



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:26 am BST

PDB ID : 6EDS
Title : Structure of Cysteine-free Human Insulin-Degrading Enzyme in complex with
Glucagon and Substrate-selective Macrocyclic Inhibitor 63
Authors : Tan, G.A.; Seeliger, M.A.; Maianti, J.P.; Liu, D.R.; Welsh, A.J.
Deposited on : 2018-08-10
Resolution : 3.18 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 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 : 2.11
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) : 2.11

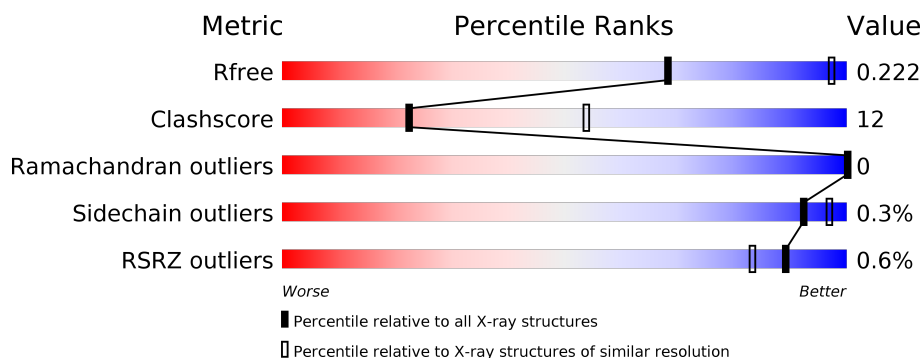
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 on 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	978	<div> <div style="width: 73%;"></div> <div style="width: 25%;"></div> <div style="width: 2%;"></div> </div>
1	B	978	<div> <div style="width: 73%;"></div> <div style="width: 25%;"></div> <div style="width: 2%;"></div> </div>
2	C	29	<div> <div style="width: 17%;"></div> <div style="width: 21%;"></div> <div style="width: 21%;"></div> <div style="width: 59%;"></div> </div>
2	D	29	<div> <div style="width: 24%;"></div> <div style="width: 17%;"></div> <div style="width: 59%;"></div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16064 atoms, of which 138 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	959	Total	C	N	O	S	0	0	0
			7798	5021	1310	1445	22			
1	B	959	Total	C	N	O	S	0	0	0
			7802	5024	1311	1445	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735

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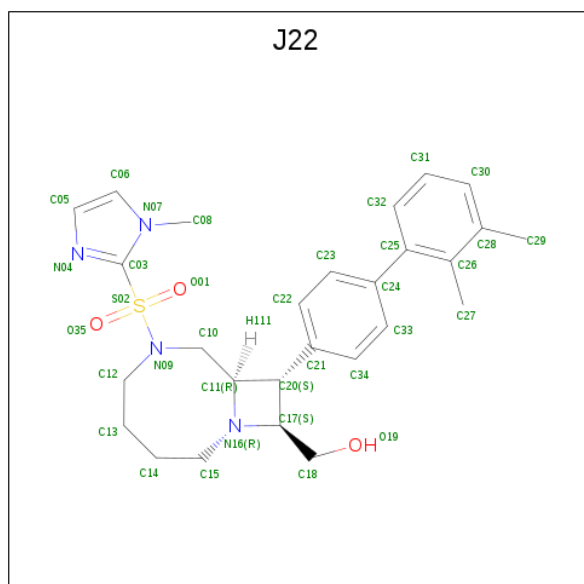
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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called Glucagon.

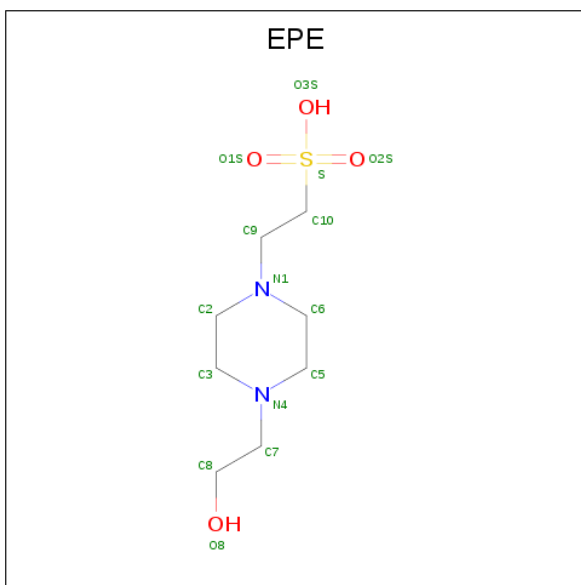
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	S	0	0	0
			100	65	17	17	1			
2	D	12	Total	C	N	O	S	0	0	0
			100	65	17	17	1			

- Molecule 3 is {(8R,9S,10S)-9-(2',3'-dimethyl[1,1'-biphenyl]-4-yl)-6-[(1-methyl-1H-imidazol-2-yl)sulfonyl]-1,6-diazabicyclo[6.2.0]decan-10-yl}methanol (three-letter code: J22) (formula: C₂₇H₃₄N₄O₃S) (labeled as "Ligand of Interest" by author).



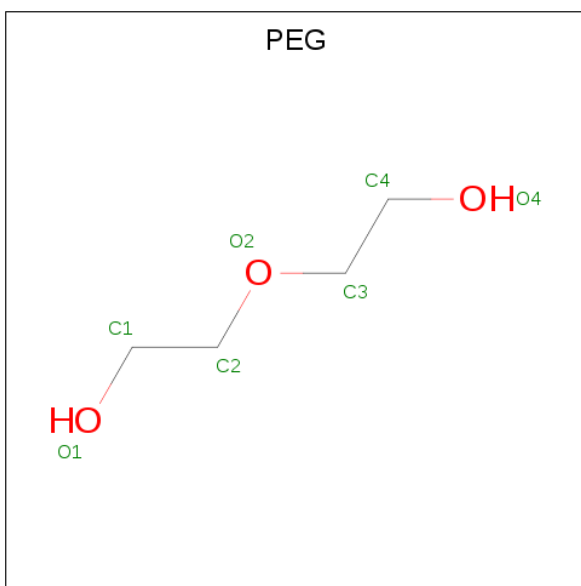
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			69	27	34	4	3		
3	B	1	Total	C	H	N	O	0	0
			69	27	34	4	3		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



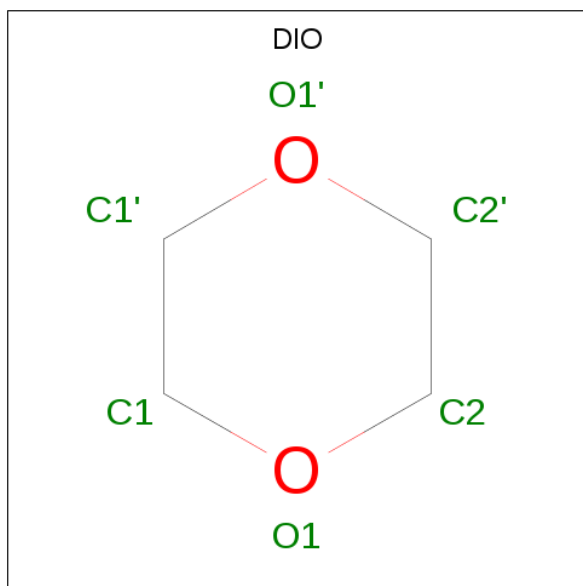
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
4	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).

