Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 01:20 PM JST

PDB ID	:	5XAR
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:

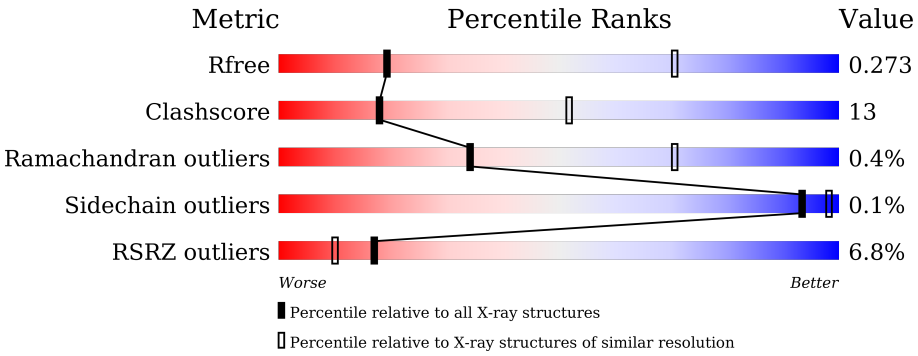
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	438	4% 75% 20% 5%
1	B	438	8% 73% 20% 7%
1	C	438	7% 75% 18% • 6%
1	D	438	7% 75% 19% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BOG	B	502	-	-	-	X

2 Entry composition (i)

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			

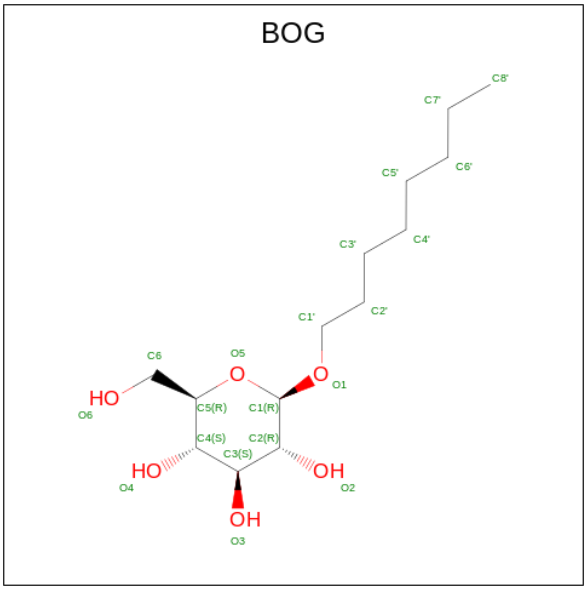
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: 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.

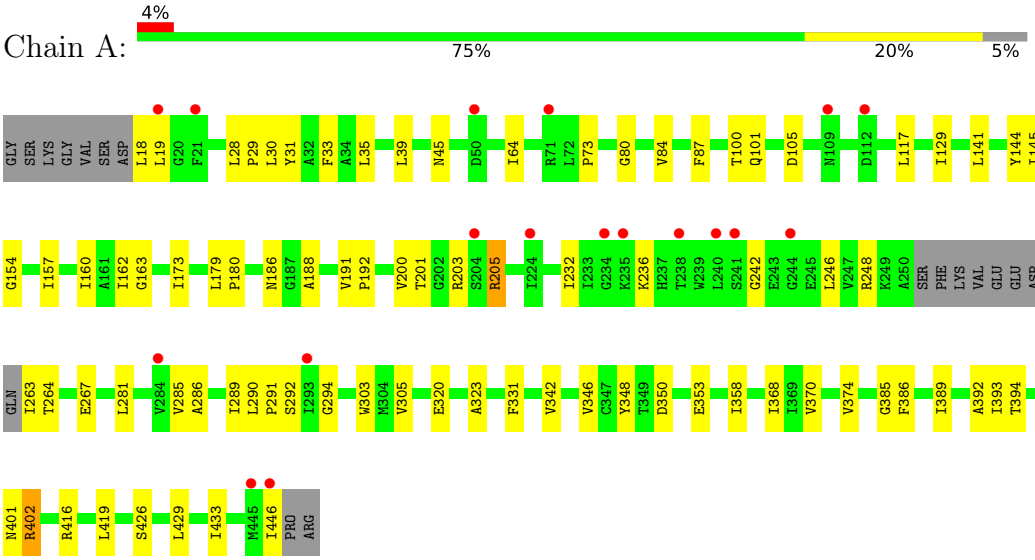
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

