



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:09 AM UTC

PDB ID : 5YLV / pdb_00005ylv
Title : Crystal structure of the gastric proton pump complexed with SCH28080
Authors : Abe, K.; Irie, K.; Nakanishi, H.; Fujiyoshi, Y.
Deposited on : 2017-10-19
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

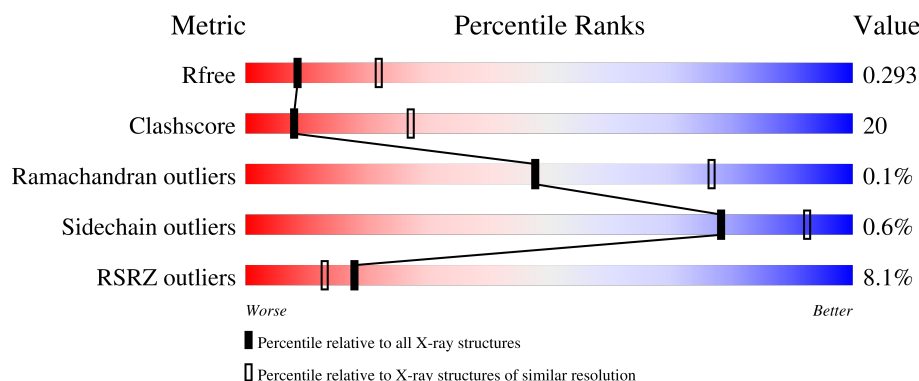
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1034	5% 64% 30% • 5%
2	B	289	18% 59% 31% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	BFD	A	385	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9937 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 Potassium-transporting ATPase alpha chain 1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	987	Total	Be	C	F	N	O	S	0	0	0
			7663	1	4890	3	1292	1423	54			

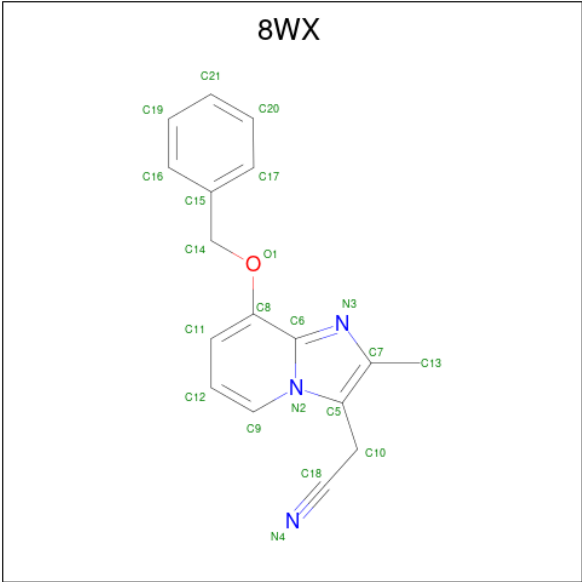
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	CYS	ARG	engineered mutation	UNP P19156
A	593	CYS	SER	engineered mutation	UNP P19156
A	1005	SER	GLY	engineered mutation	UNP P19156

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2076	1350	341	374	11			

- Molecule 3 is 2-(2-methyl-8-phenylmethoxy-imidazo[1,2-a]pyridin-3-yl)ethanenitrile (CCD ID: 8WX) (formula: C₁₇H₁₅N₃O).

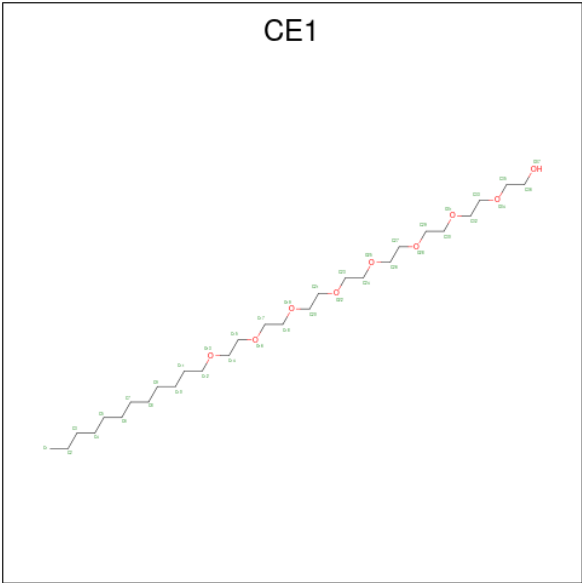


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	17	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: C₂₈H₅₈O₉).

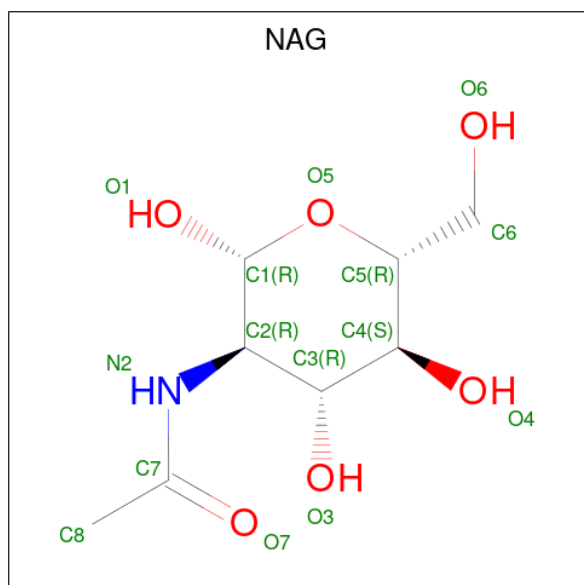


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			29	23	6		
5	B	1	Total	C	O	0	0
			19	16	3		

- Molecule 6 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

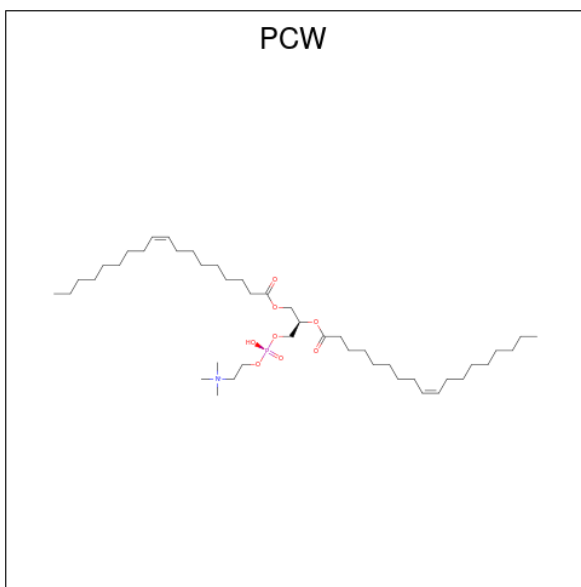
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Rb	0	0
			3	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

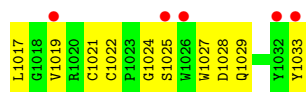
- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



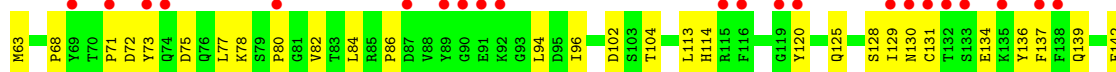
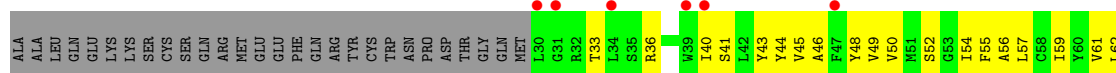
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	22	Total	O	0	0
			22	22		
9	B	7	Total	O	0	0
			7	7		



• Molecule 2: Potassium-transporting ATPase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.05Å 105.05Å 368.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.30 – 2.80 48.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (48.30-2.80) 92.2 (48.30-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.240 , 0.292 0.240 , 0.293	Depositor DCC
R_{free} test set	2746 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 18.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9937	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: 8WX, MG, PCW, CE1, NAG, RB, BFD

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	0.53	1/7808 (0.0%)	0.74	6/10604 (0.1%)
2	B	0.46	0/2143	0.69	0/2918
All	All	0.51	1/9951 (0.0%)	0.73	6/13522 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	826	PHE	C-O	-5.04	1.19	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	N-CA-C	7.96	119.95	111.28
1	A	602	ASP	N-CA-C	-6.76	99.84	109.24
1	A	825	ILE	N-CA-C	6.28	116.44	110.53
1	A	820	GLU	N-CA-C	6.04	117.86	111.28
1	A	886	GLY	N-CA-C	5.44	126.06	113.18
1	A	383	CYS	N-CA-C	-5.13	100.37	108.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	204	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7663	0	7682	310	0
2	B	2076	0	2002	98	0
3	A	21	0	0	3	0
4	A	1	0	0	1	0
5	A	29	0	45	2	0
5	B	19	0	33	1	0
6	A	3	0	0	0	0
7	B	42	0	39	2	0
8	B	54	0	84	9	0
9	A	22	0	0	1	0
9	B	7	0	0	0	0
All	All	9937	0	9885	387	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 20.