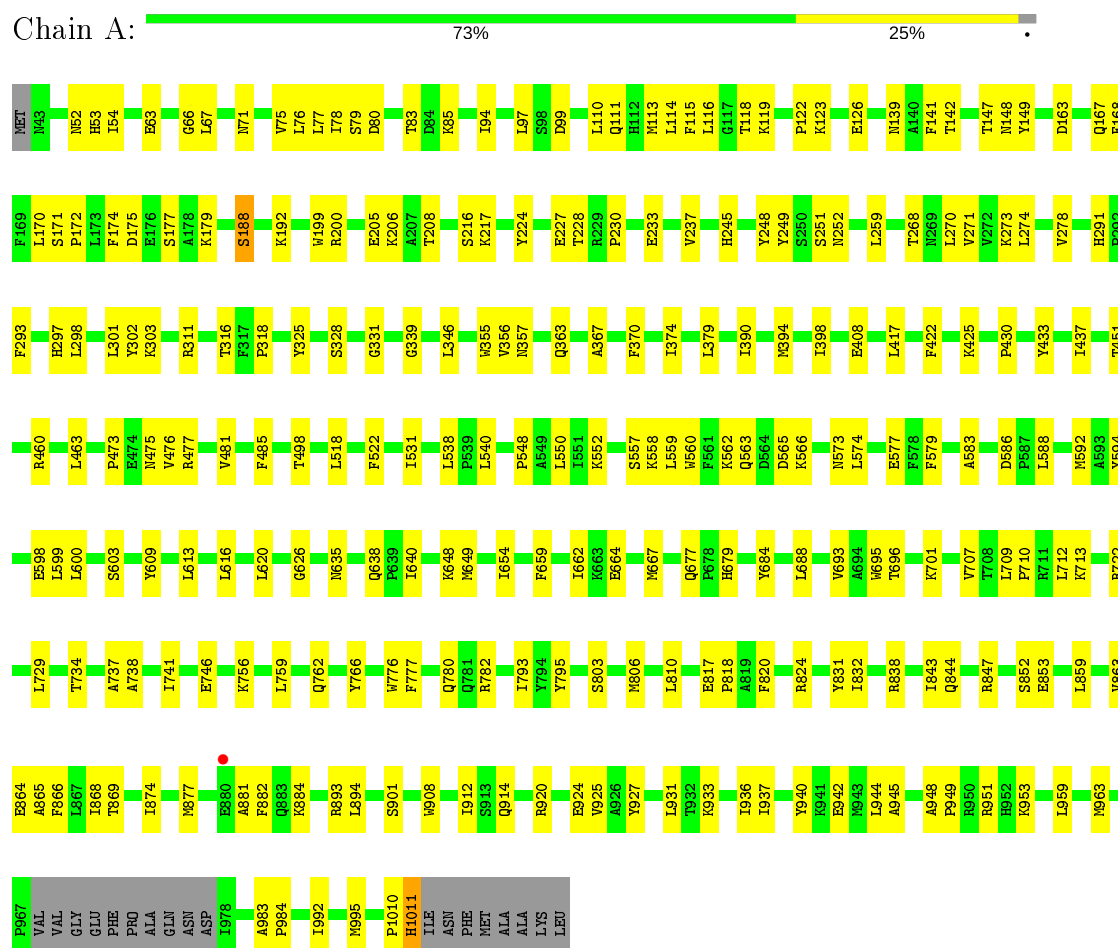


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	4	8	2		
6	B	1	Total	C	H	O	0	0
			14	4	8	2		

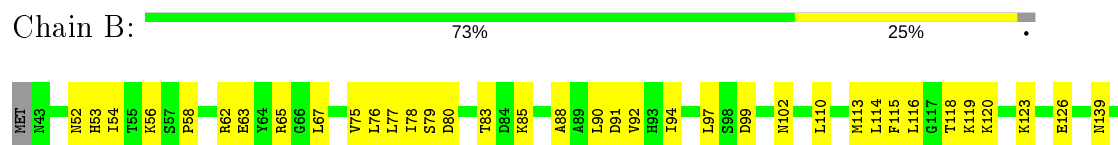
3 Residue-property plots

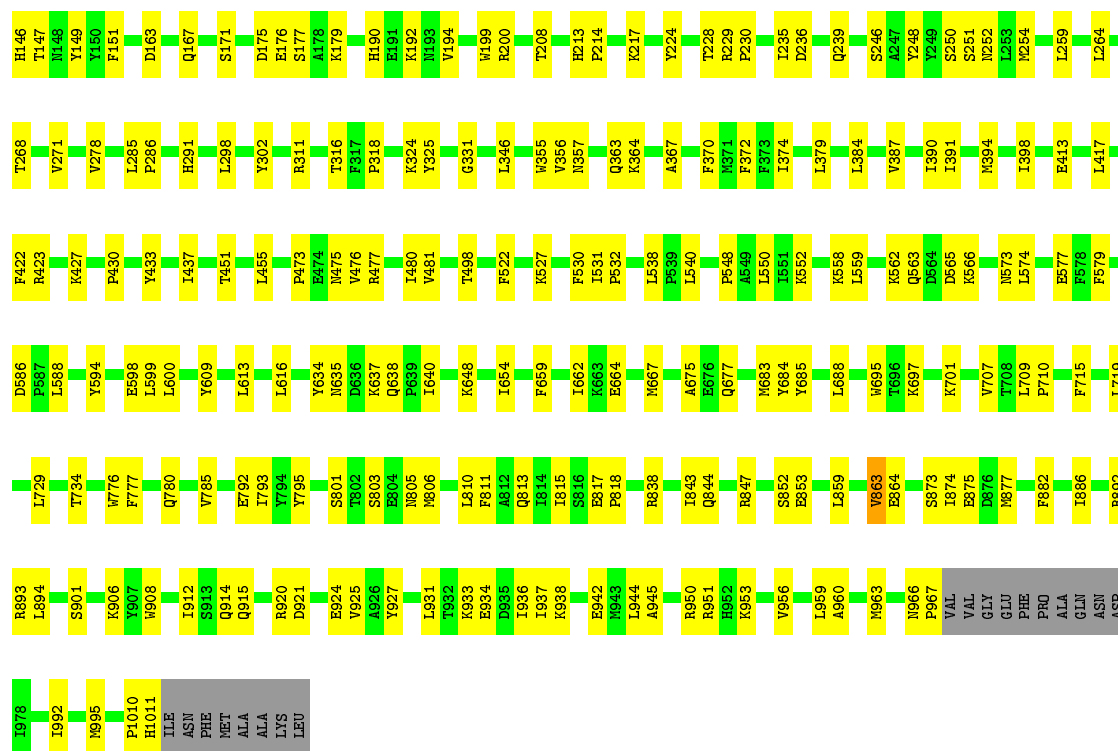
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

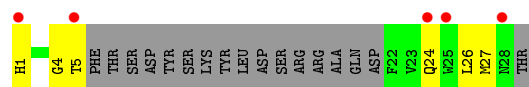


• Molecule 1: Insulin-degrading enzyme

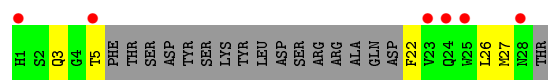




• Molecule 2: Glucagon



• Molecule 2: Glucagon



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.12Å 263.12Å 90.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	131.56 – 3.18 131.56 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (131.56-3.18) 94.2 (131.56-3.18)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.177 , 0.222 0.177 , 0.222	Depositor DCC
R_{free} test set	2869 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16064	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: EPE, PEG, DIO, J22

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	0.29	0/7994	0.46	0/10824
1	B	0.28	0/7998	0.44	0/10828
2	C	0.36	0/102	0.49	0/135
2	D	0.33	0/102	0.55	0/135
All	All	0.28	0/16196	0.45	0/21922

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	7798	0	7684	187	2
1	B	7802	0	7695	175	1
2	C	100	0	92	11	0
2	D	100	0	92	7	0
3	A	35	34	0	1	0
3	B	35	34	0	3	0
4	A	15	17	17	0	0
4	B	15	17	17	0	0
5	A	7	10	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	7	10	10	3	0
6	A	6	8	8	1	0
6	B	6	8	8	1	0
All	All	15926	138	15633	367	2

