Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 05:32 am GMT

PDB ID	:	2W1B
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:

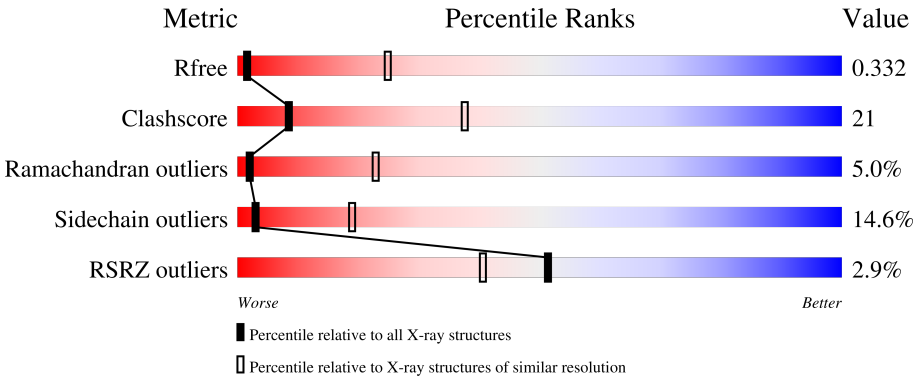
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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}	130704	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1049	3% 52% 39% 7%

2 Entry composition

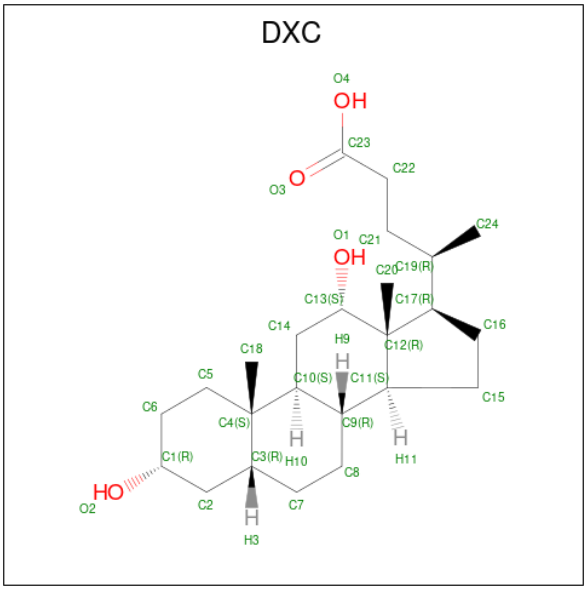
There are 2 unique types of molecules in this entry. The entry contains 7869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	1032	7841	5047	1294	1457	43	0	0	0

- Molecule 2 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: $C_{24}H_{40}O_4$).