All (387) 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:882:MET:CE	1:A:923:GLN:HE21	1.16	1.52
1:A:882:MET:CE	1:A:923:GLN:NE2	2.00	1.24
1:A:994:ARG:NH1	2:B:75:ASP:OD2	1.79	1.15
1:A:911:TYR:HE2	2:B:71:PRO:HA	1.06	1.13
1:A:882:MET:HE2	1:A:882:MET:HA	1.35	1.09
1:A:773:GLN:HA	1:A:776:LEU:HD12	1.35	1.09
2:B:139:GLN:HB3	2:B:149:LYS:HD2	1.37	1.06
1:A:882:MET:HE2	1:A:923:GLN:HE21	1.17	1.05
1:A:882:MET:HE3	1:A:923:GLN:HE21	1.24	1.02
1:A:882:MET:HE1	1:A:923:GLN:CG	1.90	1.00
1:A:911:TYR:CE2	2:B:71:PRO:HA	1.98	0.98
1:A:911:TYR:HE2	2:B:71:PRO:CA	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:MET:HE1	1:A:923:GLN:HE21	1.30	0.95
2:B:139:GLN:HE22	2:B:150:PHE:H	1.12	0.93
1:A:53:HIS:HA	1:A:213:ARG:CD	2.01	0.91
1:A:882:MET:HE1	1:A:923:GLN:HG3	1.51	0.91
2:B:136:TYR:OH	2:B:192:GLY:O	1.90	0.90
1:A:884:GLN:OE1	2:B:73:TYR:CE1	2.28	0.85
1:A:213:ARG:NH1	1:A:250:ASN:ND2	2.24	0.84
1:A:438:ASN:O	1:A:480:ARG:NH1	2.10	0.84
1:A:53:HIS:HA	1:A:213:ARG:HD2	1.59	0.82
1:A:995:PHE:HB2	5:A:1103:CE1:H212	1.61	0.82
2:B:136:TYR:HH	2:B:192:GLY:C	1.87	0.82
1:A:790:THR:HG22	1:A:862:SER:HB3	1.63	0.80
2:B:139:GLN:HE22	2:B:150:PHE:N	1.80	0.78
1:A:1016:LYS:HA	1:A:1019:VAL:HG12	1.62	0.78
1:A:908:GLN:NE2	2:B:185:ARG:NH1	2.31	0.78
1:A:530:ILE:HB	1:A:539:LEU:HD23	1.66	0.77
1:A:911:TYR:CE2	2:B:71:PRO:CA	2.63	0.76
1:A:834:GLU:OE1	1:A:960:ARG:NH1	2.18	0.76
1:A:882:MET:HE2	1:A:923:GLN:NE2	1.84	0.76
1:A:887:TRP:HH2	1:A:915:TRP:CD2	2.04	0.76
2:B:129:ILE:HD12	2:B:129:ILE:O	1.85	0.76
1:A:95:THR:HB	1:A:100:LYS:HE3	1.66	0.75
2:B:139:GLN:CB	2:B:149:LYS:HD2	2.06	0.75
1:A:300:PHE:HB2	1:A:854:VAL:HG22	1.69	0.74
1:A:826:PHE:HB3	1:A:827:PRO:HD3	1.69	0.74
2:B:154:PHE:HA	2:B:158:MET:HE1	1.69	0.74
2:B:59:ILE:HD11	8:B:304:PCW:H132	1.69	0.73
1:A:621:ARG:NE	1:A:623:ILE:HG12	2.04	0.73
1:A:320:MET:HE3	1:A:329:ALA:CB	2.18	0.73
1:A:955:GLN:HB3	1:A:956:GLN:HE21	1.53	0.72
1:A:49:GLU:HA	1:A:52:ASP:HB2	1.69	0.72
1:A:882:MET:CE	1:A:882:MET:HA	2.17	0.72
1:A:773:GLN:CA	1:A:776:LEU:HD12	2.16	0.72
2:B:80:PRO:HD2	2:B:269:VAL:HG23	1.72	0.72
1:A:1019:VAL:HG23	1:A:1028:ASP:OD1	1.89	0.71
2:B:40:ILE:HG13	2:B:43:TYR:HB3	1.72	0.71
1:A:879:PHE:HZ	8:B:304:PCW:H39	1.55	0.71
2:B:82:VAL:HG23	2:B:282:VAL:HG13	1.72	0.71
1:A:112:LEU:HD21	1:A:341:VAL:HG22	1.71	0.71
1:A:823:THR:HG22	1:A:974:ILE:CD1	2.20	0.71
1:A:908:GLN:HE22	2:B:185:ARG:NH1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:GLN:NE2	2:B:150:PHE:H	1.89	0.70
1:A:300:PHE:HB2	1:A:854:VAL:CG2	2.22	0.70
1:A:451:VAL:HA	1:A:454:ARG:HG3	1.74	0.70
1:A:916:THR:HG21	2:B:276:ASP:OD2	1.91	0.70
2:B:139:GLN:HB3	2:B:149:LYS:CD	2.20	0.70
1:A:320:MET:HE3	1:A:329:ALA:HB2	1.74	0.70
1:A:440:ALA:O	1:A:480:ARG:NH2	2.18	0.70
2:B:129:ILE:HG13	2:B:151:SER:O	1.91	0.70
1:A:276:ILE:HD13	1:A:728:VAL:HG21	1.74	0.69
1:A:213:ARG:HH12	1:A:250:ASN:HD22	1.40	0.69
1:A:884:GLN:OE1	2:B:73:TYR:HE1	1.75	0.68
1:A:942:ASP:HA	1:A:945:ILE:HG22	1.76	0.68
2:B:129:ILE:HD12	2:B:129:ILE:C	2.19	0.68
2:B:129:ILE:HD11	2:B:131:CYS:SG	2.34	0.68
1:A:777:ILE:O	1:A:781:LEU:N	2.20	0.67
1:A:624:MET:HE2	1:A:698:VAL:HG13	1.76	0.67
1:A:882:MET:HE1	1:A:923:GLN:NE2	1.91	0.67
1:A:952:SER:HB3	1:A:955:GLN:HG3	1.77	0.67
7:B:302:NAG:O7	7:B:302:NAG:O3	2.11	0.67
1:A:539:LEU:HD12	1:A:544:ARG:HE	1.60	0.67
2:B:102:ASP:OD1	2:B:104:THR:HG22	1.94	0.67
1:A:320:MET:HA	1:A:320:MET:HE2	1.77	0.67
1:A:823:THR:HG22	1:A:974:ILE:HD11	1.77	0.66
1:A:376:LEU:HD11	1:A:757:MET:HE1	1.77	0.66
1:A:213:ARG:NH1	1:A:250:ASN:HD22	1.91	0.66
1:A:930:VAL:HB	1:A:993:ILE:HD11	1.77	0.65
1:A:994:ARG:HH12	2:B:75:ASP:CG	2.04	0.65
1:A:526:ARG:O	1:A:592:LEU:HD22	1.96	0.65
1:A:385:BFD:F1	4:A:1102:MG:MG	1.29	0.65
1:A:741:VAL:HG22	1:A:757:MET:HE2	1.79	0.64
1:A:308:ALA:HB1	1:A:337:VAL:HA	1.79	0.64
1:A:882:MET:HE1	1:A:923:GLN:CD	2.23	0.64
1:A:162:LYS:O	1:A:166:ILE:HG13	1.99	0.63
1:A:826:PHE:HB3	1:A:827:PRO:CD	2.29	0.63
1:A:526:ARG:O	1:A:592:LEU:CD2	2.46	0.63
2:B:201:CYS:HA	2:B:261:VAL:O	1.99	0.63
1:A:559:GLU:HG2	1:A:601:ILE:HD13	1.81	0.63
1:A:242:HIS:ND1	1:A:247:GLU:HB2	2.14	0.62
1:A:468:PHE:O	1:A:472:THR:HG22	2.00	0.62
1:A:879:PHE:CZ	8:B:304:PCW:H39	2.33	0.62
1:A:994:ARG:CZ	2:B:73:TYR:CD2	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:BFD:HB2	1:A:389:THR:CB	2.30	0.62
2:B:212:PRO:O	2:B:251:ASN:ND2	2.32	0.62
1:A:1016:LYS:HA	1:A:1019:VAL:CG1	2.29	0.61
1:A:811:LEU:O	3:A:1101:8WX:N4	2.33	0.61
1:A:578:TYR:OH	1:A:586:ASN:ND2	2.33	0.61
1:A:993:ILE:HG12	1:A:997:TRP:HE3	1.64	0.61
1:A:993:ILE:HG12	1:A:997:TRP:CE3	2.36	0.61
1:A:473:LEU:HD23	1:A:474:GLY:O	2.01	0.61
1:A:683:ASP:HB3	1:A:686:GLU:HG3	1.84	0.60
1:A:53:HIS:CD2	1:A:54:GLN:HG3	2.36	0.60
1:A:1012:ASP:O	1:A:1016:LYS:HG2	2.01	0.60
2:B:136:TYR:CZ	2:B:192:GLY:O	2.55	0.59
2:B:45:VAL:O	2:B:49:VAL:HG13	2.01	0.59
2:B:195:THR:HG22	2:B:196:ALA:H	1.67	0.59
1:A:913:GLN:HG2	2:B:186:ILE:HA	1.83	0.59
1:A:956:GLN:HB2	1:A:960:ARG:HH21	1.67	0.59
2:B:48:TYR:O	2:B:52:SER:OG	2.12	0.59
2:B:33:THR:HG23	2:B:36:ARG:H	1.67	0.59
1:A:87:ASN:HB3	1:A:192:ASP:HA	1.85	0.59
1:A:786:ALA:O	1:A:790:THR:HG23	2.02	0.59
1:A:300:PHE:CB	1:A:854:VAL:HG22	2.33	0.58
1:A:895:LEU:HD22	1:A:899:TRP:HE3	1.69	0.58
1:A:930:VAL:CB	1:A:993:ILE:HD11	2.32	0.58
1:A:391:THR:HA	1:A:604:PRO:HA	1.84	0.58
1:A:1017:LEU:O	1:A:1021:CYS:HB2	2.03	0.58
1:A:676:GLY:HA3	1:A:701:ARG:O	2.04	0.58
1:A:648:GLU:HB3	1:A:652:ASP:HB2	1.86	0.57
1:A:902:HIS:O	1:A:905:GLN:NE2	2.36	0.57
1:A:631:ILE:HD12	1:A:631:ILE:H	1.69	0.57
2:B:215:VAL:HG22	2:B:249:LEU:HD23	1.86	0.57
1:A:385:BFD:F1	1:A:385:BFD:OD2	2.13	0.56
1:A:90:ARG:CD	1:A:272:ASP:OD1	2.54	0.56
1:A:388:GLY:O	1:A:605:ARG:NH2	2.32	0.56
1:A:621:ARG:HG3	1:A:621:ARG:HH11	1.70	0.56
1:A:53:HIS:HA	1:A:213:ARG:NE	2.20	0.56
2:B:230:PRO:HG2	2:B:232:TYR:HE1	1.70	0.56
1:A:786:ALA:HB2	1:A:858:LEU:HD11	1.88	0.56
1:A:90:ARG:HD2	1:A:272:ASP:OD1	2.06	0.56
1:A:823:THR:CB	1:A:974:ILE:HD11	2.35	0.56
1:A:97:GLU:OE2	1:A:100:LYS:NZ	2.38	0.56
2:B:217:TYR:HA	2:B:246:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:LEU:HG	1:A:895:LEU:HD12	1.88	0.55
1:A:291:THR:HG21	1:A:371:GLU:OE1	2.06	0.55
1:A:688:VAL:HG23	1:A:717:LEU:HD11	1.88	0.55
1:A:887:TRP:CH2	1:A:915:TRP:CD2	2.93	0.55
1:A:789:LEU:O	1:A:792:ASN:HB2	2.06	0.55
2:B:155:THR:H	2:B:158:MET:CE	2.20	0.55
1:A:823:THR:CG2	1:A:974:ILE:HD11	2.36	0.54
2:B:125:GLN:OE1	2:B:154:PHE:N	2.32	0.54
1:A:963:ILE:HD12	1:A:963:ILE:H	1.72	0.54
1:A:998:TRP:O	1:A:1001:PRO:HD2	2.07	0.54
2:B:159:LEU:HD22	2:B:246:ALA:HB2	1.90	0.54
1:A:511:ARG:HB2	1:A:569:LEU:O	2.08	0.54
1:A:530:ILE:HB	1:A:539:LEU:CD2	2.38	0.53
1:A:724:THR:HG22	1:A:741:VAL:HB	1.90	0.53
1:A:927:CYS:HA	1:A:930:VAL:HG12	1.91	0.53
1:A:1025:SER:O	1:A:1029:GLN:HG3	2.08	0.53
1:A:63:LYS:HD3	1:A:64:TYR:CE2	2.44	0.53
1:A:699:PHE:HB3	1:A:702:THR:HG21	1.91	0.53
1:A:114:TRP:CZ3	1:A:146:ILE:HG12	2.44	0.52
1:A:374:GLU:OE1	1:A:378:SER:OG	2.21	0.52
2:B:56:ALA:O	2:B:59:ILE:HG13	2.09	0.52
1:A:1003:PRO:HG2	5:A:1103:CE1:H31	1.91	0.52
1:A:383:CYS:HB2	1:A:723:VAL:HG12	1.91	0.52
1:A:794:PRO:HB2	1:A:935:ILE:HD11	1.91	0.52
2:B:178:CYS:SG	2:B:248:LYS:HD2	2.50	0.52
1:A:942:ASP:O	1:A:946:ARG:HG2	2.09	0.52
1:A:983:GLY:O	1:A:987:ILE:HD12	2.09	0.52
1:A:376:LEU:HA	1:A:379:THR:OG1	2.08	0.52
1:A:926:THR:N	1:A:991:MET:HE1	2.25	0.52
1:A:321:CYS:O	1:A:322:ILE:HD13	2.10	0.52
2:B:68:PRO:HG3	8:B:304:PCW:H81	1.91	0.52
1:A:385:BFD:HB2	1:A:389:THR:HB	1.92	0.52
1:A:941:ALA:HB2	1:A:1005:SER:OG	2.10	0.52
1:A:621:ARG:HH21	1:A:697:MET:HB2	1.74	0.52
2:B:139:GLN:NE2	2:B:150:PHE:HB2	2.25	0.52
1:A:385:BFD:HB2	1:A:389:THR:OG1	2.09	0.51
1:A:840:ILE:HA	1:A:843:LEU:HD12	1.92	0.51
2:B:63:MET:HG3	8:B:304:PCW:H2	1.91	0.51
2:B:125:GLN:HE22	2:B:155:THR:HA	1.76	0.51
1:A:53:HIS:O	1:A:213:ARG:CZ	2.58	0.51
1:A:356:THR:HB	1:A:373:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LEU:HD23	1:A:928:TYR:OH	2.10	0.51
1:A:422:GLN:HG2	1:A:427:TRP:NE1	2.25	0.51
1:A:956:GLN:HB3	1:A:960:ARG:HD2	1.93	0.51
1:A:443:LYS:O	1:A:446:GLN:NE2	2.40	0.51
1:A:96:PRO:HD2	1:A:99:VAL:CG1	2.41	0.51
1:A:315:PHE:CD2	1:A:800:LEU:HD22	2.46	0.51
1:A:110:GLN:HG2	1:A:149:VAL:HG23	1.93	0.51
1:A:297:ILE:HA	1:A:300:PHE:CD2	2.46	0.51
1:A:731:SER:OG	1:A:732:PRO:HD3	2.11	0.51
1:A:856:GLU:OE2	1:A:856:GLU:N	2.43	0.50
1:A:865:GLN:HE21	2:B:44:TYR:HE1	1.57	0.50
1:A:895:LEU:O	1:A:895:LEU:HD23	2.12	0.50
1:A:1015:ARG:HA	1:A:1027:TRP:CZ2	2.45	0.50
2:B:125:GLN:HE22	2:B:154:PHE:C	2.19	0.50
1:A:778:PHE:HE2	1:A:846:ARG:NH1	2.09	0.50
1:A:833:TYR:HE2	1:A:963:ILE:HG21	1.76	0.50
1:A:879:PHE:CE2	2:B:55:PHE:HZ	2.29	0.50
2:B:50:VAL:O	2:B:54:ILE:HD12	2.11	0.50
1:A:275:ILE:O	1:A:279:ILE:HG13	2.12	0.50
2:B:63:MET:HE2	2:B:63:MET:HA	1.92	0.50