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 12.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:A:167:GLN:HB3	1.22	1.17
1:B:118:THR:HG21	1:B:167:GLN:HB3	1.24	1.16
1:B:944:LEU:O	1:B:951:ARG:NH1	1.97	0.96
1:A:113:MET:HE2	1:A:116:LEU:HD12	1.52	0.92
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.49	0.90
1:B:113:MET:HE2	1:B:116:LEU:HD12	1.54	0.89
1:B:78:ILE:HB	1:B:259:LEU:HD23	1.55	0.88
1:A:777:PHE:HB3	1:A:992:ILE:HD11	1.56	0.87
1:A:864:GLU:OE2	1:A:951:ARG:NH2	2.08	0.87
1:B:777:PHE:HB3	1:B:992:ILE:HD11	1.55	0.86
1:B:864:GLU:OE2	1:B:951:ARG:NH2	2.10	0.84
1:A:67:LEU:HD11	1:A:268:THR:HG23	1.63	0.81
1:B:76:LEU:HD23	1:B:437:ILE:HG21	1.60	0.81
1:B:118:THR:CG2	1:B:167:GLN:HB3	2.07	0.80
1:A:944:LEU:O	1:A:951:ARG:NH1	2.15	0.80
1:A:777:PHE:HB3	1:A:992:ILE:CD1	2.11	0.79
1:B:777:PHE:HB3	1:B:992:ILE:CD1	2.11	0.79
1:B:118:THR:HG21	1:B:167:GLN:CB	2.09	0.78
1:A:113:MET:CE	1:A:116:LEU:HD12	2.15	0.76
1:B:906:LYS:NZ	1:B:921:ASP:OD2	2.19	0.76
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.66	0.75
1:A:139:ASN:ND2	2:C:27:MET:HB2	2.01	0.75
1:A:877:MET:O	1:A:933:LYS:NZ	2.18	0.75
2:C:4:GLY:O	2:C:5:THR:HG23	1.87	0.74
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.21	0.74
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.69	0.74
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.23	0.73
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.24	0.73
1:B:78:ILE:CB	1:B:259:LEU:HD23	2.18	0.73
1:B:311:ARG:NH1	1:B:379:LEU:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:NH1	1:A:379:LEU:O	2.22	0.72
1:B:113:MET:CE	1:B:116:LEU:HD12	2.19	0.72
1:A:874:ILE:O	1:A:933:LYS:HE3	1.90	0.71
1:A:76:LEU:HD23	1:A:437:ILE:HG21	1.73	0.71
1:B:99:ASP:O	1:B:217:LYS:NZ	2.20	0.70
1:B:236:ASP:OD2	1:B:239:GLN:HG2	1.92	0.70
1:A:795:TYR:CE1	1:A:953:LYS:HD2	2.27	0.70
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.74	0.69
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.74	0.69
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.76	0.68
1:A:99:ASP:O	1:A:217:LYS:NZ	2.25	0.67
1:A:795:TYR:HE1	1:A:953:LYS:HD2	1.59	0.67
1:B:914:GLN:O	1:B:1010:PRO:HB3	1.94	0.67
2:C:26:LEU:HG	2:C:27:MET:HG3	1.76	0.67
1:B:324:LYS:HE3	1:B:325:TYR:CZ	2.30	0.67
1:B:78:ILE:CG2	1:B:259:LEU:HD23	2.24	0.67
1:B:139:ASN:ND2	2:D:27:MET:HB2	2.10	0.67
1:B:1010:PRO:O	1:B:1011:HIS:HB2	1.95	0.66
1:A:1010:PRO:O	1:A:1011:HIS:HB2	1.95	0.66
1:B:806:MET:HE3	1:B:893:ARG:HH12	1.61	0.65
1:A:328:SER:HB3	1:A:460:ARG:HG3	1.77	0.65
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.79	0.64
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.80	0.64
1:A:118:THR:HG21	1:A:167:GLN:CB	2.15	0.64
1:A:273:LYS:HG2	1:A:274:LEU:HD12	1.79	0.64
1:A:667:MET:SD	1:A:701:LYS:HG3	2.38	0.64
1:B:635:ASN:HD22	5:B:1102:PEG:H21	1.62	0.63
1:A:71:ASN:HB2	1:A:251:SER:OG	1.98	0.63
1:B:683:MET:HA	1:B:792:GLU:OE1	1.99	0.63
1:A:868:ILE:HD11	1:A:984:PRO:HG3	1.80	0.63
1:B:813:GLN:OE1	1:B:892:ARG:NH1	2.30	0.63
1:A:200:ARG:NH2	1:A:498:THR:HA	2.13	0.63
1:A:538:LEU:CD1	1:A:734:THR:HG23	2.28	0.63
1:A:80:ASP:O	1:A:83:THR:HG22	2.00	0.62
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.80	0.62
1:B:331:GLY:HA3	1:B:363:GLN:OE1	1.99	0.62
1:B:413:GLU:OE2	1:B:527:LYS:HD2	1.99	0.62
1:B:417:LEU:HD11	1:B:531:ILE:HG12	1.82	0.61
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.32	0.61
1:B:367:ALA:HB3	1:B:370:PHE:CE1	2.36	0.61
1:B:810:LEU:HD23	1:B:936:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:HG21	1:B:302:TYR:CZ	2.36	0.60
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.83	0.60
1:A:557:SER:OG	1:A:746:GLU:OE2	2.17	0.60
1:A:806:MET:HE3	1:A:893:ARG:HH12	1.67	0.60
1:A:270:LEU:HD12	1:A:274:LEU:HD13	1.83	0.60
1:A:859:LEU:O	1:A:863:VAL:HG12	2.02	0.59
1:A:119:LYS:HB2	1:A:171:SER:HB2	1.84	0.59
1:B:67:LEU:HB2	1:B:75:VAL:HB	1.84	0.59
1:B:119:LYS:HB2	1:B:171:SER:HB2	1.83	0.59
1:A:565:ASP:OD1	1:A:566:LYS:HG3	2.02	0.59
1:A:192:LYS:HG3	1:A:677:GLN:OE1	2.03	0.58
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.85	0.58
1:B:110:LEU:HD23	1:B:114:LEU:HD13	1.84	0.58
1:A:550:LEU:HD11	1:A:558:LYS:HG2	1.86	0.58
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.85	0.58
1:B:599:LEU:CD2	1:B:662:ILE:HD12	2.28	0.57
2:D:26:LEU:HG	2:D:27:MET:HG3	1.85	0.57
1:B:795:TYR:CE1	1:B:953:LYS:HD2	2.39	0.57
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.87	0.57
1:A:417:LEU:HD21	1:A:531:ILE:HG12	1.86	0.57
1:A:297:HIS:O	1:A:477:ARG:HD2	2.05	0.57
1:A:599:LEU:CD2	1:A:662:ILE:HD12	2.34	0.57
1:A:843:ILE:HG22	1:A:844:GLN:H	1.70	0.57
1:B:118:THR:HG22	1:B:120:LYS:H	1.70	0.56
1:B:77:LEU:HD21	1:B:271:VAL:HG21	1.86	0.56
1:A:110:LEU:HD23	1:A:114:LEU:HD13	1.87	0.56
1:B:175:ASP:OD2	1:B:177:SER:HB3	2.06	0.56
1:A:709:LEU:HD21	1:A:713:LYS:HE3	1.87	0.56
1:A:820:PHE:CZ	1:A:824:ARG:HD3	2.41	0.56
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.86	0.55
1:A:63:GLU:HB2	1:A:79:SER:HB3	1.87	0.55
1:B:838:ARG:O	1:B:844:GLN:HA	2.05	0.55
1:A:118:THR:HG22	1:A:119:LYS:N	2.21	0.55
1:A:868:ILE:HD11	1:A:984:PRO:CG	2.36	0.55
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.42	0.55
1:B:118:THR:HG22	1:B:119:LYS:N	2.22	0.55
1:B:451:THR:HB	1:B:455:LEU:HD12	1.89	0.55
1:A:908:TRP:O	1:A:912:ILE:HG12	2.07	0.55
1:B:934:GLU:OE2	1:B:938:LYS:HE3	2.07	0.55
1:B:776:TRP:HA	1:B:953:LYS:O	2.06	0.54
1:A:111:GLN:HE21	2:C:26:LEU:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:SER:O	1:B:877:MET:HB2	2.07	0.54
1:B:83:THR:OG1	1:B:85:LYS:O	2.25	0.54
1:B:859:LEU:O	1:B:863:VAL:HG12	2.08	0.54
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.43	0.54
1:A:114:LEU:HD23	1:A:168:PHE:HB3	1.89	0.54
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.90	0.54
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.43	0.54
1:A:729:LEU:HD12	1:A:738:ALA:HB1	1.90	0.54
1:B:56:LYS:NZ	1:B:62:ARG:O	2.38	0.54
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.43	0.53
1:B:250:SER:O	1:B:254:MET:HG3	2.09	0.53
1:B:588:LEU:HD12	1:B:707:VAL:HG22	1.90	0.53
1:A:245:HIS:O	1:A:249:TYR:HB2	2.09	0.53
1:B:540:LEU:HD12	1:B:563:GLN:CD	2.29	0.53
1:B:960:ALA:HB3	1:B:963:MET:HB2	1.89	0.53
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.44	0.53
1:A:635:ASN:HD22	5:A:1103:PEG:H21	1.74	0.53
1:A:139:ASN:HD21	2:C:27:MET:HB2	1.70	0.53
1:B:63:GLU:HB2	1:B:79:SER:HB3	1.89	0.53
1:B:190:HIS:O	1:B:194:VAL:HG23	2.08	0.53
1:B:433:TYR:CZ	1:B:437:ILE:HD11	2.43	0.53
1:A:616:LEU:CD1	1:A:638:GLN:HG3	2.39	0.53
1:A:205:GLU:HG2	1:A:293:PHE:HZ	1.74	0.53
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.44	0.53
1:A:374:ILE:HG21	3:A:1101:J22:O01	2.09	0.52
1:B:251:SER:HB3	1:B:278:VAL:HG12	1.90	0.52
1:A:433:TYR:CE2	1:A:437:ILE:HD11	2.44	0.52
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.90	0.52
1:B:192:LYS:HG3	1:B:677:GLN:OE1	2.10	0.52
1:B:67:LEU:HD11	1:B:268:THR:HG23	1.91	0.52
1:A:206:LYS:HB3	1:A:216:SER:HA	1.91	0.52
1:B:291:HIS:CE1	1:B:318:PRO:HB3	2.44	0.52
1:B:298:LEU:HD13	1:B:475:ASN:HA	1.90	0.52
1:B:538:LEU:CD1	1:B:734:THR:HG23	2.39	0.52
1:B:236:ASP:CG	1:B:239:GLN:HG2	2.30	0.52
1:B:374:ILE:HG21	3:B:1104:J22:O01	2.09	0.52
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.10	0.52
1:B:473:PRO:O	1:B:476:VAL:HG12	2.10	0.52
1:B:852:SER:HB3	1:B:859:LEU:HD11	1.91	0.52
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.91	0.52
1:A:550:LEU:HB2	1:A:560:TRP:CZ3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LEU:HD11	5:B:1102:PEG:H12	1.91	0.52
1:B:550:LEU:HD11	1:B:558:LYS:HG2	1.92	0.51
1:B:920:ARG:O	1:B:924:GLU:HG3	2.10	0.51
1:A:301:LEU:HD12	1:A:302:TYR:N	2.26	0.51
1:A:588:LEU:HD12	1:A:707:VAL:HG22	1.91	0.51
1:A:776:TRP:HA	1:A:953:LYS:O	2.10	0.51
1:A:793:ILE:HD12	1:A:863:VAL:HG11	1.91	0.51
1:A:115:PHE:CE1	2:C:26:LEU:HD22	2.45	0.51
1:B:387:VAL:HG11	1:B:480:ILE:HD11	1.92	0.51
1:B:213:HIS:ND1	1:B:214:PRO:HD2	2.26	0.51
1:A:367:ALA:HB3	1:A:370:PHE:CE1	2.46	0.51
1:A:693:VAL:HB	1:A:766:TYR:CE1	2.46	0.51
1:B:208:THR:O	1:B:208:THR:HG22	2.10	0.51
1:B:795:TYR:HE1	1:B:953:LYS:HD2	1.76	0.51
1:A:709:LEU:HD21	1:A:713:LYS:CE	2.40	0.50
1:B:538:LEU:HD11	5:B:1102:PEG:C1	2.41	0.50
1:A:927:TYR:CE2	1:A:931:LEU:HD11	2.46	0.50
1:B:163:ASP:O	1:B:167:GLN:HG2	2.11	0.50
1:B:942:GLU:OE1	1:B:950:ARG:HD3	2.11	0.50
1:B:65:ARG:HB3	1:B:264:LEU:HD22	1.93	0.50
1:A:83:THR:OG1	1:A:85:LYS:O	2.29	0.50
1:B:1010:PRO:O	1:B:1011:HIS:CB	2.58	0.50
1:B:616:LEU:HD11	1:B:638:GLN:HG2	1.94	0.50
1:A:115:PHE:CZ	2:C:26:LEU:HD22	2.46	0.50
1:B:843:ILE:HG22	1:B:844:GLN:H	1.75	0.50
1:A:793:ILE:O	1:A:847:ARG:HA	2.12	0.50
1:A:355:TRP:HB3	1:A:390:ILE:HD11	1.94	0.49
1:B:97:LEU:CD1	1:B:367:ALA:HB2	2.42	0.49
1:B:531:ILE:O	1:B:637:LYS:HE3	2.12	0.49
1:B:565:ASP:OD1	1:B:566:LYS:HG3	2.13	0.49
1:B:58:PRO:HG2	1:B:423:ARG:HG3	1.94	0.49
1:A:1010:PRO:O	1:A:1011:HIS:CB	2.60	0.49
1:B:80:ASP:O	1:B:83:THR:HG22	2.13	0.49
1:B:139:ASN:HD21	2:D:27:MET:HB2	1.77	0.49
1:A:175:ASP:OD2	1:A:177:SER:HB3	2.12	0.49
1:B:200:ARG:NH2	1:B:498:THR:HA	2.28	0.49
1:A:433:TYR:CZ	1:A:437:ILE:HD11	2.48	0.48
1:B:259:LEU:HD12	1:B:430:PRO:HB3	1.94	0.48
1:A:594:TYR:CE2	1:A:598:GLU:HG3	2.48	0.48
1:B:311:ARG:HA	1:B:481:VAL:O	2.13	0.48
1:B:675:ALA:HA	1:B:785:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASP:OD2	1:B:427:LYS:NZ	2.34	0.48
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.44	0.48
1:B:118:THR:CG2	1:B:119:LYS:N	2.77	0.48
1:B:355:TRP:HB3	1:B:390:ILE:HD11	1.96	0.48
1:B:433:TYR:CE2	1:B:437:ILE:HD11	2.48	0.48
1:A:356:VAL:HG12	1:A:357:ASN:N	2.28	0.47
1:B:311:ARG:HD3	1:B:384:LEU:HD22	1.94	0.47
1:A:654:ILE:HD13	1:A:712:LEU:HD23	1.96	0.47
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.48	0.47
1:A:942:GLU:HA	1:A:949:PRO:HD2	1.97	0.47
1:A:111:GLN:NE2	2:C:26:LEU:HB2	2.28	0.47
1:A:540:LEU:HD12	1:A:563:GLN:CD	2.34	0.47
1:A:298:LEU:HD13	1:A:475:ASN:HA	1.96	0.47
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.97	0.47
1:B:90:LEU:HD23	1:B:91:ASP:N	2.29	0.47
1:A:301:LEU:HD12	1:A:302:TYR:H	1.79	0.47
1:A:52:ASN:O	1:A:53:HIS:C	2.53	0.47
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.97	0.47
1:B:538:LEU:HD12	1:B:734:THR:HG23	1.97	0.47
1:B:877:MET:HE1	1:B:882:PHE:HD2	1.80	0.47
1:A:573:ASN:HD21	1:A:901:SER:HA	1.79	0.47
1:A:780:GLN:NE2	1:A:959:LEU:HD11	2.29	0.47
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.50	0.47
1:B:793:ILE:O	1:B:847:ARG:HA	2.15	0.47
1:B:811:PHE:CE2	1:B:815:ILE:HD13	2.49	0.47
1:A:339:GLY:O	2:C:1:HIS:N	2.45	0.47
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.97	0.47
1:A:118:THR:CG2	1:A:119:LYS:N	2.78	0.46
1:A:270:LEU:HD12	1:A:274:LEU:CD1	2.44	0.46
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.96	0.46
1:A:866:PHE:O	1:A:869:THR:HB	2.16	0.46
1:B:208:THR:HG22	1:B:477:ARG:HH12	1.80	0.46
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.47	0.46
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.97	0.46
1:A:273:LYS:CG	1:A:274:LEU:HD12	2.45	0.46
1:B:688:LEU:HD13	1:B:995:MET:HE1	1.97	0.46
1:A:843:ILE:HG22	1:A:844:GLN:N	2.28	0.46
1:A:914:GLN:O	1:A:1010:PRO:HB3	2.14	0.46
1:B:110:LEU:HD23	1:B:110:LEU:O	2.15	0.46
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.97	0.46
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.51	0.46
1:A:920:ARG:O	1:A:924:GLU:HG3	2.16	0.46
1:B:945:ALA:O	1:B:951:ARG:HD2	2.16	0.46
1:A:473:PRO:O	1:A:476:VAL:HG12	2.16	0.46
1:A:722:ARG:HA	1:A:756:LYS:O	2.15	0.46
1:A:325:TYR:HB3	1:A:328:SER:OG	2.16	0.46
1:A:538:LEU:HD13	1:A:734:THR:CG2	2.44	0.46
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.98	0.46
1:B:316:THR:HG23	1:B:374:ILE:HG12	1.99	0.45
1:A:208:THR:CG2	1:A:302:TYR:CZ	3.00	0.45
1:A:609:TYR:CE2	1:A:613:LEU:HD11	2.51	0.45
1:B:176:GLU:OE2	1:B:179:LYS:HE2	2.16	0.45
1:B:67:LEU:HD11	1:B:77:LEU:HD11	1.98	0.45
1:A:54:ILE:HD11	1:A:66:GLY:N	2.31	0.45
1:B:573:ASN:HD21	1:B:901:SER:HA	1.81	0.45
1:A:227:GLU:C	1:A:230:PRO:HD2	2.37	0.45
1:B:364:LYS:HB3	1:B:372:PHE:HB2	1.97	0.45
1:B:859:LEU:O	1:B:863:VAL:CG1	2.65	0.45
1:A:111:GLN:OE1	1:A:142:THR:OG1	2.31	0.45
1:A:141:PHE:CE2	1:A:148:ASN:HB3	2.52	0.45
1:A:688:LEU:HB3	1:A:995:MET:HE1	1.98	0.45
1:B:115:PHE:CE1	2:D:26:LEU:HD22	2.52	0.45
1:A:640:ILE:HD13	6:A:1104:DIO:H21	1.98	0.45
1:A:311:ARG:HA	1:A:481:VAL:O	2.17	0.45
1:B:356:VAL:HG12	1:B:357:ASN:N	2.31	0.45
1:A:820:PHE:CE1	1:A:824:ARG:HD3	2.52	0.45
1:B:224:TYR:HA	1:B:228:THR:HB	1.98	0.45
1:B:573:ASN:ND2	1:B:901:SER:HA	2.32	0.45
1:A:77:LEU:HD21	1:A:271:VAL:HG21	1.98	0.44
1:A:803:SER:HA	1:A:927:TYR:CE2	2.51	0.44
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.52	0.44
1:A:224:TYR:HA	1:A:228:THR:HB	1.99	0.44
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.53	0.44
1:B:685:TYR:HB2	1:B:956:VAL:HG11	2.00	0.44
1:A:425:LYS:HE2	1:A:425:LYS:HB3	1.71	0.44
1:A:838:ARG:O	1:A:844:GLN:HA	2.18	0.44
1:B:391:ILE:O	1:B:394:MET:HB2	2.17	0.44
1:B:667:MET:SD	1:B:701:LYS:HG3	2.58	0.44
1:A:259:LEU:HD22	1:A:430:PRO:HB3	2.00	0.44
1:A:868:ILE:HD12	1:A:984:PRO:HD3	2.00	0.44
1:B:346:LEU:HA	1:B:522:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:LEU:HB3	1:B:995:MET:CE	2.48	0.44
1:A:118:THR:CG2	1:A:167:GLN:HB3	2.16	0.44
1:A:251:SER:HB3	1:A:278:VAL:HG12	1.99	0.44
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.78	0.44
1:A:67:LEU:CD1	1:A:268:THR:HG23	2.43	0.44
1:A:75:VAL:HG11	1:A:271:VAL:HG11	2.00	0.44
1:A:303:LYS:HB3	1:A:485:PHE:CD2	2.53	0.44
1:B:102:ASN:HD22	1:B:235:ILE:HD11	1.83	0.44
1:B:285:LEU:HD12	1:B:286:PRO:CD	2.48	0.44
1:A:868:ILE:CD1	1:A:984:PRO:HD3	2.48	0.44
1:B:882:PHE:CE2	1:B:933:LYS:HA	2.53	0.44
1:A:122:PRO:HG3	1:B:527:LYS:HE2	2.00	0.43
1:A:679:HIS:CE1	1:A:832:ILE:HD13	2.54	0.43
1:B:843:ILE:HG22	1:B:844:GLN:N	2.33	0.43
1:B:852:SER:OG	1:B:853:GLU:N	2.51	0.43
1:A:577:GLU:HG2	1:A:579:PHE:CZ	2.52	0.43
1:A:852:SER:HB3	1:A:859:LEU:HD11	1.98	0.43
1:B:894:LEU:HD11	1:B:925:VAL:HG11	2.00	0.43
1:A:810:LEU:HD23	1:A:936:ILE:HD11	2.00	0.43
1:B:709:LEU:HB3	1:B:710:PRO:HD3	2.00	0.43
1:A:328:SER:HB2	1:A:460:ARG:HB2	2.01	0.43
1:B:780:GLN:OE1	1:B:959:LEU:HD11	2.18	0.43
1:A:188:SER:HB3	1:A:831:TYR:HB2	2.01	0.43
1:B:422:PHE:CZ	1:B:451:THR:HG22	2.54	0.43
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.54	0.43
1:B:801:SER:O	1:B:805:ASN:HB2	2.18	0.43
1:B:882:PHE:CE1	1:B:886:ILE:HD11	2.53	0.43
1:A:600:LEU:HD23	1:A:620:LEU:HD21	2.00	0.42
1:A:78:ILE:O	1:A:259:LEU:HA	2.18	0.42
1:A:688:LEU:HB3	1:A:995:MET:CE	2.49	0.42
1:B:875:GLU:HG3	1:B:937:ILE:HD13	2.00	0.42
1:A:311:ARG:O	1:A:379:LEU:N	2.51	0.42
1:A:346:LEU:HA	1:A:522:PHE:CE1	2.55	0.42
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.19	0.42
2:C:4:GLY:O	2:C:5:THR:CG2	2.64	0.42
1:B:92:VAL:O	1:B:146:HIS:HA	2.19	0.42
1:B:577:GLU:HG2	1:B:579:PHE:CZ	2.54	0.42
1:B:640:ILE:HG21	6:B:1103:DIO:H2'2	2.01	0.42
1:A:208:THR:HG21	1:A:302:TYR:CZ	2.55	0.42
1:A:328:SER:HB3	1:A:460:ARG:CG	2.47	0.42
1:A:948:ALA:HB3	1:A:951:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1104:J22:C08	2:D:3:GLN:HB3	2.50	0.42
1:A:737:ALA:O	1:A:741:ILE:HG12	2.20	0.42
1:B:52:ASN:O	1:B:53:HIS:C	2.56	0.42
1:A:460:ARG:CB	1:A:463:LEU:HD12	2.50	0.42
1:A:603:SER:OG	1:A:648:LYS:HE2	2.20	0.42
1:A:874:ILE:HG22	1:A:937:ILE:HD11	2.02	0.42
1:B:110:LEU:HD23	1:B:110:LEU:C	2.40	0.42
1:B:530:PHE:HA	1:B:637:LYS:HD3	2.02	0.42
1:B:54:ILE:HD12	1:B:76:LEU:CD1	2.50	0.42
1:A:518:LEU:HA	1:A:518:LEU:HD23	1.85	0.42
1:B:588:LEU:CD1	1:B:707:VAL:HG22	2.48	0.42
1:B:908:TRP:O	1:B:912:ILE:HG12	2.20	0.42
1:A:274:LEU:HD12	1:A:274:LEU:N	2.35	0.42
1:A:852:SER:OG	1:A:853:GLU:N	2.52	0.42
1:A:865:ALA:HB2	1:A:983:ALA:HA	2.02	0.42
1:B:715:PHE:CZ	1:B:719:LEU:HD22	2.54	0.42
1:B:915:GLN:OE1	1:B:920:ARG:NH2	2.50	0.41
1:A:199:TRP:HH2	2:C:24:GLN:HG3	1.86	0.41
1:A:940:TYR:CE2	1:A:945:ALA:HB2	2.55	0.41
1:B:594:TYR:CE2	1:B:598:GLU:HG3	2.56	0.41
1:B:609:TYR:CE2	1:B:613:LEU:HD11	2.55	0.41
1:A:208:THR:HG22	1:A:477:ARG:HH12	1.85	0.41
1:A:600:LEU:CD2	1:A:649:MET:HG2	2.49	0.41
1:A:600:LEU:HD11	1:A:648:LYS:HB3	2.01	0.41
1:A:782:ARG:NH1	1:A:963:MET:O	2.30	0.41
1:B:538:LEU:HD13	1:B:734:THR:HG23	2.03	0.41
1:A:259:LEU:HD23	1:A:259:LEU:C	2.41	0.41
1:A:394:MET:O	1:A:398:ILE:HG13	2.20	0.41
1:B:803:SER:HA	1:B:927:TYR:CE2	2.56	0.41
1:B:394:MET:O	1:B:398:ILE:HG13	2.21	0.41
1:A:548:PRO:HA	1:A:562:LYS:HB2	2.02	0.41
1:A:894:LEU:HG	1:A:925:VAL:HG21	2.03	0.41
1:B:966:ASN:HA	1:B:967:PRO:HD3	1.70	0.41
1:A:163:ASP:O	1:A:167:GLN:HG2	2.20	0.41
3:B:1104:J22:C05	2:D:5:THR:HG21	2.50	0.41
1:A:188:SER:HB3	1:A:831:TYR:CB	2.51	0.41
1:A:881:ALA:HA	1:A:884:LYS:HB2	2.02	0.41
1:A:877:MET:HE1	1:A:882:PHE:HD2	1.86	0.41
1:B:874:ILE:HG22	1:B:937:ILE:HD11	2.02	0.41
1:A:592:MET:HE3	1:A:592:MET:HB2	1.92	0.40
1:A:599:LEU:HD21	1:A:659:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:CG2	1:B:302:TYR:CZ	3.03	0.40
1:A:170:LEU:HD21	1:A:278:VAL:HG22	2.03	0.40
1:B:548:PRO:HA	1:B:562:LYS:HB2	2.04	0.40
1:B:199:TRP:CH2	2:D:22:PHE:HB2	2.56	0.40
1:B:76:LEU:CD2	1:B:437:ILE:HG21	2.42	0.40
1:A:573:ASN:ND2	1:A:901:SER:HA	2.37	0.40
1:B:599:LEU:HD13	1:B:654:ILE:HG23	2.04	0.40
1:A:316:THR:HG23	1:A:374:ILE:CD1	2.52	0.40
1:A:97:LEU:CD1	1:A:367:ALA:HB2	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE2	1:B:246:SER:OG[1_554]	2.08	0.12
1:A:408:GLU:OE2	1:A:734:THR:OG1[2_544]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	955/978 (98%)	925 (97%)	30 (3%)	0	100	100
1	B	955/978 (98%)	922 (96%)	33 (4%)	0	100	100
2	C	8/29 (28%)	8 (100%)	0	0	100	100
2	D	8/29 (28%)	8 (100%)	0	0	100	100
All	All	1926/2014 (96%)	1863 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	842/870 (97%)	839 (100%)	3 (0%)	91	96
1	B	843/870 (97%)	841 (100%)	2 (0%)	93	98
2	C	10/27 (37%)	10 (100%)	0	100	100
2	D	10/27 (37%)	10 (100%)	0	100	100
All	All	1705/1794 (95%)	1700 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	SER
1	A	252	ASN
1	A	1011	HIS
1	B	252	ASN
1	B	863	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	HIS
1	B	134	HIS
1	B	157	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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
5	PEG	B	1102	-	6,6,6	0.48	0	5,5,5	0.24	0
6	DIO	A	1104	-	6,6,6	0.66	0	6,6,6	0.48	0
5	PEG	A	1103	-	6,6,6	0.49	0	5,5,5	0.44	0
4	EPE	A	1102	-	15,15,15	1.02	1 (6%)	18,20,20	1.94	5 (27%)
3	J22	A	1101	-	33,39,39	1.49	5 (15%)	39,58,58	2.33	7 (17%)
6	DIO	B	1103	-	6,6,6	0.65	0	6,6,6	0.47	0
3	J22	B	1104	-	33,39,39	1.44	5 (15%)	39,58,58	2.25	9 (23%)
4	EPE	B	1101	-	15,15,15	0.90	1 (6%)	18,20,20	1.82	5 (27%)