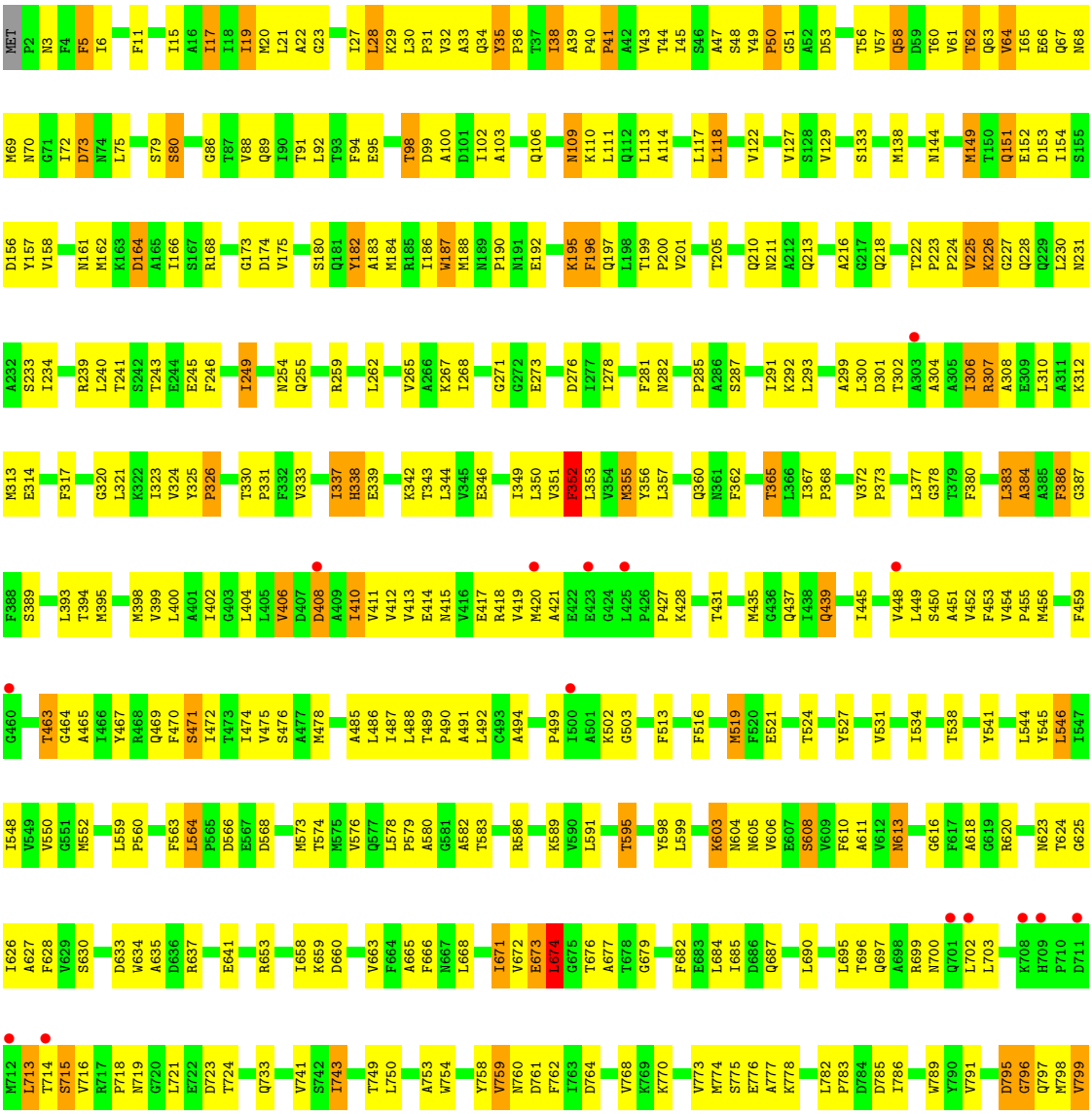
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	28	24	4	0	0

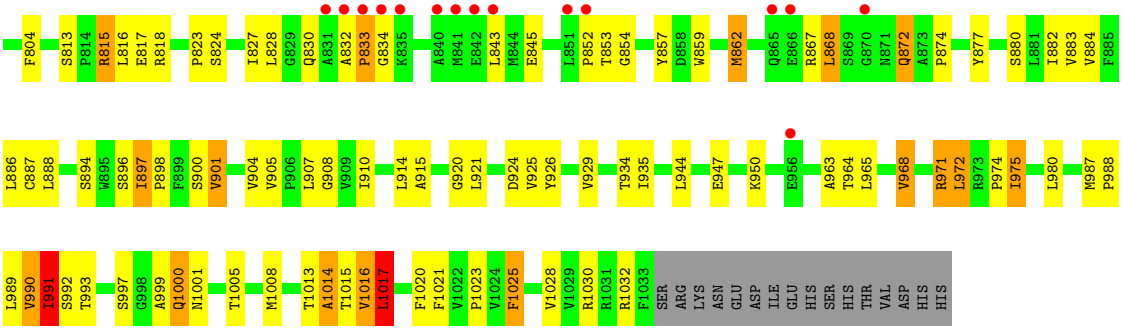
3 Residue-property plots (i)

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

• Molecule 1: ACRIFLAVIN RESISTANCE PROTEIN B

Chain A:




F804
S813
P814
R815
L816
E817
R818
P823
S824
I827
L828
G829
Q830
A831
A832
P833
G834
K835
A840
M841
E842
L843
M844
E845
L851
P852
T853
G854
Y857
D858
W859
M862
Q865
E866
R867
L868
S869
G870
N871
Q872
A873
P874
Y877
S880
L881
I882
V883
V884
F885
L886
C887
L888
S894
W895
S896
I897
P898
F899
S900
V901
V904
V905
P906
L907
G908
V909
I910
L914
A915
G920
L921
D924
V925
Y926
V929
T934
I935
L944
E947
K950
E956
A963
T964
L965
V968
R971
L972
R973
P974
I975
L980
M987
P988
L989
V990
I991
S992
T993
S997
G998
A999
Q1000
N1001
T1005
M1008
T1013
A1014
T1015
V1016
L1017
F1020
F1021
V1022
P1023
V1024
F1025
V1028
V1029
R1030
R1031
R1032
F1033
SER
ARG
LYS
ASN
GLU
ASP
ILE
GLU
HIS
SER
HIS
THR
VAL
ASP
HIS
HIS

4 Data and refinement statistics (i)

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 57.34 – 3.85	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-3.85) 95.2 (57.34-3.85)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.03%)	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)	0.31 , 79.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	2/7991 (0.0%)	0.65	2/10852 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	PHE	CG-CD2	5.22	1.46	1.38
1	A	653	ARG	CB-CG	5.19	1.66	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	713	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	972	LEU	CA-CB-CG	5.15	127.14	115.30

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	329	0
2	A	28	0	39	1	0
All	All	7869	0	8029	330	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 21.

All (330) 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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:990:VAL:HG21	1:A:1008:MET:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:904:VAL:HA	1:A:907:LEU:CD1	2.29	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: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:56:THR:O	1:A:56:THR:HG22	2.06	0.54
1:A:435:MET:C	1:A:437:GLN:H	2.11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:356:TYR:O	1:A:357:LEU:C	2.48	0.52
1:A:57:VAL:HG11	1:A:86:GLY:O	2.10	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: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:1013:THR:C	1:A:1015:THR:H	2.14	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:351:VAL:C	1:A:353:LEU:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:470:PHE:O	1:A:472:ILE:N	2.44	0.50
1:A:817:GLU:C	1:A:818:ARG:HG3	2.32	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:351:VAL:C	1:A:353:LEU:N	2.66	0.49
1:A:352:PHE:O	1:A:352:PHE:CD2	2.59	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:1030:ARG:C	1:A:1032:ARG:H	2.16	0.48
1:A:293:LEU:HD11	1:A:299:ALA:HB2	1.96	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: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: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: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:383:LEU:O	1:A:384:ALA:C	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:C	1:A:472:ILE:H	2.18	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:158:VAL:HG13	1:A:162:MET:HE2	1.97	0.46
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:98:THR:HG23	1:A:99:ASP:N	2.31	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
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: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: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: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:156:ASP:O	1:A:157:TYR:C	2.52	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:111:LEU:HD11	1:A:127:VAL:HG11	1.99	0.45
1:A:183:ALA:HB2	1:A:273:GLU:HG2	1.98	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: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:182:TYR:HD1	1:A:271:GLY:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:282:ASN:HD21	1:A:608:SER:HB3	1.83	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:758:TYR:CE1	1:A:770:LYS:HD3	2.52	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:914:LEU:O	1:A:915:ALA:C	2.57	0.43
1:A:158:VAL:HG22	1:A:162:MET:CE	2.49	0.43
1:A:410:ILE:HG22	1:A:411:VAL:N	2.34	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:925:VAL:O	1:A:926:TYR:C	2.57	0.43
1:A:1021:PHE:O	1:A:1025:PHE:N	2.46	0.43
1:A:162:MET:HA	1:A:313:MET:SD	2.60	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: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
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:310:LEU:C	1:A:312:LYS:H	2.23	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:467:TYR:CE1	1:A:868:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:963:ALA:O	1:A:964:THR:C	2.58	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: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: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: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:184:MET:HA	1:A:184:MET:CE	2.50	0.41
1:A:603:LYS:O	1:A:604:ASN:C	2.59	0.41
1:A:1015:THR:C	1:A:1017:LEU:H	2.24	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:975:ILE:H	1:A:975:ILE:HG12	1.65	0.41
1:A:616:GLY:C	1:A:618:ALA:H	2.24	0.41
1:A:883:VAL:HA	1:A:886:LEU:HD12	2.03	0.41
1:A:65:ILE:C	1:A:67:GLN:H	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:ND2	1:A:149:MET:N	2.69	0.40
1:A:157:TYR:C	1:A:157:TYR:CD2	2.95	0.40
1:A:211:ASN:HB2	1:A:240:LEU:HD12	2.03	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

