



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:31 PM UTC

PDB ID : 2W1B / pdb_00002w1b
Title : The structure of the efflux pump AcrB in complex with bile acid
Authors : Drew, D.; Klepsch, M.M.; Newstead, S.; Flaig, R.; De Gier, J.W.; Iwata, S.;
Beis, K.
Deposited on : 2008-10-17
Resolution : 3.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

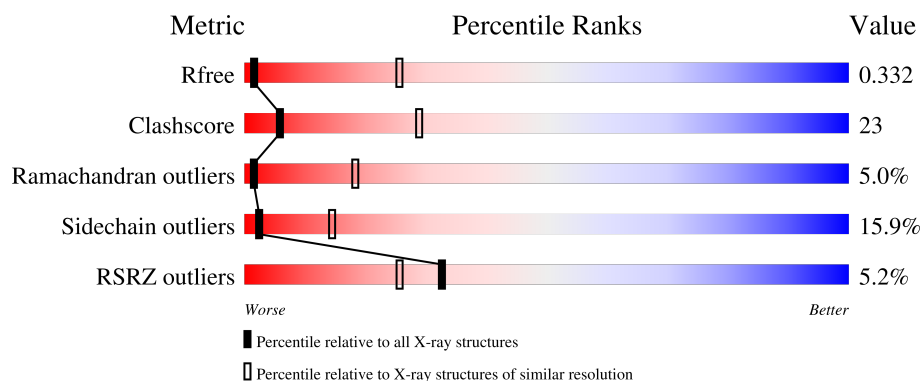
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	1049	5% 49% 41% 8% ..

2 Entry composition [i](#)

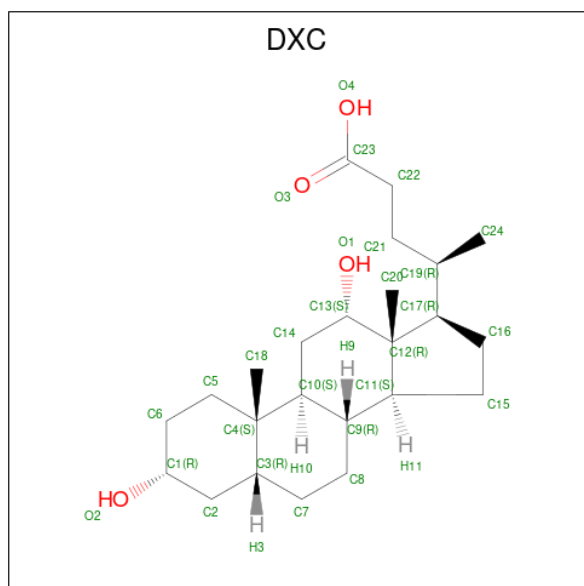
There are 2 unique types of molecules in this entry. The entry contains 7869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACRIFLAVIN RESISTANCE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			

- Molecule 2 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (CCD ID: DXC) (formula: C₂₄H₄₀O₄).