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	PEG	B	1102	-	-	1/4/4/4	-
6	DIO	A	1104	-	-	-	0/1/1/1
5	PEG	A	1103	-	-	4/4/4/4	-
4	EPE	A	1102	-	-	3/9/19/19	0/1/1/1
3	J22	A	1101	-	-	9/16/49/49	0/4/5/5
6	DIO	B	1103	-	-	-	0/1/1/1
3	J22	B	1104	-	-	7/16/49/49	0/4/5/5
4	EPE	B	1101	-	-	3/9/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	EPE	C10-S	3.62	1.82	1.77
3	B	1104	J22	C25-C24	-3.29	1.43	1.49
4	B	1101	EPE	C10-S	3.18	1.82	1.77
3	A	1101	J22	C25-C24	-3.14	1.43	1.49
3	A	1101	J22	C10-N09	2.96	1.51	1.48
3	B	1104	J22	O01-S02	2.55	1.46	1.43
3	A	1101	J22	O01-S02	2.52	1.46	1.43
3	B	1104	J22	C34-C33	2.16	1.42	1.38
3	B	1104	J22	C13-C12	2.14	1.57	1.52
3	A	1101	J22	C13-C12	2.03	1.56	1.52
3	B	1104	J22	C10-N09	2.02	1.50	1.48
3	A	1101	J22	C34-C33	2.01	1.42	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	J22	O35-S02-O01	-9.71	103.78	119.52
3	B	1104	J22	O35-S02-O01	-9.34	104.39	119.52
3	A	1101	J22	O35-S02-N09	5.91	112.08	106.69
3	B	1104	J22	O35-S02-N09	5.76	111.94	106.69
3	A	1101	J22	O01-S02-N09	5.72	111.90	106.69
3	B	1104	J22	O01-S02-N09	5.21	111.44	106.69
4	B	1101	EPE	C5-N4-C3	4.92	119.89	108.83
4	A	1102	EPE	C7-N4-C5	4.24	122.09	111.23
4	A	1102	EPE	O1S-S-C10	3.55	111.19	106.92
4	A	1102	EPE	C5-N4-C3	3.39	116.45	108.83
3	A	1101	J22	C10-N09-S02	2.88	122.90	117.70
4	A	1102	EPE	C7-N4-C3	2.76	118.28	111.23
4	B	1101	EPE	O2S-S-C10	2.57	110.01	106.92
3	B	1104	J22	C33-C24-C25	2.57	125.08	120.91
3	B	1104	J22	C12-N09-S02	2.53	120.72	116.29
3	A	1101	J22	C12-N09-S02	2.49	120.65	116.29
3	A	1101	J22	O19-C18-C17	-2.47	106.11	111.42
4	B	1101	EPE	O3S-S-C10	2.46	109.75	105.77
4	A	1102	EPE	O3S-S-C10	2.34	109.55	105.77
4	B	1101	EPE	C7-N4-C5	2.29	117.09	111.23
4	B	1101	EPE	C7-N4-C3	2.26	117.01	111.23
3	B	1104	J22	O19-C18-C17	-2.20	106.70	111.42
3	B	1104	J22	C10-N09-S02	2.10	121.49	117.70
3	B	1104	J22	C23-C24-C25	-2.03	117.62	120.91
3	A	1101	J22	C33-C24-C25	2.03	124.20	120.91
3	B	1104	J22	C13-C14-C15	-2.02	111.44	115.69