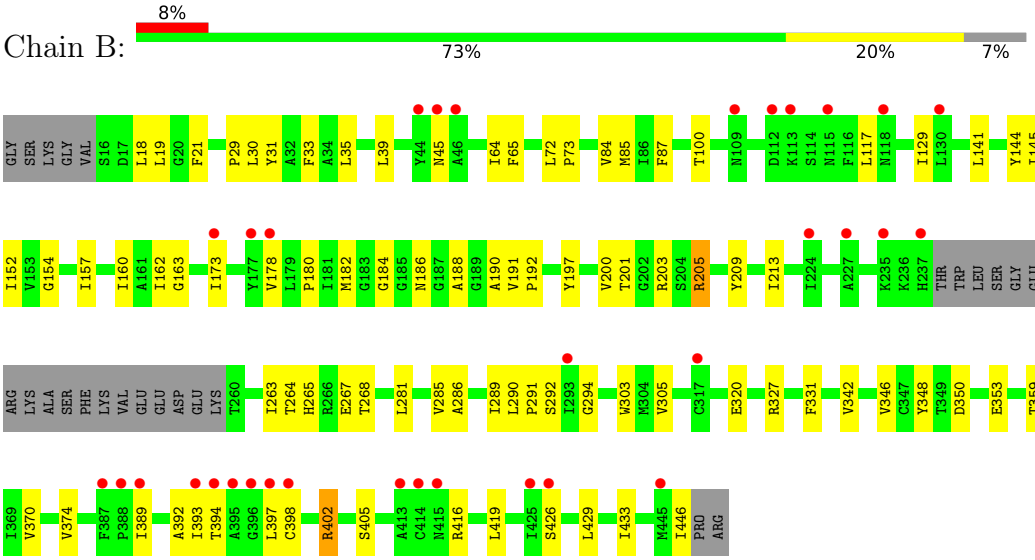
• Molecule 1: Citrate-sodium symporter

Chain A:



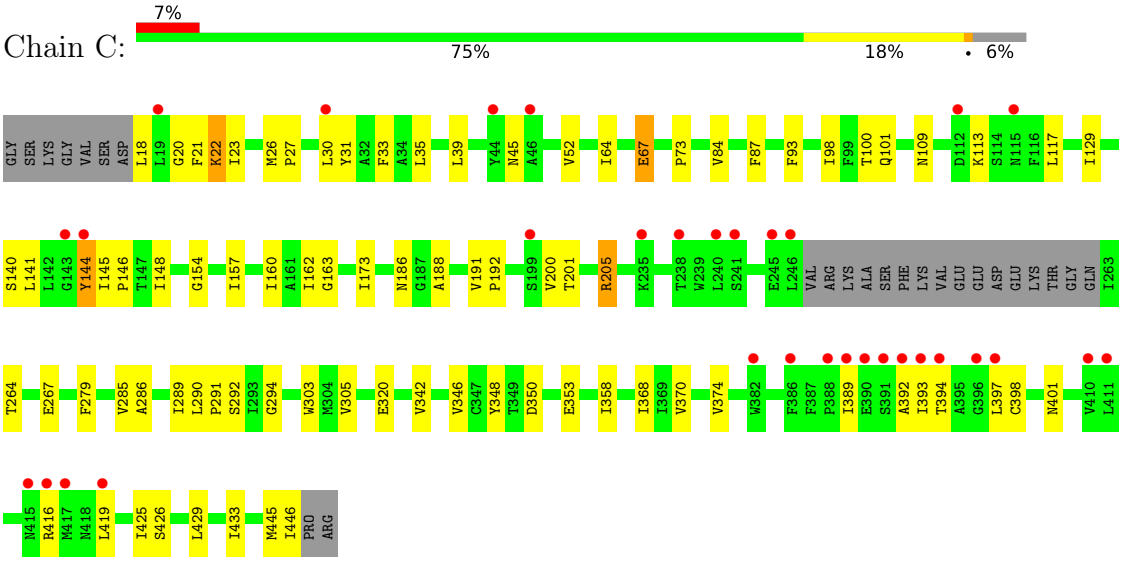
• Molecule 1: Citrate-sodium symporter

Chain B:



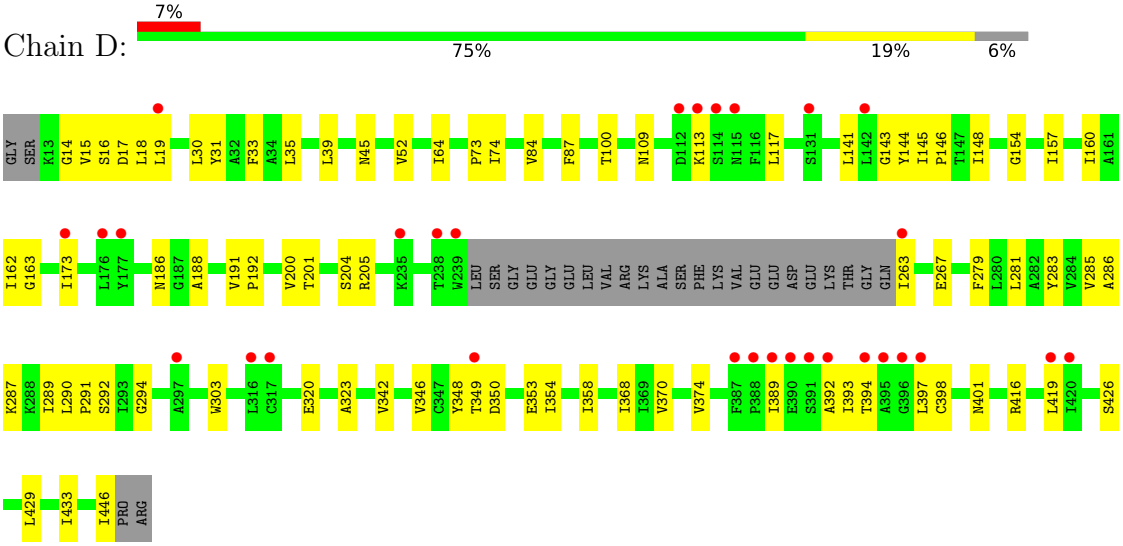
• Molecule 1: Citrate-sodium symporter

Chain C:



• Molecule 1: Citrate-sodium symporter

Chain D:



4 Data and refinement statistics (i)

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 49.97 – 3.62	Depositor EDS
% Data completeness (in resolution range)	98.5 (93.49-3.62) 98.5 (49.97-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.235 , 0.267 0.242 , 0.273	Depositor DCC
R_{free} test set	1433 reflections (4.70%)	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)	0.31 , 176.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.82	0/3186	0.92	4/4323 (0.1%)
1	B	0.80	0/3117	0.94	4/4230 (0.1%)
1	C	0.84	2/3154 (0.1%)	0.92	3/4281 (0.1%)
1	D	0.80	0/3140	0.90	1/4262 (0.0%)
All	All	0.82	2/12597 (0.0%)	0.92	12/17096 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	144	TYR	CE1-CZ	7.58	1.48	1.38
1	C	67	GLU	CD-OE1	5.08	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	402	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	22	LYS	CD-CE-NZ	7.89	129.85	111.70
1	C	205	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	205	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	205	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	205	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	205	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	205	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	402	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	242	GLY	N-CA-C	-5.47	99.42	113.10
1	D	74	ILE	CB-CA-C	-5.19	101.23	111.60
1	A	402	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3124	0	3307	82	0
1	B	3057	0	3232	102	0
1	C	3092	0	3267	94	0
1	D	3078	0	3256	76	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	344	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (344) 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:205:ARG:HD2	1:B:348:TYR:CE2	1.88	1.09
1:B:152:ILE:HG23	1:B:182:MET:HE1	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:TYR:OH	1:B:64:ILE:CG2	2.01	1.07
1:B:152:ILE:HG12	1:B:182:MET:HE3	1.34	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:359:THR:OG1	1:B:362:ASN:CG	1.96	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: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: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
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:152:ILE:CG2	1:B:182:MET:HE1	2.02	0.88
1:B:264:THR:N	1:B:267:GLU:OE1	2.07	0.88
1:D:109:ASN:CG	1:D:113:LYS:HD2	1.94	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:B:31:TYR:HH	1:B:64:ILE:HG23	1.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:152:ILE:HG23	1:B:182:MET:CE	2.14	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:248:ARG:HB3	1:A:385:GLY:O	2.01	0.60
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:22:LYS:HB3	1:C:26:MET:C	2.23	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: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:D:141:LEU:HA	1:D:145:ILE:CB	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:N	1:C:145:ILE:CD1	2.67	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: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
1:B:186:ASN:O	1:B:191:VAL:HG23	2.06	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: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:B:350:ASP:OD2	1:B:353:GLU:HG2	2.07	0.53
1:C:320:GLU:CD	1:C:320:GLU:H	2.11	0.53
1:B:320:GLU:H	1:B:320:GLU:CD	2.12	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:A:320:GLU:CD	1:A:320:GLU:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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:320:GLU:H	1:D:320:GLU:CD	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:144:TYR:OH	1:A:426:SER:OG	2.18	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:144:TYR:OH	1:D:426:SER:OG	2.15	0.45
1:D:290:LEU:HD23	1:D:303:TRP:CZ2	2.52	0.45
1:C:140:SER:C	1:C:145:ILE:HG13	2.37	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:A:246:LEU:HD23	1:A:246:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:A:148:ILE:CG2	1:A:399:MET:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:143:GLY:C	1:D:146:PRO:HD2	2.40	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
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: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: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:148:ILE:HG23	1:A:399:MET:HE3	2.03	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:263:ILE:CG2	1:A:264:THR:N	2.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:419:LEU:N	1:C:419:LEU:HD12	2.37	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	413/438 (94%)	393 (95%)	18 (4%)	2 (0%)	29	67
1	B	405/438 (92%)	387 (96%)	17 (4%)	1 (0%)	47	79
1	C	409/438 (93%)	389 (95%)	18 (4%)	2 (0%)	29	67
1	D	407/438 (93%)	388 (95%)	17 (4%)	2 (0%)	29	67
All	All	1634/1752 (93%)	1557 (95%)	70 (4%)	7 (0%)	34	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	358	ILE
1	A	73	PRO
1	A	358	ILE
1	B	73	PRO
1	D	73	PRO
1	D	358	ILE
1	C	73	PRO

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	325/343 (95%)	325 (100%)	0	100 100
1	B	319/343 (93%)	318 (100%)	1 (0%)	92 97
1	C	322/343 (94%)	322 (100%)	0	100 100
1	D	321/343 (94%)	321 (100%)	0	100 100
All	All	1287/1372 (94%)	1286 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	180	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
1	B	265	HIS
1	B	362	ASN
1	C	101	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)

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	B	502	-	20,20,20	0.61	1 (5%)	25,25,25	0.92	1 (4%)
3	BOG	A	502	-	20,20,20	0.52	0	25,25,25	0.99	1 (4%)

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	B	502	-	-	3/11/31/31	0/1/1/1
3	BOG	A	502	-	-	6/11/31/31	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	2.17	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	BOG	C6-C5-C4	-2.23	107.78	113.00
3	B	502	BOG	C4-C3-C2	-2.00	107.33	110.82

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	A	502	BOG	O5-C1-O1-C1'
3	A	502	BOG	C3'-C4'-C5'-C6'