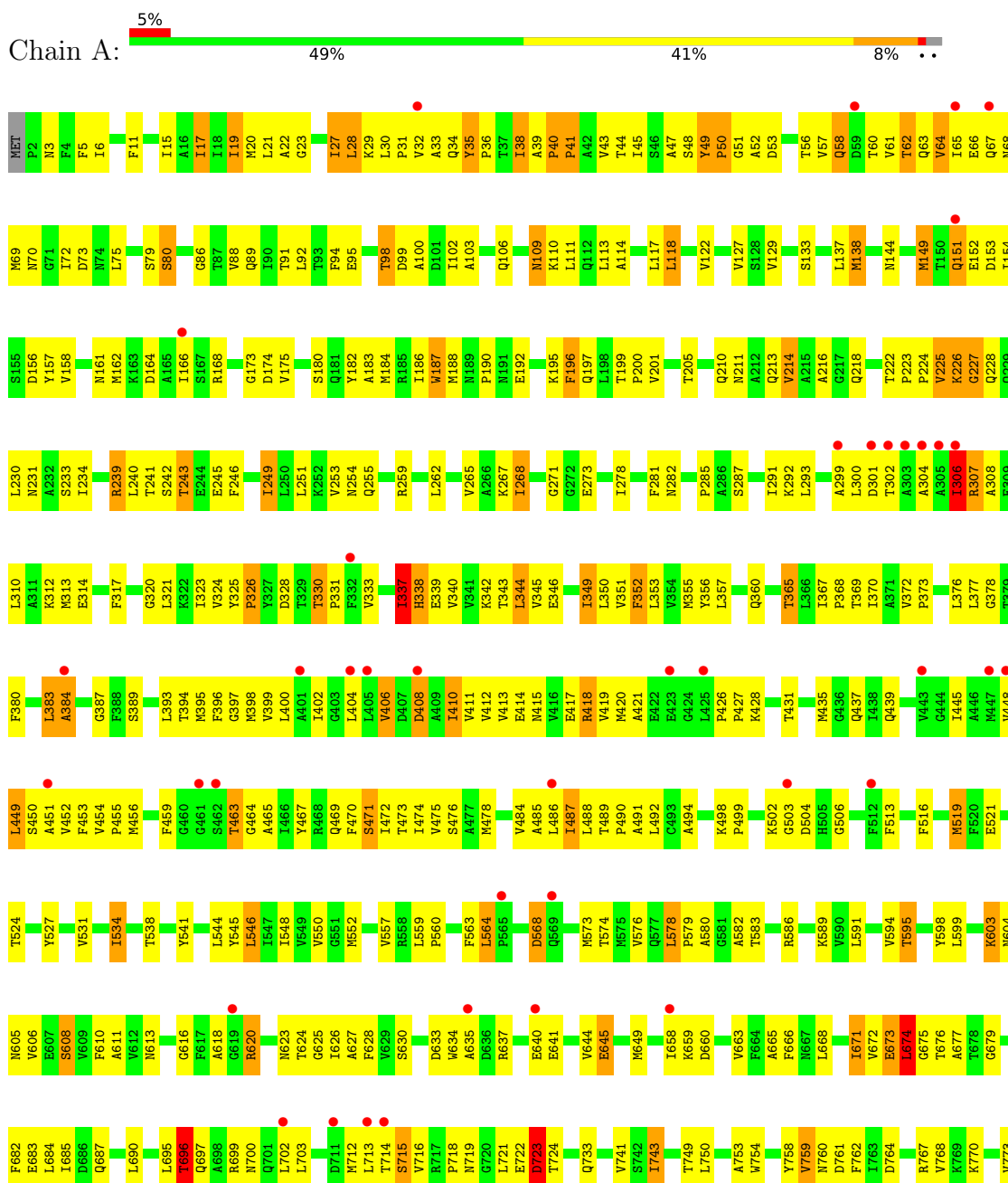


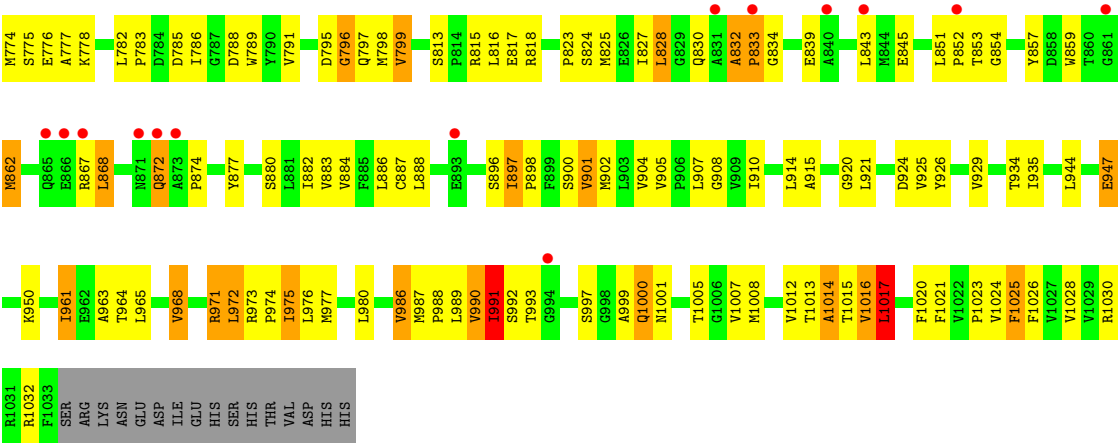
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	24	4		

3 Residue-property plots

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

• Molecule 1: ACRIFLAVIN RESISTANCE PROTEIN B





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	145.49Å 145.49Å 515.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.85 40.00 – 3.85	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-3.85) 95.1 (40.00-3.85)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.278 , 0.349 0.270 , 0.332	Depositor DCC
R_{free} test set	978 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	96.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7869	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