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	EPE	C10-C9-N1-C2
3	A	1101	J22	N16-C17-C18-O19
3	A	1101	J22	C12-N09-S02-O01
3	B	1104	J22	N16-C17-C18-O19
5	B	1102	PEG	O2-C3-C4-O4
3	B	1104	J22	C10-N09-S02-O01
3	B	1104	J22	C12-N09-S02-O01
4	A	1102	EPE	C8-C7-N4-C5
5	A	1103	PEG	O2-C3-C4-O4
4	B	1101	EPE	C10-C9-N1-C6
3	B	1104	J22	C12-N09-S02-C03
4	A	1102	EPE	N4-C7-C8-O8
5	A	1103	PEG	C1-C2-O2-C3
3	B	1104	J22	C20-C17-C18-O19
3	A	1101	J22	C10-N09-S02-O01
5	A	1103	PEG	O1-C1-C2-O2
5	A	1103	PEG	C4-C3-O2-C2
3	B	1104	J22	C12-N09-S02-O35
3	A	1101	J22	C23-C24-C25-C26
4	B	1101	EPE	C10-C9-N1-C2
3	A	1101	J22	C33-C24-C25-C26
4	B	1101	EPE	C8-C7-N4-C3
3	B	1104	J22	C10-N09-S02-C03
3	A	1101	J22	C23-C24-C25-C32
3	A	1101	J22	C33-C24-C25-C32
3	A	1101	J22	C20-C17-C18-O19
3	A	1101	J22	C12-N09-S02-C03