1:A:272:ASP:HA	1:A:277:GLY:HA3	1.93	0.50
1:A:320:MET:HE3	1:A:329:ALA:HB3	1.93	0.50
1:A:866:ILE:O	1:A:870:GLN:HG3	2.12	0.50
1:A:875:PHE:CD2	8:B:304:PCW:H432	2.46	0.50
1:A:929:THR:OG1	1:A:990:PHE:HA	2.12	0.50
1:A:219:GLY:O	1:A:261:GLY:HA3	2.12	0.50
1:A:792:ASN:HA	1:A:795:GLU:OE1	2.12	0.50
1:A:526:ARG:HB3	1:A:592:LEU:HD23	1.94	0.49
1:A:526:ARG:HB3	1:A:592:LEU:CD2	2.43	0.49
1:A:885:GLU:OE2	2:B:75:ASP:HB2	2.12	0.49
2:B:129:ILE:C	2:B:129:ILE:CD1	2.85	0.49
2:B:41:SER:O	2:B:45:VAL:HG23	2.12	0.49
2:B:59:ILE:HA	2:B:62:LEU:HB3	1.94	0.49
2:B:120:TYR:CZ	2:B:244:LEU:HD11	2.48	0.49
1:A:882:MET:HE3	1:A:923:GLN:NE2	2.00	0.49
1:A:944:LEU:CD2	1:A:964:LEU:HD21	2.43	0.49
1:A:885:GLU:OE2	2:B:75:ASP:OD2	2.30	0.49
1:A:1016:LYS:CA	1:A:1019:VAL:HG12	2.40	0.49
1:A:218:GLN:HB2	1:A:262:THR:HG22	1.94	0.48
1:A:64:TYR:CE1	1:A:196:VAL:CG1	2.96	0.48
1:A:707:LYS:O	1:A:711:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:HD2	1:A:99:VAL:HG11	1.94	0.48
1:A:489:ILE:HD11	1:A:585:MET:HE1	1.94	0.48
1:A:609:PRO:O	1:A:613:LEU:HG	2.14	0.48
1:A:621:ARG:HD3	1:A:622:VAL:N	2.28	0.48
1:A:916:THR:CG2	1:A:919:GLN:H	2.25	0.48
1:A:520:PRO:HG2	1:A:551:TYR:CE1	2.47	0.48
1:A:522:ARG:O	1:A:525:GLU:HG2	2.13	0.48
1:A:61:GLU:HB2	1:A:66:THR:O	2.14	0.48
1:A:216:GLN:HA	1:A:238:PRO:HG3	1.96	0.48
1:A:123:ALA:O	1:A:127:GLN:HG3	2.14	0.47
1:A:858:LEU:HB2	1:A:1033:TYR:HB2	1.97	0.47
2:B:255:ASN:OD1	2:B:289:GLN:HA	2.14	0.47
1:A:826:PHE:O	1:A:827:PRO:C	2.55	0.47
1:A:621:ARG:HD3	1:A:621:ARG:C	2.39	0.47
1:A:158:TYR:O	1:A:161:PHE:HB3	2.15	0.47
1:A:407:HIS:HB3	1:A:420:PHE:HB2	1.96	0.47
1:A:833:TYR:CE2	1:A:963:ILE:HG21	2.49	0.47
1:A:930:VAL:HA	1:A:993:ILE:CD1	2.45	0.47
1:A:955:GLN:HB3	1:A:956:GLN:NE2	2.24	0.47
1:A:613:LEU:O	1:A:617:THR:HG23	2.15	0.47
2:B:59:ILE:O	2:B:62:LEU:HB3	2.15	0.47
1:A:723:VAL:HG22	1:A:734:LEU:HA	1.97	0.47
2:B:134:GLU:O	2:B:134:GLU:HG3	2.15	0.47
1:A:504:LEU:HD13	1:A:511:ARG:O	2.16	0.46
1:A:526:ARG:CB	1:A:592:LEU:HD23	2.45	0.46
1:A:785:ILE:HG21	1:A:854:VAL:HG11	1.97	0.46
1:A:792:ASN:ND2	1:A:820:GLU:OE2	2.49	0.46
1:A:865:GLN:O	1:A:869:ILE:HG13	2.16	0.46
1:A:823:THR:HB	1:A:974:ILE:HD11	1.97	0.46
1:A:879:PHE:HZ	8:B:304:PCW:C39	2.25	0.46
1:A:879:PHE:CZ	8:B:304:PCW:H372	2.51	0.46
1:A:241:THR:HB	1:A:249:ARG:H	1.80	0.46
2:B:137:PHE:CE1	2:B:139:GLN:HG3	2.50	0.46
1:A:621:ARG:HG3	1:A:621:ARG:NH1	2.30	0.46
2:B:114:HIS:ND1	2:B:170:PHE:HE1	2.14	0.46
1:A:545:GLU:O	1:A:549:THR:HG23	2.16	0.46
1:A:743:MET:HE3	1:A:762:ASP:CG	2.41	0.45
1:A:773:GLN:HA	1:A:776:LEU:CD1	2.25	0.45
1:A:335:ALA:HA	3:A:1101:8WX:C19	2.46	0.45
1:A:936:GLU:O	1:A:939:GLN:N	2.46	0.45
1:A:1010:VAL:O	1:A:1014:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HB	1:A:100:LYS:CE	2.41	0.45
1:A:335:ALA:HB2	3:A:1101:8WX:C17	2.46	0.45
1:A:915:TRP:CE2	2:B:77:LEU:HD21	2.50	0.45
2:B:86:PRO:HD2	2:B:179:PHE:CD1	2.51	0.45
2:B:125:GLN:HE22	2:B:155:THR:CA	2.30	0.45
1:A:812:GLY:O	1:A:816:ILE:HG23	2.16	0.45
2:B:137:PHE:O	2:B:137:PHE:CD1	2.70	0.45
1:A:147:ALA:O	1:A:151:VAL:HG23	2.16	0.45
1:A:790:THR:C	1:A:792:ASN:H	2.25	0.45
1:A:964:LEU:C	1:A:964:LEU:HD23	2.41	0.45
2:B:142:PHE:HB2	2:B:147:HIS:NE2	2.32	0.45
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.86	0.45
1:A:235:THR:C	1:A:236:ARG:HD2	2.42	0.45
1:A:621:ARG:HE	1:A:623:ILE:HG12	1.80	0.45
1:A:783:LYS:NZ	1:A:837:GLU:OE1	2.50	0.45
1:A:858:LEU:HD13	1:A:1033:TYR:CD1	2.52	0.45
1:A:627:GLY:HA2	1:A:702:THR:H	1.81	0.45
1:A:685:SER:O	1:A:688:VAL:HG12	2.17	0.44
1:A:1006:LEU:O	1:A:1010:VAL:HG23	2.17	0.44
1:A:370:LEU:O	1:A:373:VAL:HB	2.17	0.44
1:A:235:THR:O	1:A:236:ARG:HD2	2.17	0.44
1:A:526:ARG:O	1:A:592:LEU:HD23	2.16	0.44
2:B:113:LEU:HD23	2:B:113:LEU:HA	1.67	0.44
1:A:90:ARG:HD3	1:A:272:ASP:OD1	2.16	0.44
1:A:117:ALA:O	1:A:120:CYS:HB2	2.17	0.44
2:B:136:TYR:HE1	2:B:191:PRO:HD2	1.82	0.44
1:A:367:VAL:HG11	1:A:373:VAL:HG23	1.99	0.44
1:A:887:TRP:CH2	1:A:915:TRP:CE2	3.05	0.44
1:A:945:ILE:HG12	1:A:1012:ASP:HB3	1.99	0.44
1:A:621:ARG:NE	1:A:623:ILE:CG1	2.79	0.44
1:A:790:THR:O	1:A:794:PRO:HD2	2.18	0.44
1:A:556:GLY:C	1:A:558:GLY:H	2.26	0.44
1:A:255:SER:HB3	1:A:276:ILE:HG13	2.00	0.44
1:A:908:GLN:NE2	2:B:185:ARG:CZ	2.81	0.44
1:A:996:GLN:HG2	5:B:305:CE1:H91	2.00	0.44
2:B:130:ASN:HB2	7:B:302:NAG:H2	2.00	0.44
1:A:786:ALA:CB	1:A:858:LEU:HD11	2.48	0.43
2:B:46:ALA:O	2:B:50:VAL:HG23	2.18	0.43
2:B:136:TYR:HH	2:B:192:GLY:H	1.63	0.43
2:B:142:PHE:HA	2:B:149:LYS:HD3	1.99	0.43
1:A:437:CYS:SG	1:A:498:GLN:HG2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:TRP:HH2	1:A:915:TRP:CG	2.36	0.43
1:A:896:ARG:HB3	1:A:897:PRO:HD3	2.00	0.43
2:B:216:GLU:HG2	2:B:218:PHE:CZ	2.53	0.43
1:A:984:MET:HE2	1:A:987:ILE:HD13	1.99	0.43
1:A:318:VAL:O	1:A:322:ILE:HG12	2.18	0.43
1:A:516:MET:HB3	1:A:565:CYS:SG	2.59	0.43
1:A:916:THR:HG23	1:A:918:GLY:N	2.33	0.43
2:B:204:LEU:HD13	2:B:204:LEU:HA	1.77	0.43
1:A:605:ARG:O	1:A:606:ALA:C	2.62	0.43
1:A:945:ILE:CD1	1:A:1012:ASP:HB3	2.49	0.43
1:A:673:VAL:HG22	1:A:698:VAL:HB	2.01	0.43
1:A:691:LEU:HD23	1:A:697:MET:HE3	2.00	0.43
1:A:794:PRO:HB2	1:A:935:ILE:CD1	2.48	0.43
1:A:120:CYS:SG	1:A:141:LEU:HB3	2.59	0.43
1:A:393:ASN:HA	1:A:602:ASP:OD1	2.18	0.43
1:A:618:ALA:O	1:A:845:PRO:HD3	2.19	0.43
1:A:96:PRO:O	1:A:99:VAL:HG12	2.19	0.43
1:A:624:MET:HE1	1:A:633:ALA:HB1	2.00	0.43
1:A:984:MET:N	1:A:985:PRO:HD2	2.34	0.43
2:B:96:ILE:HD13	2:B:179:PHE:CE1	2.53	0.43
1:A:818:PHE:CE1	1:A:978:LEU:HD21	2.54	0.42
1:A:861:TYR:CE1	1:A:1015:ARG:HD3	2.54	0.42
1:A:132:ASP:O	1:A:135:THR:HG23	2.19	0.42
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.83	0.42
1:A:797:THR:N	1:A:798:PRO:HD2	2.34	0.42
1:A:907:LEU:O	1:A:914:GLU:HA	2.20	0.42
1:A:933:ILE:O	1:A:937:MET:HG2	2.19	0.42
2:B:226:LEU:HD12	2:B:226:LEU:H	1.83	0.42
1:A:723:VAL:CG2	1:A:734:LEU:HA	2.50	0.42
2:B:154:PHE:HA	2:B:158:MET:CE	2.46	0.42
2:B:264:ILE:HG22	2:B:269:VAL:HG11	2.02	0.42
1:A:623:ILE:HG23	1:A:697:MET:HB3	2.00	0.42
1:A:911:TYR:CD2	2:B:71:PRO:HB3	2.55	0.42
1:A:930:VAL:CA	1:A:993:ILE:HD11	2.49	0.42
1:A:365:CYS:SG	1:A:757:MET:SD	3.18	0.42
1:A:166:ILE:O	1:A:169:SER:HB3	2.20	0.42
1:A:882:MET:HE2	1:A:882:MET:CA	2.25	0.42
1:A:1022:CYS:O	1:A:1024:GLY:N	2.49	0.42
2:B:149:LYS:N	2:B:236:ALA:O	2.38	0.42
2:B:253:PRO:CB	2:B:256:ARG:HH21	2.33	0.42
1:A:358:LYS:O	1:A:358:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:O	1:A:121:LEU:N	2.53	0.41
1:A:943:VAL:CG1	1:A:968:ILE:HD11	2.50	0.41
2:B:84:LEU:HD22	2:B:94:LEU:HD13	2.02	0.41
1:A:236:ARG:HD2	1:A:236:ARG:N	2.35	0.41
1:A:884:GLN:HE21	1:A:884:GLN:HB2	1.52	0.41
1:A:945:ILE:HG12	1:A:1012:ASP:CB	2.50	0.41
1:A:765:ALA:O	1:A:768:VAL:HG12	2.19	0.41
1:A:789:LEU:HD23	1:A:789:LEU:HA	1.86	0.41
1:A:884:GLN:HG3	2:B:72:ASP:HB2	2.02	0.41
2:B:63:MET:HG3	8:B:304:PCW:C2	2.49	0.41
2:B:243:PRO:C	2:B:244:LEU:HD12	2.44	0.41
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.88	0.41
1:A:673:VAL:HG13	1:A:698:VAL:HG12	2.03	0.41
1:A:987:ILE:HG22	1:A:988:PHE:CE1	2.56	0.41
1:A:472:THR:HG23	1:A:473:LEU:N	2.35	0.41
1:A:607:THR:HB	9:A:1215:HOH:O	2.20	0.41
1:A:855:ASN:OD1	1:A:855:ASN:N	2.54	0.41
1:A:882:MET:HE1	1:A:923:GLN:HG2	1.93	0.41
1:A:993:ILE:HG23	1:A:997:TRP:HB2	2.02	0.41
2:B:57:LEU:O	2:B:61:VAL:HG23	2.21	0.41
2:B:114:HIS:ND1	2:B:170:PHE:CE1	2.88	0.41
1:A:492:ASN:HB3	1:A:495:ASN:HB2	2.01	0.41
1:A:790:THR:C	1:A:792:ASN:N	2.77	0.41
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.88	0.41
1:A:127:GLN:HE21	1:A:135:THR:HG22	1.85	0.41
1:A:213:ARG:NH1	1:A:250:ASN:CG	2.79	0.41
1:A:383:CYS:O	1:A:723:VAL:HA	2.21	0.41
1:A:895:LEU:HD21	1:A:907:LEU:HD21	2.03	0.41
1:A:227:LEU:HA	1:A:227:LEU:HD13	1.88	0.41
1:A:233:PRO:HG3	1:A:259:LEU:HD13	2.03	0.41
1:A:616:ARG:NH1	1:A:641:GLY:O	2.53	0.41
2:B:82:VAL:HG11	2:B:264:ILE:HD13	2.01	0.41
2:B:142:PHE:HB2	2:B:147:HIS:CD2	2.55	0.41
1:A:181:ILE:HA	1:A:185:ASP:O	2.21	0.40
1:A:790:THR:HG21	1:A:946:ARG:HH21	1.86	0.40
1:A:817:LEU:HD23	1:A:817:LEU:HA	1.77	0.40
1:A:853:LEU:HD23	1:A:853:LEU:HA	1.92	0.40
1:A:879:PHE:HE2	2:B:55:PHE:HZ	1.69	0.40
1:A:386:LYS:HG3	1:A:636:ILE:HG21	2.02	0.40
1:A:847:ASN:OD1	1:A:849:LYS:HD2	2.22	0.40
1:A:875:PHE:O	1:A:878:TYR:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:LYS:H	2:B:78:LYS:HG3	1.68	0.40
1:A:54:GLN:NE2	1:A:243:GLU:HG2	2.37	0.40
1:A:503:THR:HG22	1:A:512:HIS:CE1	2.57	0.40
1:A:726:ASP:OD1	1:A:727:GLY:N	2.54	0.40
1:A:847:ASN:OD1	1:A:847:ASN:C	2.64	0.40
2:B:139:GLN:HB3	2:B:149:LYS:NZ	2.36	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	984/1034 (95%)	906 (92%)	77 (8%)	1 (0%)	48 77
2	B	259/289 (90%)	238 (92%)	21 (8%)	0	100 100
All	All	1243/1323 (94%)	1144 (92%)	98 (8%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	901	ASN