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

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	0.67	0/7991	1.02	25/10852 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PRO	CA-C-N	9.26	131.41	119.84
1	A	40	PRO	C-N-CA	9.26	131.41	119.84
1	A	49	TYR	CA-C-N	8.51	130.48	119.84
1	A	49	TYR	C-N-CA	8.51	130.48	119.84
1	A	986	VAL	N-CA-C	-7.38	105.39	113.43
1	A	214	VAL	N-CA-C	6.92	118.44	108.48
1	A	972	LEU	N-CA-C	-6.79	104.99	113.55
1	A	788	ASP	N-CA-C	-6.67	105.29	113.50
1	A	851	LEU	CA-C-N	6.66	128.16	119.84
1	A	851	LEU	C-N-CA	6.66	128.16	119.84
1	A	345	VAL	N-CA-C	-6.34	107.69	113.71
1	A	832	ALA	CA-C-N	6.10	127.46	119.84
1	A	832	ALA	C-N-CA	6.10	127.46	119.84
1	A	723	ASP	N-CA-C	6.00	118.24	108.63
1	A	27	ILE	N-CA-C	-5.91	104.16	110.36
1	A	426	PRO	CA-C-N	5.77	127.05	119.84
1	A	426	PRO	C-N-CA	5.77	127.05	119.84
1	A	306	ILE	CA-C-N	5.70	131.96	121.70
1	A	306	ILE	C-N-CA	5.70	131.96	121.70
1	A	340	VAL	N-CA-C	-5.44	107.49	111.90
1	A	696	THR	N-CA-C	-5.37	105.43	111.28
1	A	498	LYS	CA-C-N	5.29	125.23	119.78
1	A	498	LYS	C-N-CA	5.29	125.23	119.78
1	A	487	ILE	N-CA-C	5.24	116.52	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	620	ARG	N-CA-C	5.13	116.72	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7841	0	7990	365	0
2	A	28	0	39	1	0
All	All	7869	0	8029	366	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 23.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2034:DXC:C15	2:A:2034:DXC:C16	1.84	1.41
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.30	1.08
1:A:971:ARG:HB2	1:A:971:ARG:NH1	1.74	1.02
1:A:552:MET:HA	1:A:910:ILE:HD13	1.43	0.97
1:A:33:ALA:HA	1:A:300:LEU:HD13	1.44	0.95
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.50	0.94
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.52	0.91
1:A:897:ILE:H	1:A:898:PRO:HD2	1.38	0.88
1:A:676:THR:HA	1:A:862:MET:HB2	1.55	0.88
1:A:239:ARG:HG3	1:A:239:ARG:HH11	1.40	0.86
1:A:453:PHE:O	1:A:471:SER:OG	1.96	0.84
1:A:306:ILE:HG22	1:A:306:ILE:O	1.76	0.84
1:A:971:ARG:HB2	1:A:971:ARG:CZ	2.07	0.83
1:A:158:VAL:HG22	1:A:162:MET:HE2	1.59	0.82
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.63	0.81
1:A:393:LEU:HD23	1:A:470:PHE:HE1	1.45	0.81
1:A:684:LEU:O	1:A:824:SER:HA	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD23	1:A:470:PHE:CE1	2.15	0.81
1:A:451:ALA:HB1	1:A:883:VAL:HG13	1.64	0.80
1:A:330:THR:H	1:A:331:PRO:HD2	1.46	0.80
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.63	0.79
1:A:578:LEU:HB2	1:A:623:ASN:HB2	1.65	0.78
1:A:465:ALA:O	1:A:469:GLN:HG2	1.84	0.77
1:A:944:LEU:HB3	1:A:971:ARG:HH21	1.48	0.77
1:A:415:ASN:O	1:A:419:VAL:HG23	1.85	0.77
1:A:225:VAL:O	1:A:226:LYS:O	2.03	0.77
1:A:19:ILE:HG22	1:A:378:GLY:HA2	1.68	0.75
1:A:64:VAL:HG11	1:A:117:LEU:HB3	1.70	0.74
1:A:342:LYS:HG2	1:A:346:GLU:OE2	1.89	0.73
1:A:576:VAL:HA	1:A:663:VAL:HG22	1.71	0.73
1:A:626:ILE:HG12	1:A:628:PHE:CE1	2.24	0.73
1:A:696:THR:HG23	1:A:825:MET:HE1	1.70	0.73
1:A:743:ILE:HD12	1:A:743:ILE:H	1.53	0.72
1:A:144:ASN:HD22	1:A:149:MET:HG2	1.53	0.72
1:A:352:PHE:HD2	1:A:352:PHE:O	1.72	0.71
1:A:184:MET:HE3	1:A:184:MET:HA	1.70	0.71
1:A:758:TYR:HE1	1:A:770:LYS:HB3	1.53	0.71
1:A:907:LEU:HD23	1:A:1017:LEU:HB3	1.73	0.71
1:A:402:ILE:O	1:A:406:VAL:HG23	1.91	0.69
1:A:915:ALA:HB1	1:A:1005:THR:HG22	1.73	0.69
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.74	0.69
1:A:35:TYR:CE1	1:A:671:ILE:HG12	2.27	0.68
1:A:36:PRO:HG2	1:A:38:ILE:HG12	1.74	0.68
1:A:70:ASN:O	1:A:72:ILE:HG13	1.93	0.67
1:A:564:LEU:HG	1:A:926:TYR:CE1	2.30	0.67
1:A:356:TYR:O	1:A:360:GLN:N	2.24	0.67
1:A:411:VAL:O	1:A:415:ASN:HB2	1.95	0.67
1:A:989:LEU:O	1:A:1001:ASN:ND2	2.29	0.66
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.77	0.66
1:A:344:LEU:HD21	1:A:399:VAL:HA	1.77	0.66
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.76	0.66
1:A:817:GLU:O	1:A:818:ARG:HG3	1.95	0.65
1:A:330:THR:N	1:A:331:PRO:HD2	2.12	0.65
1:A:897:ILE:N	1:A:898:PRO:HD2	2.12	0.65
1:A:697:GLN:O	1:A:700:ASN:HB2	1.95	0.64
1:A:58:GLN:HA	1:A:62:THR:OG1	1.98	0.64
1:A:1020:PHE:O	1:A:1023:PRO:HD2	1.98	0.64
1:A:449:LEU:O	1:A:453:PHE:HD1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HB3	1:A:196:PHE:CD1	2.34	0.63
1:A:149:MET:HG3	1:A:154:ILE:HG13	1.81	0.63
1:A:408:ASP:O	1:A:412:VAL:HG23	1.99	0.62
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.81	0.62
1:A:758:TYR:CE1	1:A:770:LYS:HB3	2.34	0.62
1:A:68:ASN:O	1:A:110:LYS:HD2	2.00	0.62
1:A:368:PRO:HG3	1:A:413:VAL:HG21	1.80	0.62
1:A:239:ARG:HG3	1:A:239:ARG:NH1	2.14	0.61
1:A:758:TYR:OH	1:A:761:ASP:OD1	2.13	0.61
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.82	0.61
1:A:987:MET:HA	1:A:1008:MET:HE1	1.81	0.61
1:A:41:PRO:HB2	1:A:94:PHE:HB2	1.82	0.61
1:A:230:LEU:HG	1:A:231:ASN:N	2.15	0.61
1:A:888:LEU:HB2	1:A:898:PRO:HB3	1.83	0.61
1:A:23:GLY:HA3	1:A:377:LEU:O	2.01	0.60
1:A:971:ARG:HB2	1:A:971:ARG:HH11	1.66	0.60
1:A:733:GLN:HE22	1:A:743:ILE:HG21	1.67	0.60
1:A:95:GLU:O	1:A:98:THR:HB	2.02	0.60
1:A:5:PHE:HE2	1:A:11:PHE:HD1	1.51	0.59
1:A:73:ASP:HB2	1:A:106:GLN:HE22	1.66	0.59
1:A:200:PRO:HD2	1:A:749:THR:CG2	2.33	0.59
1:A:190:PRO:HG3	1:A:789:TRP:CH2	2.38	0.59
1:A:35:TYR:HB3	1:A:36:PRO:CD	2.33	0.59
1:A:741:VAL:HG21	1:A:799:VAL:HG21	1.84	0.59
1:A:971:ARG:CZ	1:A:971:ARG:CB	2.81	0.59
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.33	0.59
1:A:5:PHE:CE1	1:A:487:ILE:HG12	2.38	0.58
1:A:679:GLY:HA3	1:A:830:GLN:HG2	1.85	0.58
1:A:527:TYR:O	1:A:531:VAL:HG23	2.04	0.58
1:A:411:VAL:HG22	1:A:974:PRO:HB3	1.85	0.58
1:A:874:PRO:HA	1:A:877:TYR:HB2	1.85	0.58
1:A:997:SER:HA	1:A:1000:GLN:HB2	1.85	0.58
1:A:58:GLN:HE22	1:A:63:GLN:HE21	1.52	0.58
1:A:753:ALA:O	1:A:775:SER:HB3	2.04	0.58
1:A:435:MET:C	1:A:437:GLN:H	2.11	0.57
1:A:552:MET:CA	1:A:910:ILE:HD13	2.27	0.57
1:A:35:TYR:HB3	1:A:36:PRO:HD2	1.86	0.57
1:A:337:ILE:HG22	1:A:338:HIS:H	1.69	0.57
1:A:356:TYR:O	1:A:357:LEU:C	2.48	0.56
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.41	0.56