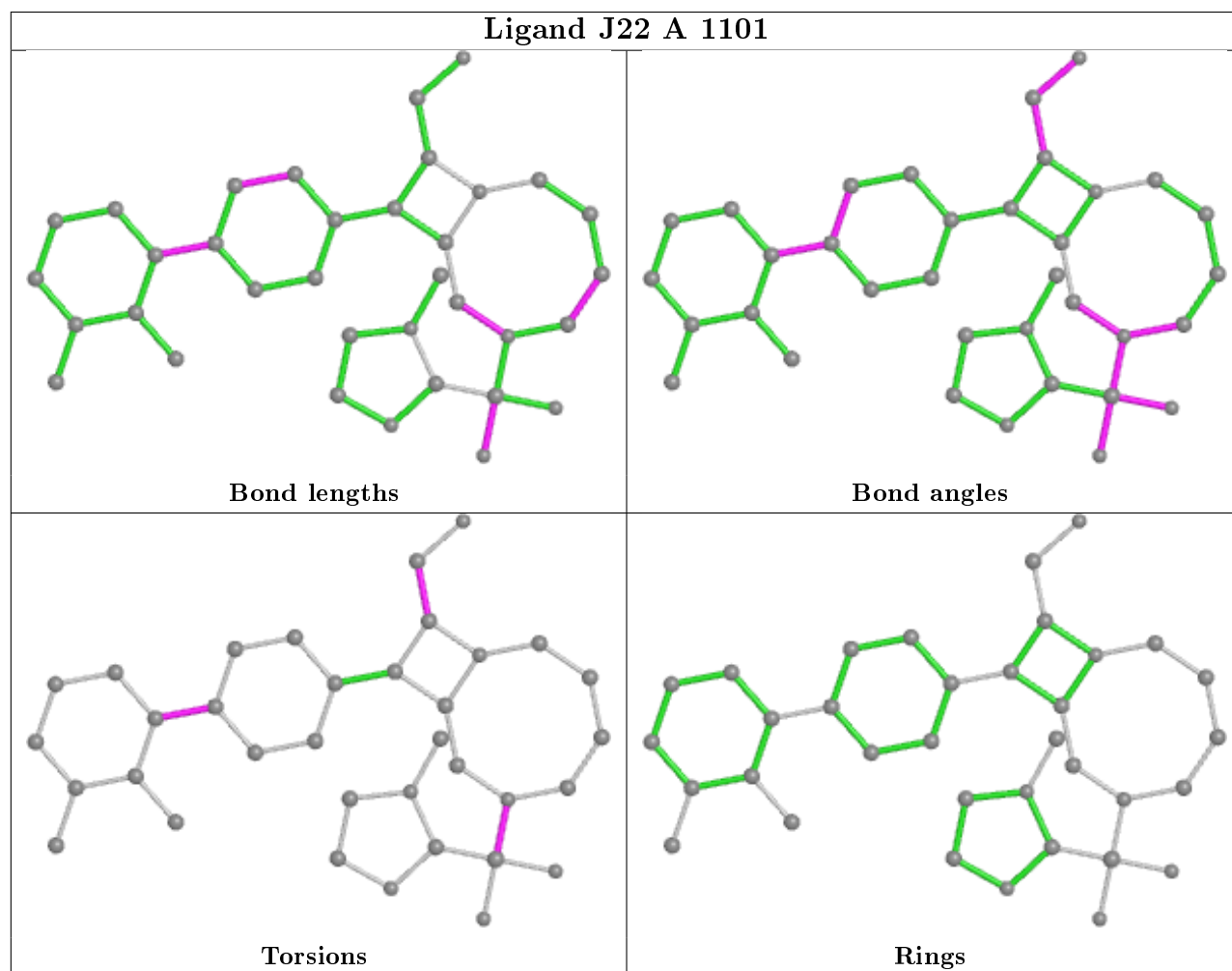
There are no ring outliers.

