 280	0
1	C	413/438 (94%)	-0.09	11 (2%) 56 34	124, 190, 245, 282	0
1	D	411/438 (93%)	-0.13	12 (2%) 53 32	132, 197, 253, 296	0
All	All	1650/1752 (94%)	-0.09	49 (2%) 52 31	117, 186, 245, 296	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	GLY	6.6
1	D	205	ARG	4.9
1	A	405	SER	4.9
1	A	234	GLY	4.5
1	A	240	LEU	4.5
1	D	206	GLU	4.4
1	D	348	TYR	4.0
1	D	347	CYS	3.8
1	D	195	GLU	3.7
1	B	317	CYS	3.4
1	A	446	ILE	3.4
1	A	238	THR	3.3
1	B	425	ILE	3.1
1	B	182	MET	3.1
1	C	144	TYR	2.9
1	C	397	LEU	2.9
1	C	354	ILE	2.9
1	D	97	GLY	2.8
1	D	349	THR	2.8
1	D	408	LEU	2.7
1	A	241	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	260	THR	2.7
1	C	393	ILE	2.6
1	A	245	GLU	2.6
1	B	132	VAL	2.6
1	C	20	GLY	2.6
1	B	178	VAL	2.6
1	C	411	LEU	2.6
1	D	95	TYR	2.5
1	B	59	PHE	2.5
1	C	295	GLY	2.5
1	A	51	ILE	2.4
1	B	119	LEU	2.3