1:A:527:TYR:OH	1:A:968:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:VAL:HA	1:A:907:LEU:CD1	2.29	0.56
1:A:1013:THR:C	1:A:1015:THR:H	2.14	0.56
1:A:372:VAL:HB	1:A:373:PRO:CD	2.33	0.56
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.41	0.56
1:A:750:LEU:HD12	1:A:754:TRP:CD1	2.41	0.56
1:A:32:VAL:O	1:A:300:LEU:HB2	2.05	0.56
1:A:228:GLN:HG2	1:A:230:LEU:H	1.71	0.56
1:A:337:ILE:CG2	1:A:338:HIS:N	2.69	0.55
1:A:449:LEU:O	1:A:453:PHE:CD1	2.58	0.55
1:A:882:ILE:O	1:A:886:LEU:HG	2.06	0.55
1:A:395:MET:O	1:A:398:MET:HB2	2.07	0.55
1:A:714:THR:HG22	1:A:715:SER:H	1.72	0.55
1:A:393:LEU:HD13	1:A:469:GLN:HG3	1.88	0.55
1:A:351:VAL:C	1:A:353:LEU:H	2.14	0.55
1:A:513:PHE:O	1:A:516:PHE:HB2	2.06	0.55
1:A:144:ASN:ND2	1:A:149:MET:H	2.04	0.55
1:A:174:ASP:O	1:A:292:LYS:HB2	2.07	0.55
1:A:712:MET:HE3	1:A:839:GLU:HB3	1.88	0.55
1:A:817:GLU:C	1:A:818:ARG:HG3	2.32	0.55
1:A:56:THR:O	1:A:56:THR:HG22	2.06	0.54
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.26	0.54
1:A:414:GLU:HA	1:A:417:GLU:HG2	1.90	0.54
1:A:351:VAL:O	1:A:353:LEU:N	2.41	0.54
1:A:827:ILE:O	1:A:828:LEU:HD22	2.08	0.54
1:A:1030:ARG:C	1:A:1032:ARG:H	2.16	0.53
1:A:53:ASP:O	1:A:57:VAL:HG23	2.09	0.53
1:A:109:ASN:O	1:A:113:LEU:HG	2.08	0.53
1:A:394:THR:O	1:A:398:MET:HG2	2.09	0.53
1:A:406:VAL:HG13	1:A:410:ILE:HD12	1.91	0.53
1:A:563:PHE:O	1:A:924:ASP:HB2	2.09	0.53
1:A:35:TYR:CB	1:A:36:PRO:CD	2.86	0.53
1:A:598:TYR:HB3	1:A:606:VAL:HG11	1.89	0.53
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.09	0.53
1:A:35:TYR:CB	1:A:36:PRO:HD2	2.39	0.53
1:A:408:ASP:N	1:A:408:ASP:OD1	2.41	0.53
1:A:69:MET:O	1:A:70:ASN:HB3	2.09	0.53
1:A:671:ILE:HD12	1:A:674:LEU:HD22	1.91	0.53
1:A:210:GLN:OE1	1:A:249:ILE:HA	2.08	0.52
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.40	0.52
1:A:5:PHE:CE2	1:A:11:PHE:HD1	2.27	0.52
1:A:456:MET:O	1:A:467:TYR:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:ND2	1:A:149:MET:HG2	2.22	0.52
1:A:3:ASN:HA	1:A:6:ILE:HG12	1.91	0.52
1:A:351:VAL:C	1:A:353:LEU:N	2.66	0.52
1:A:699:ARG:HE	1:A:718:PRO:HB3	1.75	0.52
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.90	0.52
1:A:57:VAL:HG11	1:A:86:GLY:O	2.10	0.52
1:A:383:LEU:O	1:A:384:ALA:C	2.52	0.52
1:A:872:GLN:O	1:A:872:GLN:HG2	2.10	0.52
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.92	0.52
1:A:79:SER:OG	1:A:80:SER:N	2.43	0.52
1:A:470:PHE:C	1:A:472:ILE:H	2.18	0.52
1:A:546:LEU:O	1:A:550:VAL:HG23	2.10	0.52
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.45	0.51
1:A:34:GLN:HA	1:A:333:VAL:HG11	1.92	0.51
1:A:563:PHE:CE2	1:A:674:LEU:HD21	2.44	0.51
1:A:489:THR:HB	1:A:490:PRO:CD	2.40	0.51
1:A:582:ALA:HB1	1:A:586:ARG:NE	2.26	0.51
1:A:684:LEU:O	1:A:824:SER:CA	2.57	0.51
1:A:195:LYS:HB3	1:A:196:PHE:HD1	1.73	0.51
1:A:367:ILE:HB	1:A:368:PRO:CD	2.35	0.51
1:A:563:PHE:HE2	1:A:674:LEU:HD21	1.75	0.51
1:A:184:MET:HB2	1:A:762:PHE:CE2	2.46	0.51
1:A:88:VAL:O	1:A:88:VAL:HG13	2.10	0.51
1:A:897:ILE:H	1:A:898:PRO:CD	2.18	0.51
1:A:1017:LEU:O	1:A:1021:PHE:HD1	1.93	0.50
1:A:187:TRP:CE3	1:A:187:TRP:HA	2.46	0.50
1:A:699:ARG:O	1:A:703:LEU:HG	2.11	0.50
1:A:183:ALA:HB2	1:A:273:GLU:CG	2.42	0.50
1:A:187:TRP:HZ3	1:A:774:MET:HB3	1.76	0.50
1:A:310:LEU:O	1:A:314:GLU:HG3	2.12	0.50
1:A:896:SER:O	1:A:897:ILE:HG13	2.11	0.50
1:A:156:ASP:O	1:A:157:TYR:C	2.52	0.50
1:A:470:PHE:O	1:A:472:ILE:N	2.44	0.50
1:A:485:ALA:HA	1:A:489:THR:HB	1.93	0.50
1:A:68:ASN:O	1:A:110:LYS:CD	2.60	0.50
1:A:971:ARG:CG	1:A:974:PRO:HG2	2.22	0.50
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.94	0.50
1:A:337:ILE:CG2	1:A:338:HIS:H	2.25	0.49
1:A:905:VAL:HG22	1:A:935:ILE:HG23	1.92	0.49
1:A:545:TYR:O	1:A:548:ILE:HB	2.13	0.49
1:A:352:PHE:O	1:A:352:PHE:CD2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.13	0.49
1:A:306:ILE:O	1:A:306:ILE:CG2	2.47	0.49
1:A:187:TRP:HA	1:A:187:TRP:HE3	1.77	0.48
1:A:947:GLU:O	1:A:950:LYS:HB3	2.12	0.48
1:A:450:SER:HA	1:A:453:PHE:HB2	1.94	0.48
1:A:61:VAL:HG13	1:A:118:LEU:HD22	1.95	0.48
1:A:188:MET:HB2	1:A:775:SER:HA	1.95	0.48
1:A:999:ALA:O	1:A:1001:ASN:N	2.46	0.48
1:A:564:LEU:HG	1:A:926:TYR:HE1	1.78	0.48
1:A:293:LEU:HD11	1:A:299:ALA:HB2	1.96	0.48
1:A:914:LEU:O	1:A:915:ALA:C	2.57	0.48
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.94	0.48
1:A:314:GLU:HA	1:A:317:PHE:CE2	2.49	0.48
1:A:344:LEU:HD21	1:A:402:ILE:HD11	1.96	0.47
1:A:414:GLU:HB2	1:A:977:MET:HE1	1.95	0.47
1:A:791:VAL:O	1:A:798:MET:HA	2.14	0.47
1:A:166:ILE:HG22	1:A:175:VAL:HG21	1.95	0.47
1:A:404:LEU:HD23	1:A:478:MET:HG3	1.97	0.47
1:A:591:LEU:HD13	1:A:611:ALA:HB1	1.94	0.47
1:A:925:VAL:O	1:A:926:TYR:C	2.57	0.47
1:A:576:VAL:HB	1:A:625:GLY:HA3	1.95	0.47
1:A:218:GLN:HG2	1:A:233:SER:HA	1.95	0.47
1:A:355:MET:HE3	1:A:355:MET:HA	1.96	0.47
1:A:421:ALA:O	1:A:503:GLY:HA2	2.14	0.47
1:A:817:GLU:O	1:A:818:ARG:CG	2.62	0.47
1:A:534:ILE:HG22	1:A:541:TYR:CE1	2.49	0.47
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.96	0.47
1:A:719:ASN:HB2	1:A:828:LEU:HD23	1.96	0.47
1:A:192:GLU:O	1:A:265:VAL:HG12	2.15	0.47
1:A:310:LEU:C	1:A:312:LYS:H	2.23	0.47
1:A:346:GLU:O	1:A:350:LEU:HD12	2.15	0.47
1:A:448:VAL:HG22	1:A:887:CYS:CB	2.38	0.47
1:A:699:ARG:NE	1:A:718:PRO:HB3	2.30	0.47
1:A:351:VAL:O	1:A:355:MET:HB2	2.15	0.47
1:A:677:ALA:HA	1:A:867:ARG:HH21	1.80	0.47
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.49	0.47
1:A:888:LEU:CB	1:A:898:PRO:HB3	2.45	0.47
1:A:832:ALA:HA	1:A:833:PRO:HD3	1.79	0.46
1:A:49:TYR:HA	1:A:50:PRO:HD2	1.64	0.46
1:A:578:LEU:O	1:A:580:ALA:N	2.49	0.46
1:A:611:ALA:HA	1:A:627:ALA:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:CD1	1:A:196:PHE:N	2.84	0.46
1:A:17:ILE:O	1:A:20:MET:HB2	2.16	0.46
1:A:603:LYS:O	1:A:604:ASN:C	2.59	0.46
1:A:1015:THR:C	1:A:1017:LEU:H	2.24	0.46
1:A:30:LEU:HD12	1:A:31:PRO:HD2	1.97	0.46
1:A:33:ALA:HA	1:A:300:LEU:CD1	2.32	0.46
1:A:963:ALA:O	1:A:964:THR:C	2.58	0.46
1:A:467:TYR:HE1	1:A:868:LEU:HD21	1.81	0.46
1:A:521:GLU:O	1:A:524:THR:HG22	2.16	0.46
1:A:98:THR:HG23	1:A:99:ASP:N	2.31	0.45
1:A:240:LEU:HB3	1:A:245:GLU:HG3	1.98	0.45