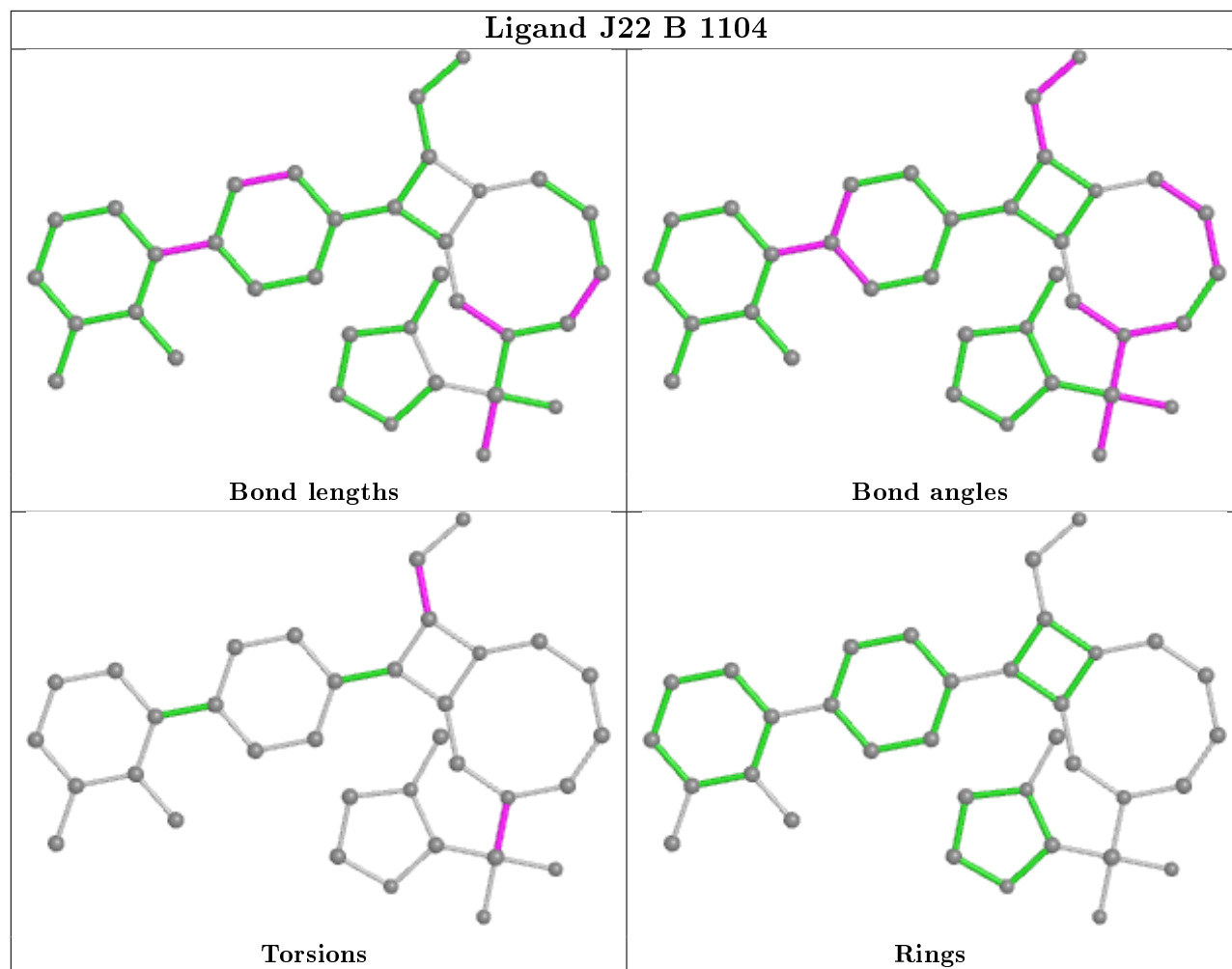
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	PEG	3	0
6	A	1104	DIO	1	0
5	A	1103	PEG	1	0
3	A	1101	J22	1	0
6	B	1103	DIO	1	0
3	B	1104	J22	3	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, 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	959/978 (98%)	-0.19	1 (0%) 95 95	21, 41, 67, 110	0
1	B	959/978 (98%)	0.05	0 100 100	29, 55, 79, 136	0
2	C	12/29 (41%)	1.75	5 (41%) 0 0	63, 95, 116, 118	0
2	D	12/29 (41%)	2.14	6 (50%) 0 0	73, 112, 134, 155	0
All	All	1942/2014 (96%)	-0.04	12 (0%) 89 83	21, 48, 78, 155	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	24	GLN	4.1
2	D	25	TRP	3.4
2	D	28	ASN	3.0
2	C	25	TRP	2.8
2	D	1	HIS	2.8
2	D	5	THR	2.7
2	C	24	GLN	2.7
2	C	1	HIS	2.6
2	C	28	ASN	2.6
2	D	23	VAL	2.6
2	C	5	THR	2.4
1	A	880	GLU	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](#)