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	833/869 (96%)	828 (99%)	5 (1%)	78	92
2	B	224/253 (88%)	223 (100%)	1 (0%)	84	94
All	All	1057/1122 (94%)	1051 (99%)	6 (1%)	78	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	A	585	MET
1	A	823	THR
1	A	882	MET
1	A	993	ILE
2	B	128	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	176	GLN
1	A	299	HIS
1	A	407	HIS
1	A	495	ASN
1	A	548	GLN
1	A	566	GLN
1	A	792	ASN
1	A	884	GLN
1	A	908	GLN
1	A	923	GLN
1	A	939	GLN
1	A	956	GLN
1	A	986	ASN
1	A	1029	GLN
2	B	160	GLN
2	B	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	BFD	A	385	1,4	8,11,12	5.95	3 (37%)	2,15,17	1.31	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
1	BFD	A	385	1,4	-	2/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	BFD	F1-BE	10.77	1.78	1.54
1	A	385	BFD	F2-BE	9.38	1.75	1.54
1	A	385	BFD	F3-BE	8.67	1.73	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	385	BFD	O-C-CA-CB
1	A	385	BFD	CA-CB-CG-OD1

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	385	BFD	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z > 2$
5	CE1	A	1103	-	28,28,36	0.42	0	27,27,35	0.53	0
8	PCW	B	304	-	53,53,53	0.99	2 (3%)	59,61,61	0.94	3 (5%)
5	CE1	B	305	-	18,18,36	0.39	0	17,17,35	0.56	0
7	NAG	B	303	2	14,14,15	0.41	0	17,19,21	0.67	0
3	8WX	A	1101	-	20,23,23	2.41	5 (25%)	21,31,31	5.81	5 (23%)
7	NAG	B	302	2	14,14,15	0.30	0	17,19,21	0.56	0
7	NAG	B	301	2	14,14,15	0.56	0	17,19,21	0.93	1 (5%)