1:A:448:VAL:O	1:A:884:VAL:HG22	2.14	0.45
1:A:65:ILE:C	1:A:67:GLN:H	2.24	0.45
1:A:576:VAL:HG21	1:A:591:LEU:HD23	1.98	0.45
1:A:149:MET:HB2	1:A:153:ASP:HB3	1.97	0.45
1:A:905:VAL:HG13	1:A:935:ILE:HD12	1.98	0.45
1:A:338:HIS:CD2	1:A:339:GLU:HG2	2.51	0.45
1:A:559:LEU:HA	1:A:560:PRO:HD3	1.81	0.45
1:A:157:TYR:O	1:A:161:ASN:HB2	2.17	0.45
1:A:616:GLY:C	1:A:618:ALA:H	2.24	0.45
1:A:111:LEU:HD11	1:A:127:VAL:HG11	1.99	0.45
1:A:157:TYR:C	1:A:157:TYR:CD2	2.95	0.45
1:A:183:ALA:HB2	1:A:273:GLU:HG2	1.98	0.45
1:A:435:MET:C	1:A:437:GLN:N	2.75	0.45
1:A:463:THR:HG23	1:A:563:PHE:HE1	1.82	0.45
1:A:199:THR:OG1	1:A:201:VAL:HB	2.17	0.45
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.81	0.44
1:A:239:ARG:NH1	1:A:239:ARG:CG	2.80	0.44
1:A:228:GLN:HG2	1:A:230:LEU:N	2.32	0.44
1:A:902:MET:C	1:A:904:VAL:H	2.23	0.44
1:A:226:LYS:O	1:A:227:GLY:C	2.60	0.44
1:A:782:LEU:O	1:A:785:ASP:HB2	2.17	0.44
1:A:19:ILE:HA	1:A:22:ALA:HB3	1.99	0.44
1:A:633:ASP:O	1:A:635:ALA:N	2.50	0.44
1:A:795:ASP:OD2	1:A:796:GLY:N	2.42	0.44
1:A:987:MET:N	1:A:988:PRO:CD	2.81	0.44
1:A:971:ARG:HG2	1:A:974:PRO:CG	2.23	0.44
1:A:1025:PHE:O	1:A:1026:PHE:C	2.61	0.44
1:A:182:TYR:HD1	1:A:271:GLY:O	2.00	0.44
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.52	0.44
1:A:420:MET:SD	1:A:499:PRO:HA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ALA:HA	1:A:623:ASN:CG	2.43	0.44
1:A:40:PRO:HA	1:A:41:PRO:HD2	1.67	0.44
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.00	0.44
1:A:1020:PHE:C	1:A:1023:PRO:HD2	2.43	0.44
1:A:300:LEU:H	1:A:300:LEU:HD12	1.82	0.44
1:A:626:ILE:HG12	1:A:628:PHE:HE1	1.76	0.44
1:A:897:ILE:HD11	1:A:1030:ARG:HH11	1.83	0.44
1:A:28:LEU:O	1:A:30:LEU:N	2.50	0.43
1:A:377:LEU:O	1:A:380:PHE:HB2	2.19	0.43
1:A:924:ASP:OD1	1:A:924:ASP:C	2.61	0.43
1:A:396:PHE:O	1:A:397:GLY:C	2.60	0.43
1:A:491:ALA:O	1:A:494:ALA:HB3	2.18	0.43
1:A:43:VAL:HG12	1:A:44:THR:N	2.33	0.43
1:A:109:ASN:OD1	1:A:109:ASN:C	2.61	0.43
1:A:673:GLU:C	1:A:675:GLY:H	2.26	0.43
1:A:282:ASN:HD21	1:A:608:SER:HB3	1.83	0.43
1:A:504:ASP:C	1:A:506:GLY:H	2.26	0.43
1:A:594:VAL:O	1:A:595:THR:C	2.61	0.43
1:A:901:VAL:O	1:A:904:VAL:HG23	2.18	0.43
1:A:183:ALA:N	1:A:271:GLY:O	2.41	0.43
1:A:469:GLN:O	1:A:473:THR:OG1	2.26	0.43
1:A:758:TYR:CE1	1:A:770:LYS:HD3	2.52	0.43
1:A:904:VAL:O	1:A:905:VAL:C	2.61	0.43
1:A:672:VAL:O	1:A:673:GLU:HB3	2.18	0.43
1:A:783:PRO:O	1:A:786:ILE:HG12	2.18	0.43
1:A:431:THR:O	1:A:435:MET:N	2.48	0.43
1:A:813:SER:HB3	1:A:816:LEU:HD23	2.01	0.43
1:A:610:PHE:N	1:A:628:PHE:O	2.44	0.43
1:A:1021:PHE:O	1:A:1025:PHE:N	2.46	0.43
1:A:973:ARG:HG2	1:A:977:MET:HE2	2.01	0.42
1:A:162:MET:HA	1:A:313:MET:SD	2.60	0.42
1:A:164:ASP:CG	1:A:767:ARG:HH22	2.28	0.42
1:A:644:VAL:O	1:A:645:GLU:C	2.62	0.42
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.48	0.42
1:A:944:LEU:HB3	1:A:971:ARG:NH2	2.27	0.42
1:A:1012:VAL:O	1:A:1015:THR:OG1	2.34	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.89	0.42
1:A:445:ILE:HB	1:A:449:LEU:HD11	2.01	0.42
1:A:180:SER:OG	1:A:273:GLU:HB2	2.19	0.42
1:A:304:ALA:HA	1:A:307:ARG:HH21	1.84	0.42
1:A:325:TYR:HA	1:A:326:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LEU:O	1:A:492:LEU:HG	2.20	0.42
1:A:897:ILE:O	1:A:900:SER:HB3	2.20	0.42
1:A:915:ALA:HB1	1:A:1005:THR:CG2	2.45	0.42
1:A:568:ASP:OD2	1:A:568:ASP:C	2.62	0.42
1:A:965:LEU:O	1:A:968:VAL:HG12	2.19	0.42
1:A:365:THR:O	1:A:368:PRO:HD2	2.19	0.42
1:A:776:GLU:HG2	1:A:777:ALA:H	1.84	0.42
1:A:986:VAL:C	1:A:988:PRO:HD2	2.44	0.42
1:A:467:TYR:CE1	1:A:868:LEU:HD21	2.54	0.42
1:A:564:LEU:HD12	1:A:925:VAL:HB	2.01	0.42
1:A:23:GLY:O	1:A:27:ILE:HG13	2.20	0.42
1:A:330:THR:N	1:A:331:PRO:CD	2.80	0.42
1:A:454:VAL:HB	1:A:455:PRO:HD3	2.00	0.42
1:A:45:ILE:HG23	1:A:129:VAL:HG22	2.00	0.41
1:A:988:PRO:O	1:A:991:ILE:HG12	2.19	0.41
1:A:50:PRO:C	1:A:52:ALA:H	2.28	0.41
1:A:278:ILE:HG13	1:A:613:ASN:HB3	2.01	0.41
1:A:519:MET:H	1:A:519:MET:HG2	1.58	0.41
1:A:722:GLU:CD	1:A:723:ASP:H	2.28	0.41
1:A:75:LEU:CD1	1:A:92:LEU:HD23	2.50	0.41
1:A:114:ALA:HA	1:A:117:LEU:HD12	2.02	0.41
1:A:300:LEU:HD12	1:A:300:LEU:N	2.34	0.41
1:A:721:LEU:HD13	1:A:815:ARG:HB2	2.02	0.41
1:A:151:GLN:HB3	1:A:285:PRO:HB3	2.03	0.41
1:A:216:ALA:HB1	1:A:234:ILE:O	2.21	0.41
1:A:410:ILE:HG22	1:A:411:VAL:N	2.34	0.41
1:A:456:MET:HE1	1:A:877:TYR:HA	2.01	0.41
1:A:474:ILE:O	1:A:478:MET:N	2.49	0.41
1:A:605:ASN:HB3	1:A:637:ARG:HD3	2.02	0.41
1:A:1013:THR:O	1:A:1015:THR:N	2.53	0.41
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.51	0.41
1:A:372:VAL:O	1:A:373:PRO:C	2.61	0.41
1:A:183:ALA:HB2	1:A:273:GLU:HG3	2.02	0.41
1:A:326:PRO:O	1:A:630:SER:HB2	2.20	0.41
1:A:367:ILE:CB	1:A:368:PRO:HD3	2.37	0.41
1:A:475:VAL:O	1:A:478:MET:HB3	2.21	0.41
1:A:605:ASN:ND2	1:A:637:ARG:HG2	2.35	0.41
1:A:961:ILE:C	1:A:963:ALA:H	2.28	0.41
1:A:975:ILE:H	1:A:975:ILE:HG12	1.65	0.41
1:A:337:ILE:O	1:A:338:HIS:C	2.64	0.41
1:A:990:VAL:HG21	1:A:1008:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:C	1:A:472:ILE:N	2.79	0.41
1:A:883:VAL:HA	1:A:886:LEU:HD12	2.03	0.41
1:A:100:ALA:O	1:A:103:ALA:HB3	2.21	0.41
1:A:349:ILE:O	1:A:353:LEU:HG	2.21	0.41
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.36	0.41
1:A:902:MET:C	1:A:904:VAL:N	2.79	0.41
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	2.03	0.41
1:A:445:ILE:O	1:A:449:LEU:HG	2.21	0.41
1:A:685:ILE:HG22	1:A:687:GLN:HG3	2.02	0.41
1:A:574:THR:HB	1:A:665:ALA:CB	2.51	0.40
1:A:845:GLU:HG3	1:A:859:TRP:HE1	1.86	0.40
1:A:610:PHE:HB3	1:A:628:PHE:HB2	2.03	0.40
1:A:1001:ASN:O	1:A:1005:THR:N	2.50	0.40
1:A:242:SER:O	1:A:243:THR:C	2.64	0.40
1:A:144:ASN:ND2	1:A:149:MET:N	2.69	0.40
1:A:211:ASN:HB2	1:A:240:LEU:HD12	2.03	0.40
1:A:367:ILE:C	1:A:369:THR:N	2.80	0.40
1:A:164:ASP:O	1:A:168:ARG:NH2	2.55	0.40
1:A:184:MET:HB2	1:A:762:PHE:CD2	2.57	0.40
1:A:782:LEU:HB3	1:A:783:PRO:HD2	2.03	0.40
1:A:1013:THR:C	1:A:1015:THR:N	2.79	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	1030/1049 (98%)	782 (76%)	196 (19%)	52 (5%)	1 18