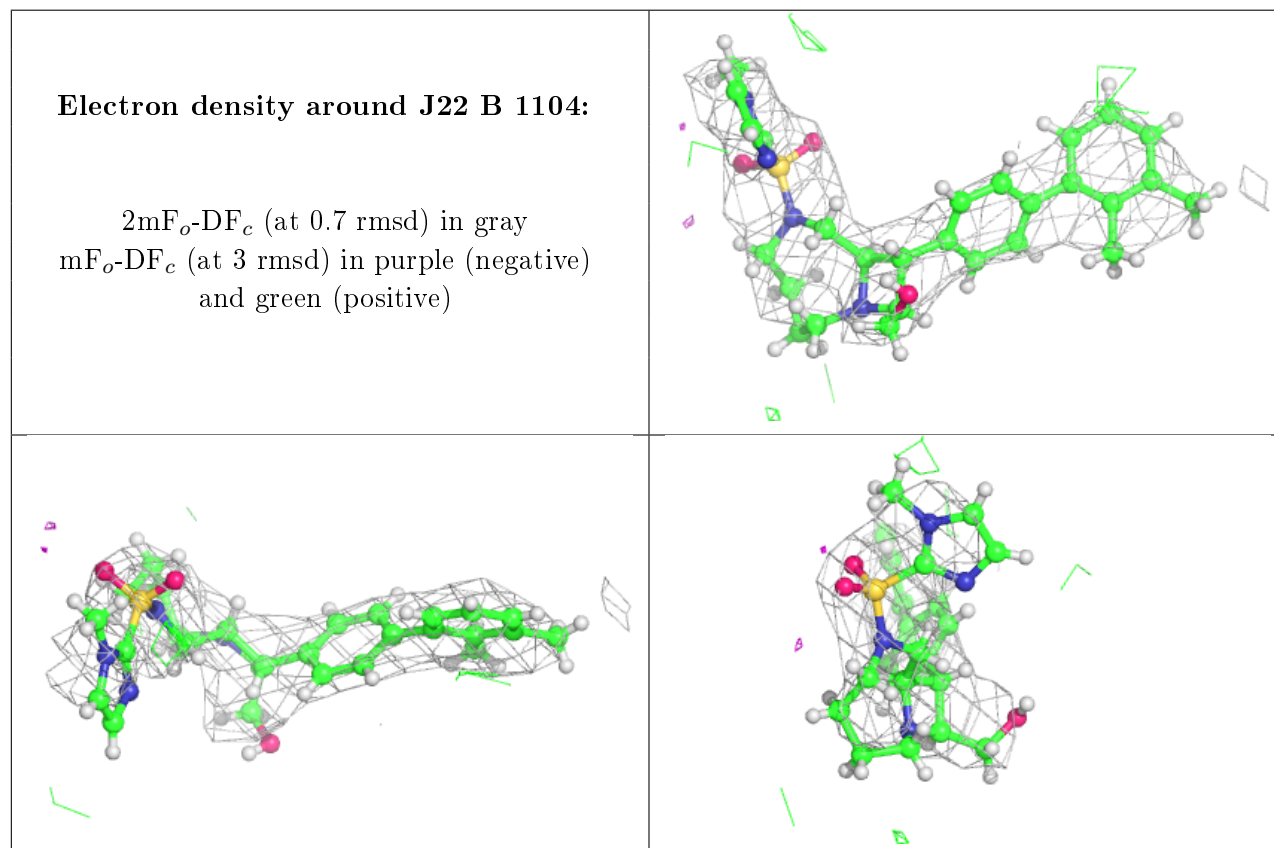
There are no carbohydrates in this entry.

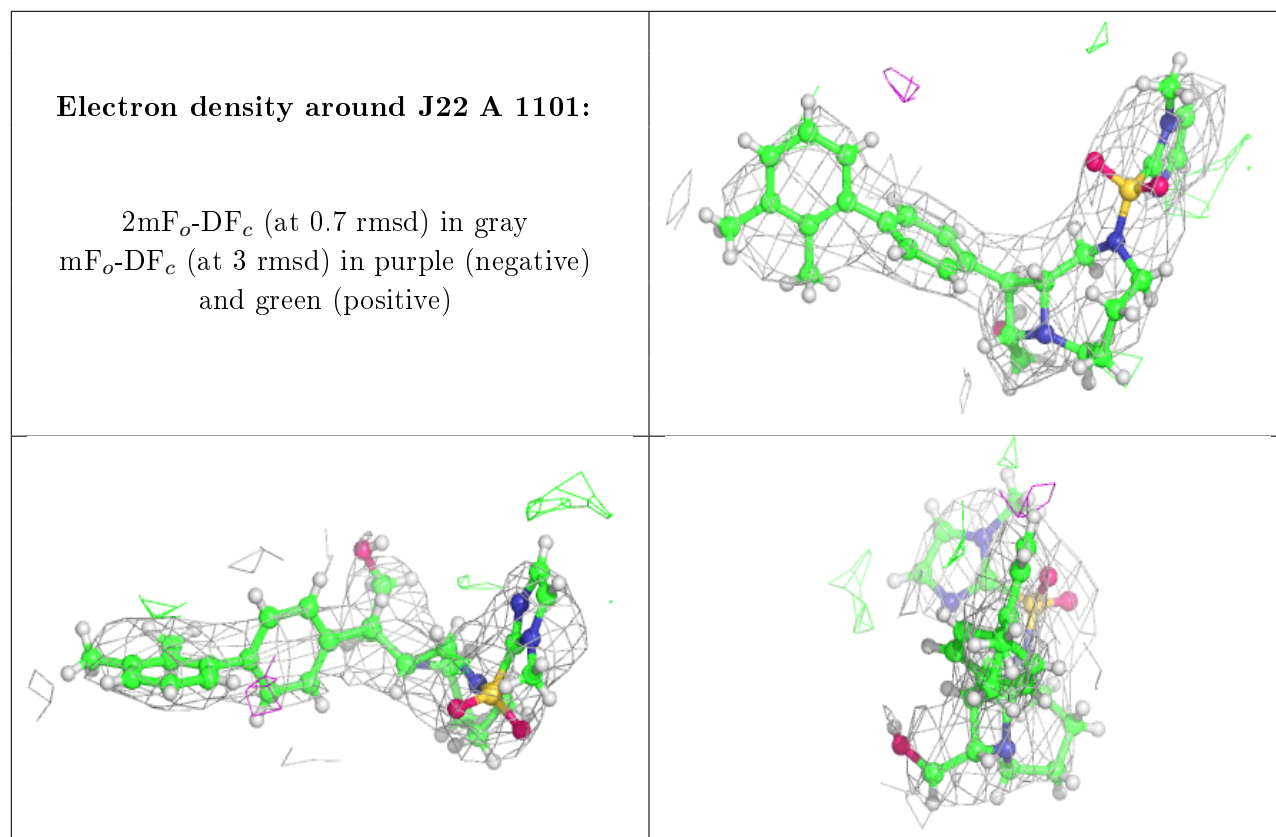
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	1103	7/7	0.81	0.49	57,73,87,87	0
6	DIO	A	1104	6/6	0.86	0.38	85,102,112,112	0
5	PEG	B	1102	7/7	0.86	0.85	82,100,122,123	0
6	DIO	B	1103	6/6	0.87	0.34	99,119,121,121	0
4	EPE	A	1102	15/15	0.90	0.33	80,96,109,111	0
4	EPE	B	1101	15/15	0.92	0.36	73,88,100,101	0
3	J22	B	1104	35/35	0.94	0.40	43,70,94,102	69
3	J22	A	1101	35/35	0.95	0.33	42,59,75,76	69

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.