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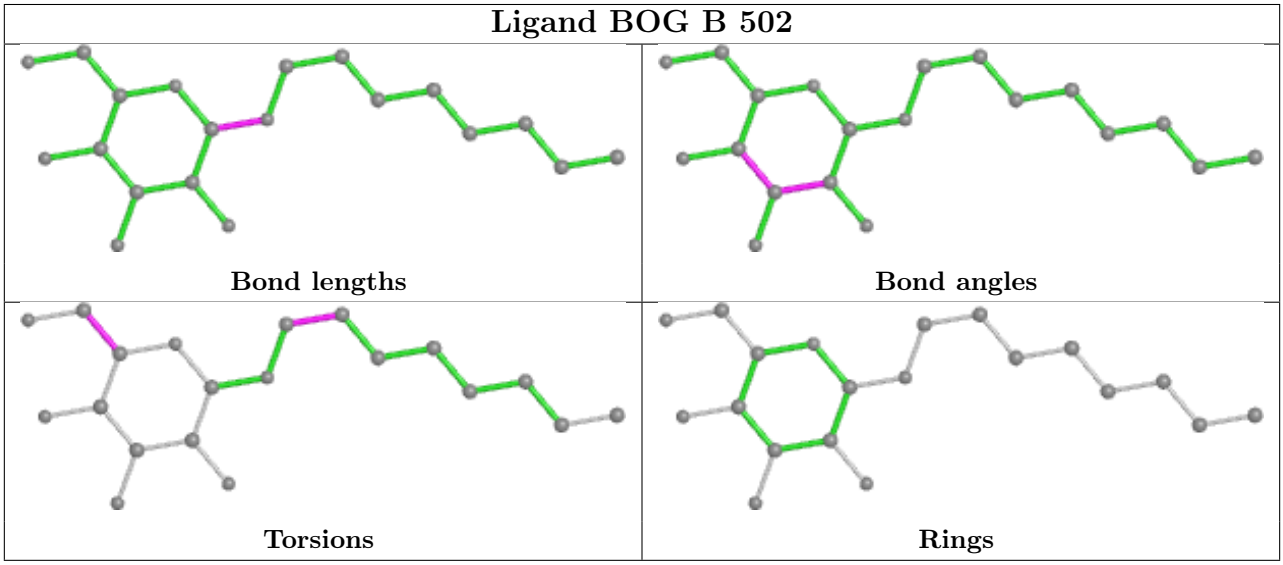
Mol	Chain	Res	Type	Atoms
3	B	502	BOG	O1-C1'-C2'-C3'
3	A	502	BOG	C5'-C6'-C7'-C8'
3	A	502	BOG	O5-C5-C6-O6

There are no ring outliers.

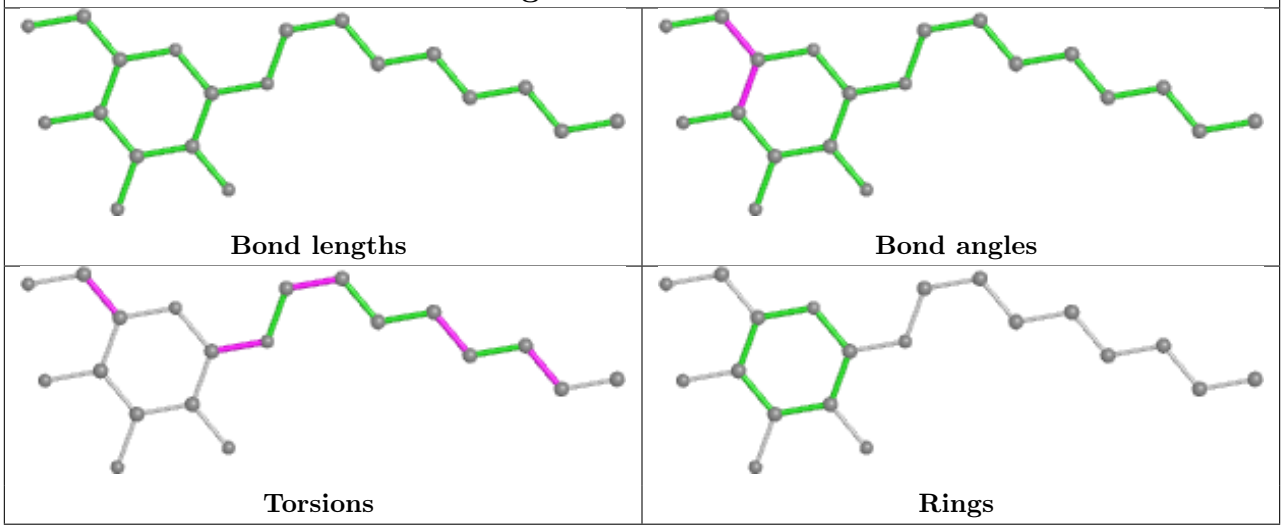
1 monomer is involved in 5 short contacts:

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand BOG A 502



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, 95^{th} 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%)	0.25	18 (4%)	35	23	117, 176, 227, 272	0
1	B	409/438 (93%)	0.32	33 (8%)	12	7	131, 187, 243, 280	0
1	C	413/438 (94%)	0.30	32 (7%)	13	8	124, 190, 245, 282	0
1	D	411/438 (93%)	0.30	30 (7%)	15	9	132, 197, 253, 296	0
All	All	1650/1752 (94%)	0.29	113 (6%)	17	10	117, 186, 245, 296	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	397	LEU	5.7
1	C	235	LYS	5.0
1	A	240	LEU	4.4
1	D	395	ALA	4.4
1	D	396	GLY	4.4
1	A	19	LEU	4.3
1	A	446	ILE	4.3
1	C	246	LEU	4.3
1	C	397	LEU	4.3
1	D	235	LYS	4.2
1	B	397	LEU	4.0
1	C	389	ILE	4.0
1	B	115	ASN	3.8
1	C	390	GLU	3.7
1	C	393	ILE	3.7
1	C	411	LEU	3.7
1	A	293	ILE	3.6
1	B	413	ALA	3.6
1	C	240	LEU	3.6
1	D	173	ILE	3.5
1	C	394	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	419	LEU	3.3
1	B	224	ILE	3.3
1	D	263	ILE	3.3
1	B	396	GLY	3.2
1	A	241	SER	3.2
1	B	414	CYS	3.2
1	D	239	TRP	3.2
1	D	392	ALA	3.2
1	A	244	GLY	3.2
1	C	386	PHE	3.1
1	D	420	ILE	3.0
1	B	426	SER	3.0
1	B	44	TYR	3.0
1	B	398	CYS	3.0
1	B	177	TYR	2.9
1	D	388	PRO	2.9
1	B	395	ALA	2.9
1	C	46	ALA	2.9
1	C	415	ASN	2.9
1	C	388	PRO	2.8
1	B	293	ILE	2.8
1	A	112	ASP	2.8
1	B	173	ILE	2.8
1	D	389	ILE	2.8
1	A	50	ASP	2.7
1	B	112	ASP	2.7
1	B	389	ILE	2.7
1	D	115	ASN	2.7
1	D	391	SER	2.7
1	B	317	CYS	2.7
1	B	178	VAL	2.7
1	A	109	ASN	2.7
1	B	388	PRO	2.7
1	C	245	GLU	2.7
1	B	394	THR	2.7
1	D	394	THR	2.7
1	D	238	THR	2.6
1	A	224	ILE	2.6
1	C	396	GLY	2.6
1	D	112	ASP	2.6
1	C	382	TRP	2.6
1	B	46	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	425	ILE	2.6
1	B	113	LYS	2.6
1	C	115	ASN	2.6
1	D	177	TYR	2.6
1	A	235	LYS	2.6
1	D	317	CYS	2.6
1	C	391	SER	2.6
1	B	227	ALA	2.5
1	B	118	ASN	2.5
1	C	143	GLY	2.5
1	B	393	ILE	2.5
1	D	387	PHE	2.5
1	D	113	LYS	2.5
1	D	316	LEU	2.4
1	C	19	LEU	2.4
1	C	416	ARG	2.4
1	A	238	THR	2.4
1	B	45	ASN	2.4
1	C	241	SER	2.4
1	C	417	MET	2.4
1	C	419	LEU	2.4
1	B	237	HIS	2.4
1	C	112	ASP	2.4
1	C	199	SER	2.3
1	C	410	VAL	2.3
1	B	387	PHE	2.3
1	B	415	ASN	2.3
1	A	71	ARG	2.3
1	A	21	PHE	2.3
1	D	142	LEU	2.3
1	A	445	MET	2.2
1	D	114	SER	2.2
1	A	234	GLY	2.2
1	B	235	LYS	2.2
1	A	284	VAL	2.2
1	D	349	THR	2.2
1	C	392	ALA	2.2
1	D	297	ALA	2.1
1	B	130	LEU	2.1
1	C	144	TYR	2.1
1	B	445	MET	2.1
1	C	238	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	131	SER	2.1
1	B	109	ASN	2.1
1	A	204	SER	2.0
1	C	44	TYR	2.0
1	D	390	GLU	2.0
1	D	176	LEU	2.0
1	C	30	LEU	2.0
1	D	19	LEU	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)