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	133	SER
1	A	226	LYS
1	A	227	GLY
1	A	255	GLN
1	A	352	PHE
1	A	471	SER
1	A	634	TRP
1	A	868	LEU
1	A	992	SER
1	A	29	LYS
1	A	41	PRO
1	A	80	SER
1	A	254	ASN
1	A	308	ALA
1	A	383	LEU
1	A	406	VAL
1	A	674	LEU
1	A	862	MET
1	A	897	ILE
1	A	1000	GLN
1	A	1014	ALA
1	A	35	TYR
1	A	50	PRO
1	A	384	ALA
1	A	1017	LEU
1	A	66	GLU
1	A	387	GLY
1	A	439	GLN
1	A	579	PRO
1	A	671	ILE
1	A	991	ILE
1	A	1025	PHE
1	A	62	THR
1	A	306	ILE
1	A	716	VAL
1	A	796	GLY
1	A	833	PRO
1	A	834	GLY
1	A	1016	VAL
1	A	428	LYS
1	A	464	GLY
1	A	759	VAL

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Mol	Chain	Res	Type
1	A	852	PRO
1	A	51	GLY
1	A	320	GLY
1	A	427	PRO
1	A	173	GLY
1	A	920	GLY
1	A	249	ILE
1	A	326	PRO
1	A	337	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	838/855 (98%)	705 (84%)	133 (16%)	2 14

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	17	ILE
1	A	19	ILE
1	A	21	LEU
1	A	38	ILE
1	A	48	SER
1	A	58	GLN
1	A	60	THR
1	A	64	VAL
1	A	89	GLN
1	A	91	THR
1	A	98	THR
1	A	102	ILE
1	A	109	ASN
1	A	118	LEU
1	A	122	VAL
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	138	MET
1	A	149	MET
1	A	151	GLN
1	A	152	GLU
1	A	187	TRP
1	A	196	PHE
1	A	197	GLN
1	A	205	THR
1	A	214	VAL
1	A	222	THR
1	A	225	VAL
1	A	239	ARG
1	A	241	THR
1	A	243	THR
1	A	246	PHE
1	A	251	LEU
1	A	253	VAL
1	A	259	ARG
1	A	267	LYS
1	A	268	ILE
1	A	291	ILE
1	A	301	ASP
1	A	302	THR
1	A	307	ARG
1	A	321	LEU
1	A	323	ILE
1	A	330	THR
1	A	337	ILE
1	A	338	HIS
1	A	343	THR
1	A	344	LEU
1	A	349	ILE
1	A	365	THR
1	A	370	ILE
1	A	376	LEU
1	A	389	SER
1	A	400	LEU
1	A	408	ASP
1	A	410	ILE
1	A	418	ARG
1	A	449	LEU
1	A	452	VAL