1	C	214	ALA	2.3
1	D	94	VAL	2.3
1	C	391	SER	2.3
1	C	357	ALA	2.3
1	B	177	TYR	2.3
1	B	388	PRO	2.2
1	B	217	THR	2.2
1	B	328	LEU	2.2
1	A	418	ASN	2.2
1	B	45	ASN	2.2
1	C	398	CYS	2.1
1	B	387	PHE	2.1
1	D	159	GLY	2.1
1	D	132	VAL	2.1
1	A	243	GLU	2.1
1	B	219	ALA	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.

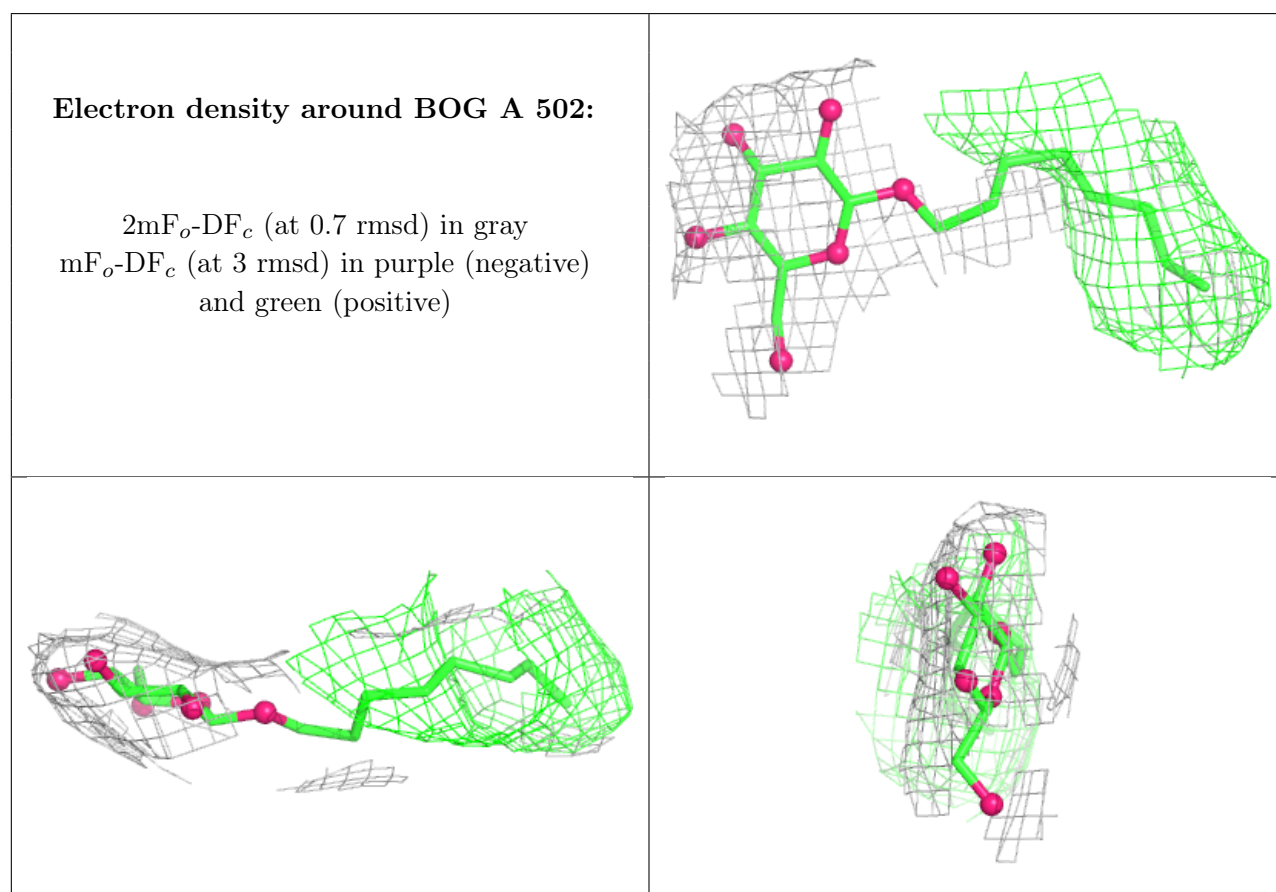
6.4 Ligands [i](#)

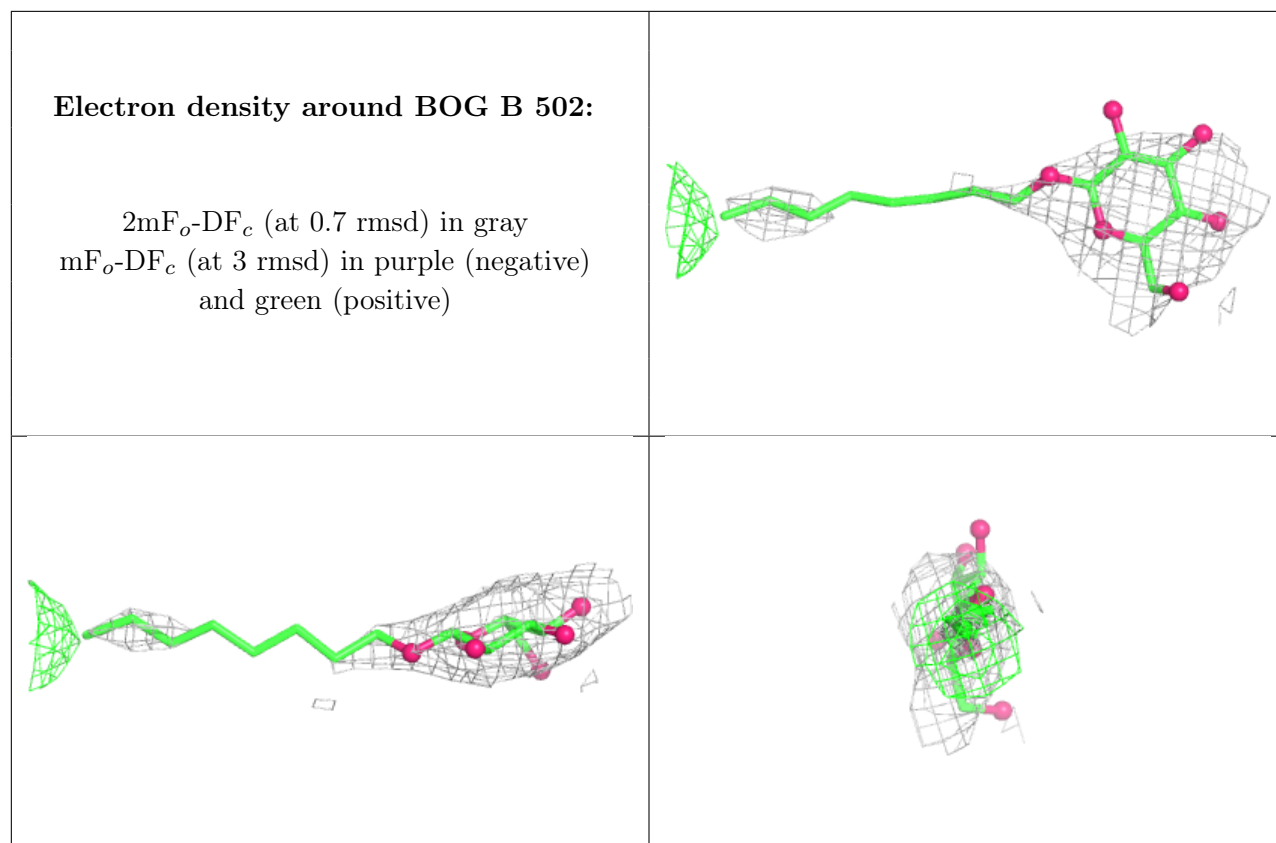
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å ²)	Q<0.9
3	BOG	A	502	20/20	0.20	0.16	213,241,270,270	0
3	BOG	B	502	20/20	0.91	0.14	141,213,250,254	0
2	NA	B	501	1/1	0.95	0.06	228,228,228,228	0
2	NA	D	501	1/1	0.95	0.08	148,148,148,148	0
2	NA	C	501	1/1	0.98	0.04	205,205,205,205	0
2	NA	A	501	1/1	0.99	0.05	193,193,193,193	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.