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	CE1	A	1103	-	-	14/26/26/34	-
8	PCW	B	304	-	-	20/57/57/57	-
5	CE1	B	305	-	-	7/16/16/34	-
7	NAG	B	303	2	-	0/6/23/26	0/1/1/1
3	8WX	A	1101	-	-	2/8/8/8	0/3/3/3
7	NAG	B	302	2	-	2/6/23/26	0/1/1/1
7	NAG	B	301	2	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	8WX	C18-N4	8.45	1.46	1.14
8	B	304	PCW	O2-C31	4.51	1.47	1.34
8	B	304	PCW	O3-C11	4.36	1.46	1.33
3	A	1101	8WX	C10-C18	3.81	1.53	1.45
3	A	1101	8WX	C6-N2	-3.21	1.35	1.39
3	A	1101	8WX	C9-C12	2.41	1.40	1.35
3	A	1101	8WX	C5-N2	-2.34	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	8WX	C10-C18-N4	-25.05	109.63	177.87
3	A	1101	8WX	C6-N3-C7	6.10	108.43	105.74
3	A	1101	8WX	C13-C7-N3	3.49	126.33	119.32
8	B	304	PCW	O2-C31-C32	3.45	118.94	111.48
3	A	1101	8WX	N2-C6-N3	-3.22	108.34	111.55
8	B	304	PCW	O3-C11-C12	3.14	121.42	111.83
3	A	1101	8WX	C14-O1-C8	2.95	121.15	116.36
8	B	304	PCW	O3-C11-O11	-2.55	117.24	123.63
7	B	301	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	304	PCW	O4P-C4-C5-N
8	B	304	PCW	C4-O4P-P-O1P
8	B	304	PCW	C4-O4P-P-O3P
5	A	1103	CE1	O25-C26-C27-O28
5	A	1103	CE1	O22-C23-C24-O25
5	A	1103	CE1	O19-C20-C21-O22
5	B	305	CE1	C7-C8-C9-C10
8	B	304	PCW	C33-C34-C35-C36
8	B	304	PCW	C34-C35-C36-C37
8	B	304	PCW	C12-C13-C14-C15
5	B	305	CE1	C2-C3-C4-C5
5	B	305	CE1	C3-C4-C5-C6
8	B	304	PCW	C20-C21-C22-C23
5	A	1103	CE1	C2-C3-C4-C5
8	B	304	PCW	C35-C36-C37-C38
8	B	304	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
7	B	302	NAG	O5-C5-C6-O6
7	B	302	NAG	C3-C2-N2-C7
5	B	305	CE1	C11-C10-C9-C8
8	B	304	PCW	C43-C44-C45-C46
5	A	1103	CE1	C10-C11-C12-O13
5	A	1103	CE1	C9-C10-C11-C12
8	B	304	PCW	O11-C11-O3-C3
5	B	305	CE1	C6-C7-C8-C9
3	A	1101	8WX	C11-C8-O1-C14
8	B	304	PCW	O3P-C1-C2-C3
5	A	1103	CE1	C17-C18-O19-C20
3	A	1101	8WX	C6-C8-O1-C14
8	B	304	PCW	O3P-C1-C2-O2
5	B	305	CE1	C18-C17-O16-C15
5	A	1103	CE1	C20-C21-O22-C23
8	B	304	PCW	C15-C16-C17-C18
5	A	1103	CE1	C11-C12-O13-C14
5	A	1103	CE1	C1-C2-C3-C4
5	B	305	CE1	C11-C12-O13-C14
8	B	304	PCW	C41-C42-C43-C44
5	A	1103	CE1	C14-C15-O16-C17
8	B	304	PCW	C21-C22-C23-C24
8	B	304	PCW	C17-C18-C19-C20
5	A	1103	CE1	O16-C17-C18-O19
5	A	1103	CE1	C15-C14-O13-C12
8	B	304	PCW	O3-C11-C12-C13
8	B	304	PCW	C13-C14-C15-C16
5	A	1103	CE1	C23-C24-O25-C26
8	B	304	PCW	O11-C11-C12-C13