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Mol	Chain	Res	Type
1	A	459	PHE
1	A	463	THR
1	A	476	SER
1	A	484	VAL
1	A	486	LEU
1	A	502	LYS
1	A	519	MET
1	A	534	ILE
1	A	538	THR
1	A	544	LEU
1	A	546	LEU
1	A	557	VAL
1	A	564	LEU
1	A	568	ASP
1	A	573	MET
1	A	578	LEU
1	A	583	THR
1	A	589	LYS
1	A	595	THR
1	A	603	LYS
1	A	608	SER
1	A	620	ARG
1	A	624	THR
1	A	640	GLU
1	A	641	GLU
1	A	645	GLU
1	A	649	MET
1	A	658	ILE
1	A	659	LYS
1	A	660	ASP
1	A	666	PHE
1	A	668	LEU
1	A	673	GLU
1	A	674	LEU
1	A	683	GLU
1	A	695	LEU
1	A	696	THR
1	A	702	LEU
1	A	713	LEU
1	A	715	SER
1	A	723	ASP
1	A	724	THR

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Mol	Chain	Res	Type
1	A	743	ILE
1	A	759	VAL
1	A	760	ASN
1	A	768	VAL
1	A	773	VAL
1	A	778	LYS
1	A	797	GLN
1	A	799	VAL
1	A	828	LEU
1	A	843	LEU
1	A	853	THR
1	A	872	GLN
1	A	880	SER
1	A	901	VAL
1	A	921	LEU
1	A	934	THR
1	A	947	GLU
1	A	961	ILE
1	A	968	VAL
1	A	971	ARG
1	A	972	LEU
1	A	975	ILE
1	A	976	LEU
1	A	980	LEU
1	A	990	VAL
1	A	991	ILE
1	A	993	THR
1	A	1007	VAL
1	A	1016	VAL
1	A	1017	LEU
1	A	1024	VAL
1	A	1028	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	63	GLN
1	A	67	GLN
1	A	106	GLN
1	A	125	GLN
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	229	GLN
1	A	237	GLN
1	A	517	ASN
1	A	588	GLN
1	A	605	ASN
1	A	613	ASN
1	A	642	ASN
1	A	697	GLN
1	A	700	ASN
1	A	733	GLN
1	A	846	GLN
1	A	871	ASN
1	A	928	GLN
1	A	1001	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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
2	DXC	A	2034	-	31,31,31	2.23	3 (9%)	49,49,49	1.77	10 (20%)

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
2	DXC	A	2034	-	-	9/9/71/71	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2034	DXC	C16-C15	11.22	1.84	1.54
2	A	2034	DXC	C15-C11	2.97	1.60	1.54
2	A	2034	DXC	C16-C17	2.68	1.59	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2034	DXC	C15-C11-C12	6.76	110.09	103.54
2	A	2034	DXC	C15-C16-C17	-3.75	97.81	105.14
2	A	2034	DXC	C16-C17-C19	3.34	117.23	112.18
2	A	2034	DXC	C4-C10-C9	3.20	115.68	112.43
2	A	2034	DXC	C16-C15-C11	-2.90	99.46	105.14
2	A	2034	DXC	C21-C19-C17	2.58	115.68	110.33
2	A	2034	DXC	C24-C19-C17	-2.05	109.81	112.88
2	A	2034	DXC	C18-C4-C5	-2.05	105.05	108.31
2	A	2034	DXC	C6-C5-C4	2.04	116.18	112.74
2	A	2034	DXC	C5-C4-C3	2.03	110.66	107.75

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2034	DXC	C12-C17-C19-C24
2	A	2034	DXC	C12-C17-C19-C21
2	A	2034	DXC	C16-C17-C19-C24
2	A	2034	DXC	C16-C17-C19-C21
2	A	2034	DXC	C19-C21-C22-C23
2	A	2034	DXC	C17-C19-C21-C22