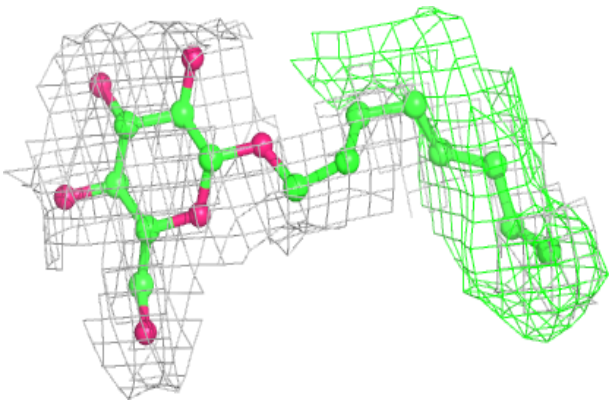
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

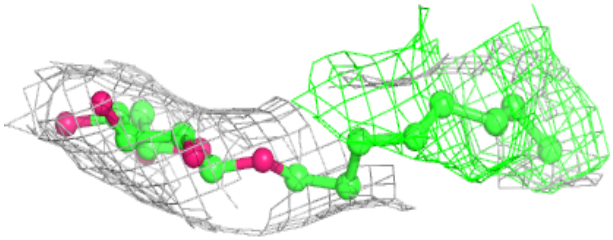
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BOG	A	502	20/20	0.64	0.26	213,241,270,270	0
3	BOG	B	502	20/20	0.66	0.51	141,213,250,254	0
2	NA	D	501	1/1	0.94	0.16	148,148,148,148	0
2	NA	B	501	1/1	0.96	0.10	228,228,228,228	0
2	NA	A	501	1/1	0.96	0.11	193,193,193,193	0
2	NA	C	501	1/1	0.98	0.08	205,205,205,205	0

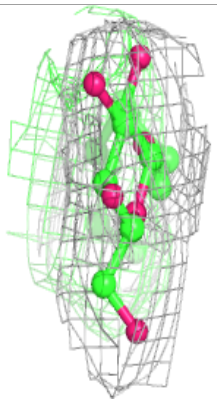
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 502:

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

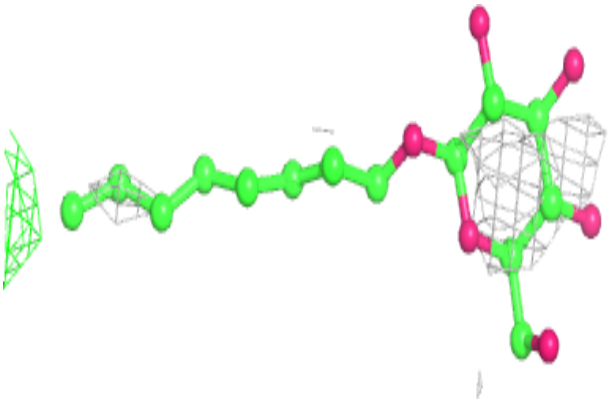


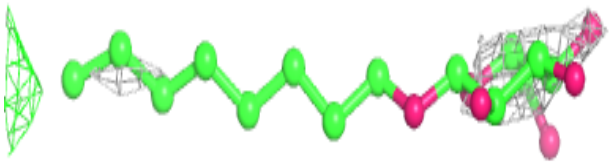


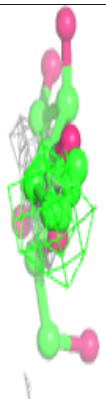


Electron density around BOG B 502:

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







6.5 Other polymers (i)

There are no such residues in this entry.