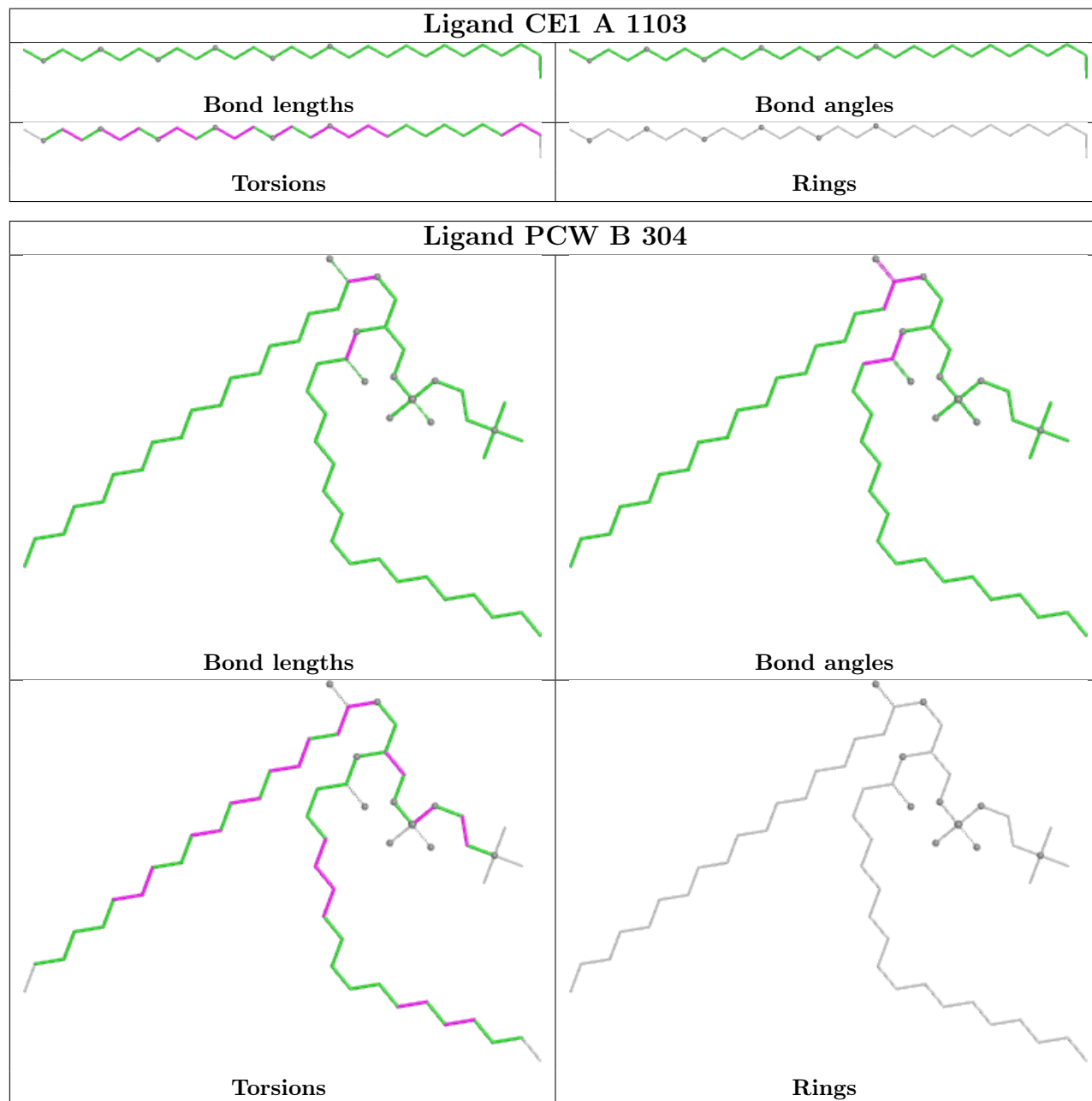
There are no ring outliers.