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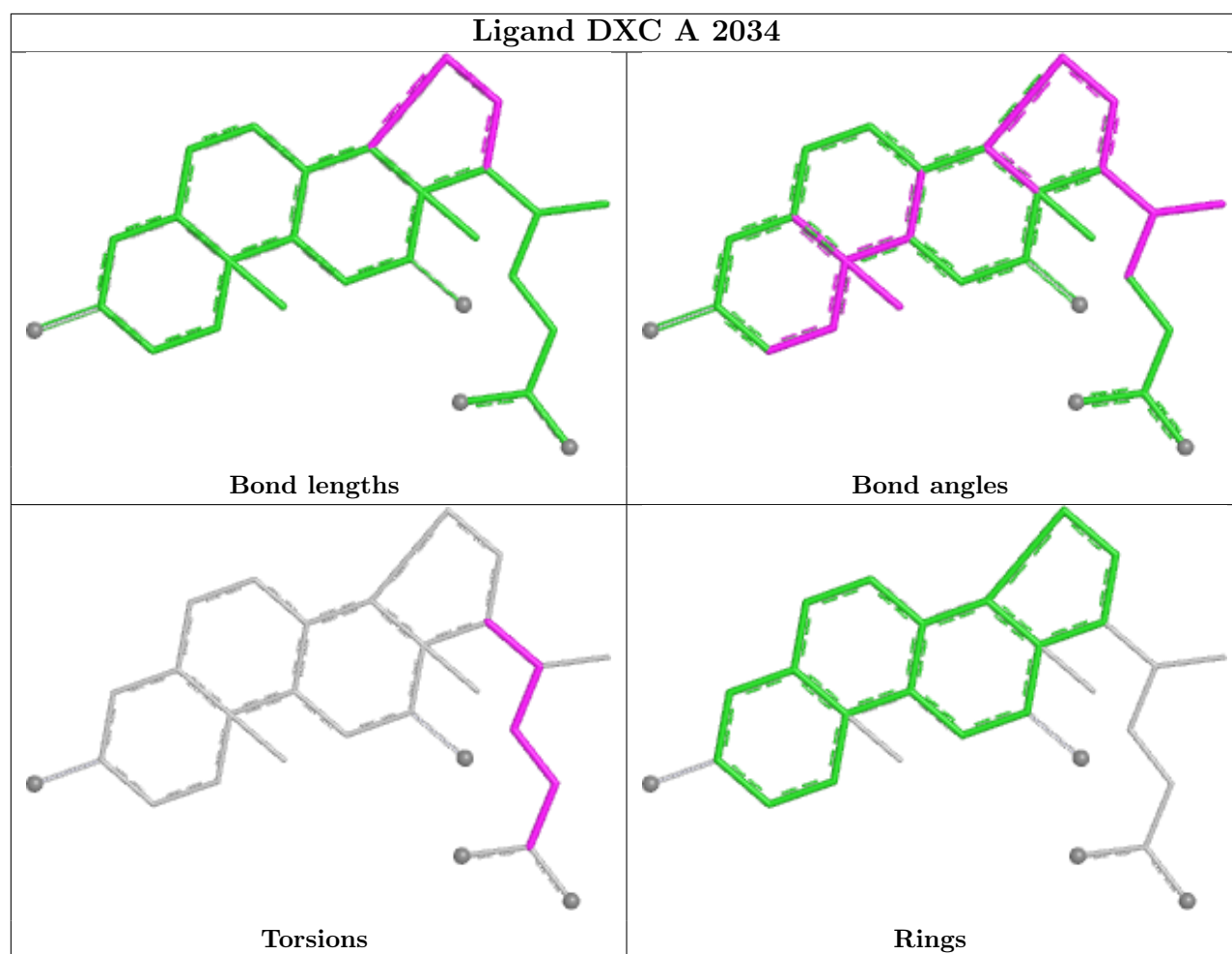
Mol	Chain	Res	Type	Atoms
2	A	2034	DXC	C21-C22-C23-O3
2	A	2034	DXC	C21-C22-C23-O4
2	A	2034	DXC	C24-C19-C21-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2034	DXC	1	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	1032/1049 (98%)	0.46	54 (5%)	33 26	48, 74, 98, 106	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	635	ALA	6.2
1	A	401	ALA	6.0
1	A	305	ALA	5.8
1	A	831	ALA	5.3
1	A	408	ASP	4.6
1	A	448	VAL	4.2
1	A	461	GLY	4.0
1	A	866	GLU	3.9
1	A	714	THR	3.7
1	A	302	THR	3.6
1	A	443	VAL	3.4
1	A	67	GLN	3.3
1	A	405	LEU	3.2
1	A	640	GLU	3.2
1	A	852	PRO	3.1
1	A	569	GLN	3.1
1	A	425	LEU	3.1
1	A	873	ALA	3.0
1	A	299	ALA	3.0
1	A	59	ASP	2.9
1	A	404	LEU	2.9
1	A	840	ALA	2.9
1	A	994	GLY	2.8
1	A	871	ASN	2.6
1	A	151	GLN	2.6
1	A	423	GLU	2.6
1	A	833	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	332	PHE	2.6
1	A	893	GLU	2.5
1	A	711	ASP	2.5
1	A	65	ILE	2.4
1	A	486	LEU	2.3
1	A	565	PRO	2.3
1	A	447	MET	2.3
1	A	301	ASP	2.3
1	A	303	ALA	2.3
1	A	872	GLN	2.2
1	A	306	ILE	2.2
1	A	384	ALA	2.2
1	A	619	GLY	2.2
1	A	865	GLN	2.1
1	A	867	ARG	2.1
1	A	166	ILE	2.1
1	A	32	VAL	2.1
1	A	512	PHE	2.1
1	A	658	ILE	2.1
1	A	451	ALA	2.1
1	A	462	SER	2.1
1	A	702	LEU	2.1
1	A	843	LEU	2.1
1	A	304	ALA	2.0
1	A	713	LEU	2.0
1	A	503	GLY	2.0
1	A	861	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

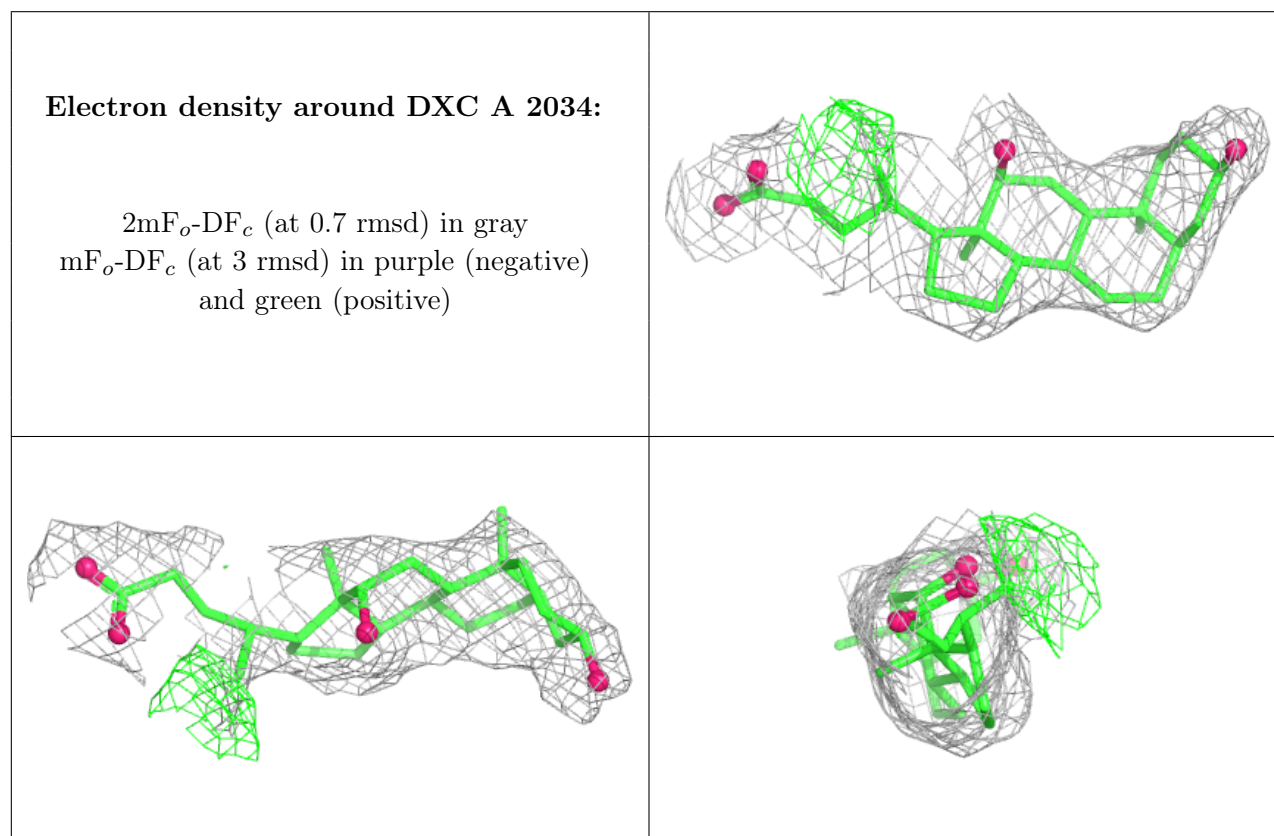
6.4 Ligands [i](#)

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DXC	A	2034	28/28	0.77	0.18	99,104,105,105	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.