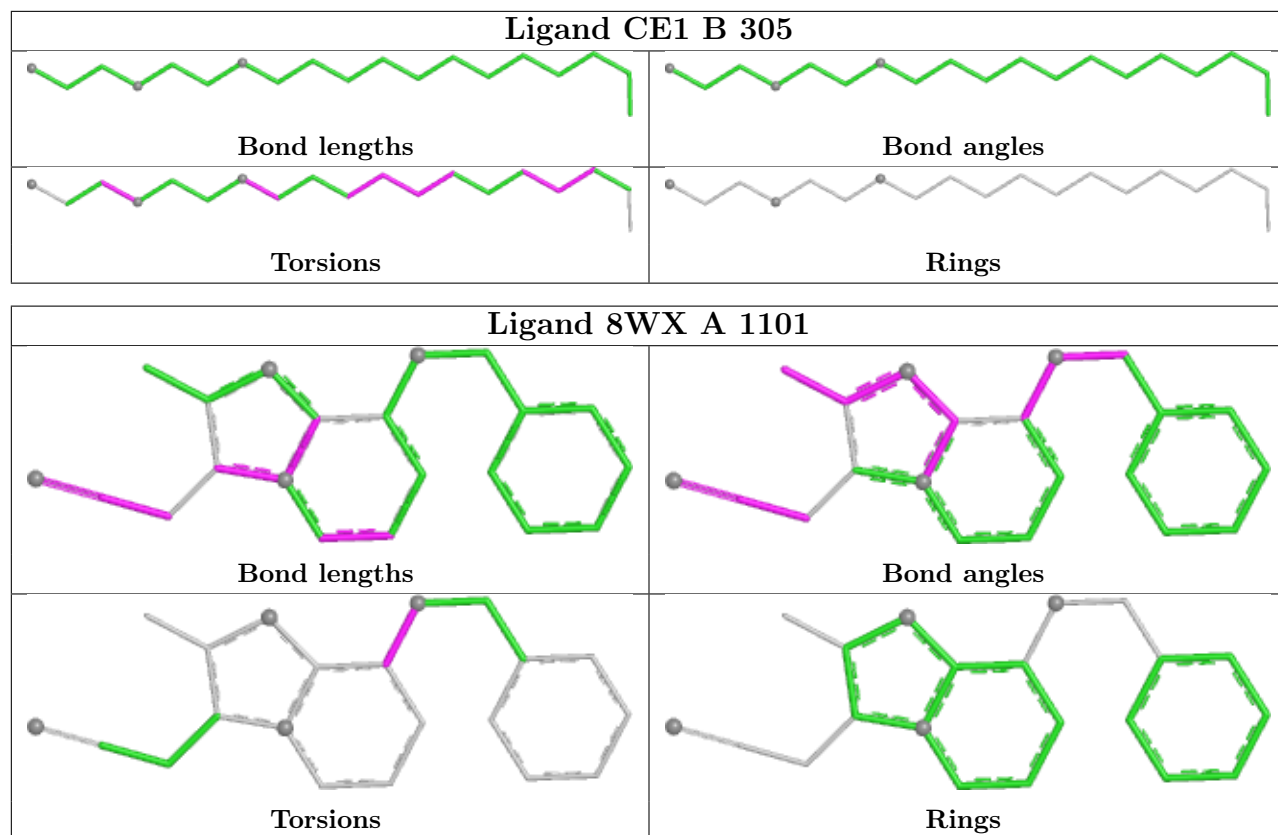
5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1103	CE1	2	0
8	B	304	PCW	9	0
5	B	305	CE1	1	0
3	A	1101	8WX	3	0
7	B	302	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	986/1034 (95%)	0.29	50 (5%) 33 25	39, 60, 98, 148	0
2	B	261/289 (90%)	1.14	51 (19%) 3 2	55, 83, 127, 151	0
All	All	1247/1323 (94%)	0.47	101 (8%) 18 13	39, 64, 105, 151	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	150	PHE	6.5
2	B	229	PHE	6.2
1	A	134	THR	5.8
2	B	236	ALA	5.7
1	A	50	ILE	5.7
1	A	558	GLY	4.8
1	A	92	PRO	4.6
2	B	186	ILE	4.5
1	A	48	MET	4.5
1	A	621	ARG	4.4
2	B	30	LEU	4.2
2	B	204	LEU	4.2
1	A	47	GLU	4.0
1	A	49	GLU	4.0
2	B	120	TYR	4.0
1	A	944	LEU	4.0
2	B	69	TYR	3.9
1	A	101	PHE	3.7
1	A	677	MET	3.7
1	A	102	ALA	3.6
1	A	439	ARG	3.5
1	A	557	LEU	3.5
2	B	91	GLU	3.5
2	B	90	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	152	CYS	3.4
1	A	158	TYR	3.3
2	B	245	VAL	3.3
2	B	237	GLN	3.2
1	A	1004	PHE	3.2
2	B	154	PHE	3.1
1	A	448	ALA	3.1
1	A	958	PHE	3.0
2	B	39	TRP	3.0
2	B	116	PHE	3.0
2	B	92	LYS	2.9
1	A	555	GLY	2.9
1	A	1026	TRP	2.9
2	B	130	ASN	2.9
2	B	224	TYR	2.9
1	A	510	PRO	2.9
2	B	129	ILE	2.9
2	B	153	LYS	2.8
2	B	232	TYR	2.8
2	B	80	PRO	2.8
1	A	404	ASN	2.8
2	B	243	PRO	2.7
2	B	89	TYR	2.7
2	B	131	CYS	2.7
2	B	138	PHE	2.7
1	A	758	ILE	2.7
1	A	836	ALA	2.7
2	B	135	LYS	2.7
2	B	228	TYR	2.6
2	B	132	THR	2.6
2	B	87	ASP	2.6
1	A	600	MET	2.6
2	B	74	GLN	2.6
2	B	31	GLY	2.5
2	B	207	PRO	2.5
1	A	870	GLN	2.5
1	A	241	THR	2.5
1	A	98	TYR	2.5
2	B	252	VAL	2.5
1	A	584	ALA	2.5
2	B	47	PHE	2.5
1	A	601	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	559	GLU	2.4
1	A	154	CYS	2.4
1	A	95	THR	2.4
1	A	995	PHE	2.4
2	B	240	TYR	2.3
1	A	327	LEU	2.3
1	A	1033	TYR	2.3
2	B	137	PHE	2.3
1	A	213	ARG	2.3
2	B	34	LEU	2.3
1	A	970	PHE	2.3
2	B	241	SER	2.2
2	B	222	GLY	2.2
2	B	214	GLN	2.2
1	A	646	GLY	2.2
1	A	851	ASP	2.2
1	A	890	LEU	2.2
1	A	943	VAL	2.2
2	B	73	TYR	2.2
2	B	206	GLN	2.2
2	B	133	SER	2.2
1	A	99	VAL	2.1
2	B	189	PHE	2.1
1	A	1032	TYR	2.1
1	A	550	ALA	2.1
1	A	507	PRO	2.1
2	B	181	ILE	2.1
1	A	103	ARG	2.1
2	B	115	ARG	2.1
2	B	119	GLY	2.1
2	B	40	ILE	2.1
2	B	71	PRO	2.0
1	A	1019	VAL	2.0
1	A	1025	SER	2.0
1	A	1008	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	BFD	A	385	12/13	0.92	0.10	38,46,49,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

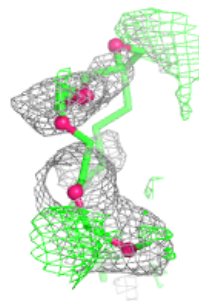
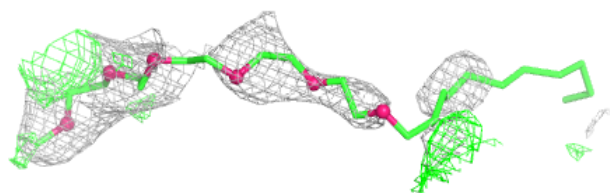
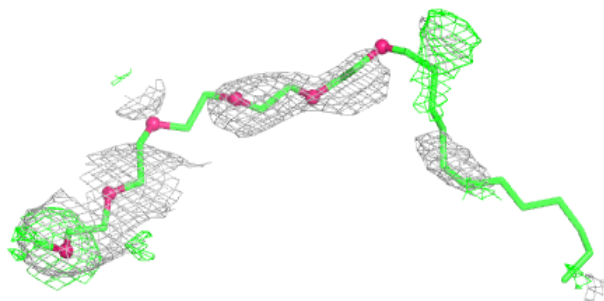
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	302	14/15	0.55	0.22	110,123,126,129	0
5	CE1	A	1103	29/37	0.74	0.36	85,117,134,138	0
5	CE1	B	305	19/37	0.86	0.21	83,94,99,101	0
7	NAG	B	303	14/15	0.86	0.13	98,104,108,109	0
8	PCW	B	304	54/54	0.88	0.21	86,106,128,131	0
7	NAG	B	301	14/15	0.94	0.09	54,59,65,66	0
3	8WX	A	1101	21/21	0.95	0.09	52,63,66,68	0
4	MG	A	1102	1/1	0.98	0.04	38,38,38,38	0
6	RB	A	1104	1/1	0.98	0.04	98,98,98,98	0
6	RB	A	1105	1/1	0.99	0.14	93,93,93,93	0
6	RB	A	1106	1/1	0.99	0.02	60,60,60,60	0

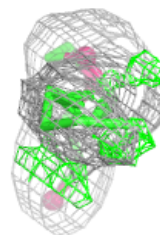
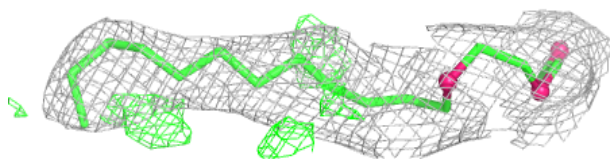
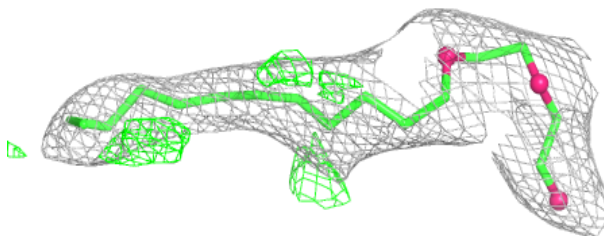
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CE1 A 1103:

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

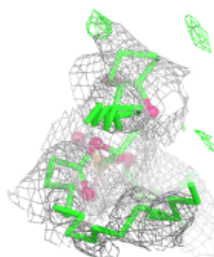
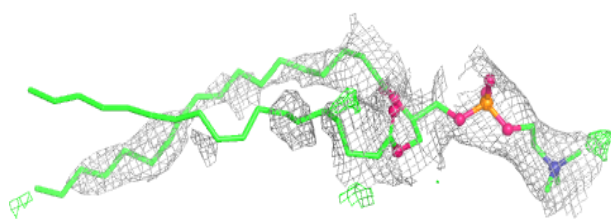
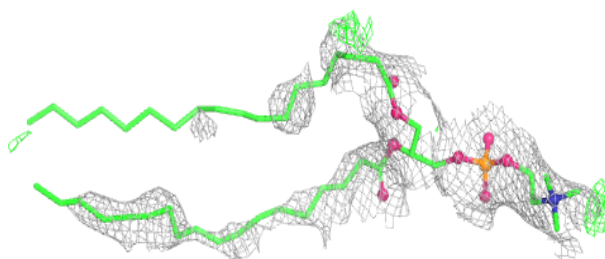
**Electron density around CE1 B 305:**

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

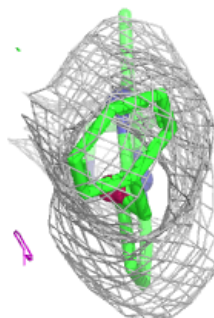
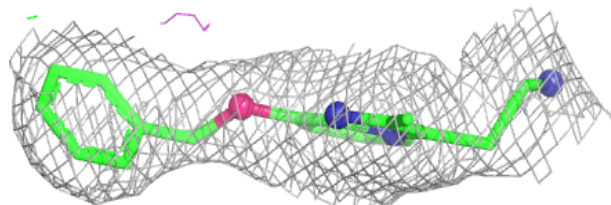
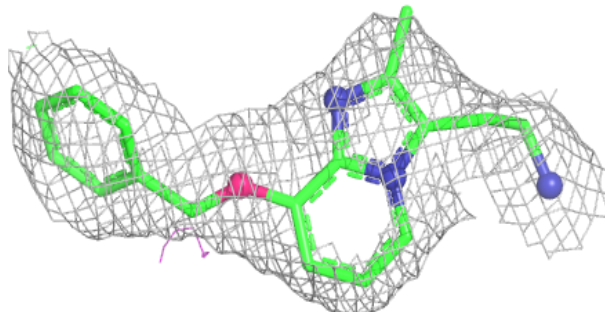


Electron density around PCW B 304:

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

**Electron density around 8WX A 1101:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.