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%)	2 23

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

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Mol	Chain	Res	Type
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
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 (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	838/855 (98%)	716 (85%)	122 (15%)	3 19

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
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	73	ASP
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	138	MET
1	A	149	MET
1	A	151	GLN
1	A	152	GLU
1	A	164	ASP
1	A	182	TYR
1	A	187	TRP
1	A	195	LYS
1	A	196	PHE
1	A	197	GLN
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	241	THR
1	A	243	THR
1	A	246	PHE

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Mol	Chain	Res	Type
1	A	259	ARG
1	A	267	LYS
1	A	276	ASP
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	338	HIS
1	A	343	THR
1	A	352	PHE
1	A	355	MET
1	A	362	PHE
1	A	365	THR
1	A	386	PHE
1	A	389	SER
1	A	400	LEU
1	A	408	ASP
1	A	410	ILE
1	A	439	GLN
1	A	452	VAL
1	A	459	PHE
1	A	463	THR
1	A	476	SER
1	A	486	LEU
1	A	502	LYS
1	A	519	MET
1	A	538	THR
1	A	544	LEU
1	A	546	LEU
1	A	564	LEU
1	A	566	ASP
1	A	568	ASP
1	A	573	MET
1	A	583	THR
1	A	589	LYS
1	A	595	THR
1	A	603	LYS
1	A	608	SER
1	A	613	ASN
1	A	620	ARG

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Mol	Chain	Res	Type
1	A	624	THR
1	A	641	GLU
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	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
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	795	ASP
1	A	797	GLN
1	A	799	VAL
1	A	804	PHE
1	A	815	ARG
1	A	843	LEU
1	A	853	THR
1	A	872	GLN
1	A	880	SER
1	A	894	SER
1	A	901	VAL
1	A	921	LEU
1	A	934	THR
1	A	968	VAL
1	A	971	ARG
1	A	972	LEU
1	A	975	ILE
1	A	980	LEU
1	A	990	VAL
1	A	991	ILE

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Mol	Chain	Res	Type
1	A	993	THR
1	A	1016	VAL
1	A	1017	LEU
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	63	GLN
1	A	67	GLN
1	A	68	ASN
1	A	106	GLN
1	A	124	GLN
1	A	125	GLN
1	A	176	GLN
1	A	194	ASN
1	A	218	GLN
1	A	229	GLN
1	A	237	GLN
1	A	517	ASN
1	A	604	ASN
1	A	605	ASN
1	A	622	GLN
1	A	642	ASN
1	A	692	HIS
1	A	733	GLN
1	A	871	ASN
1	A	928	GLN
1	A	1001	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	2.22	3 (9%)	49,49,49	1.74	7 (14%)

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	11.17	1.84	1.54
2	A	2034	DXC	C15-C11	2.93	1.60	1.54
2	A	2034	DXC	C16-C17	2.64	1.59	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2034	DXC	C15-C11-C12	6.67	110.09	103.55
2	A	2034	DXC	C15-C16-C17	-3.69	97.81	105.13
2	A	2034	DXC	C16-C17-C19	3.28	117.23	112.15
2	A	2034	DXC	C4-C10-C9	3.10	115.68	112.42
2	A	2034	DXC	C16-C15-C11	-2.86	99.46	105.13
2	A	2034	DXC	C21-C19-C17	2.61	115.68	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2034	DXC	C24-C19-C17	-2.04	109.81	112.92

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2034	DXC	C16-C17-C19-C24
2	A	2034	DXC	C12-C17-C19-C24
2	A	2034	DXC	C12-C17-C19-C21
2	A	2034	DXC	C19-C21-C22-C23
2	A	2034	DXC	C16-C17-C19-C21
2	A	2034	DXC	C17-C19-C21-C22
2	A	2034	DXC	C21-C22-C23-O3
2	A	2034	DXC	C21-C22-C23-O4
2	A	2034	DXC	C24-C19-C21-C22

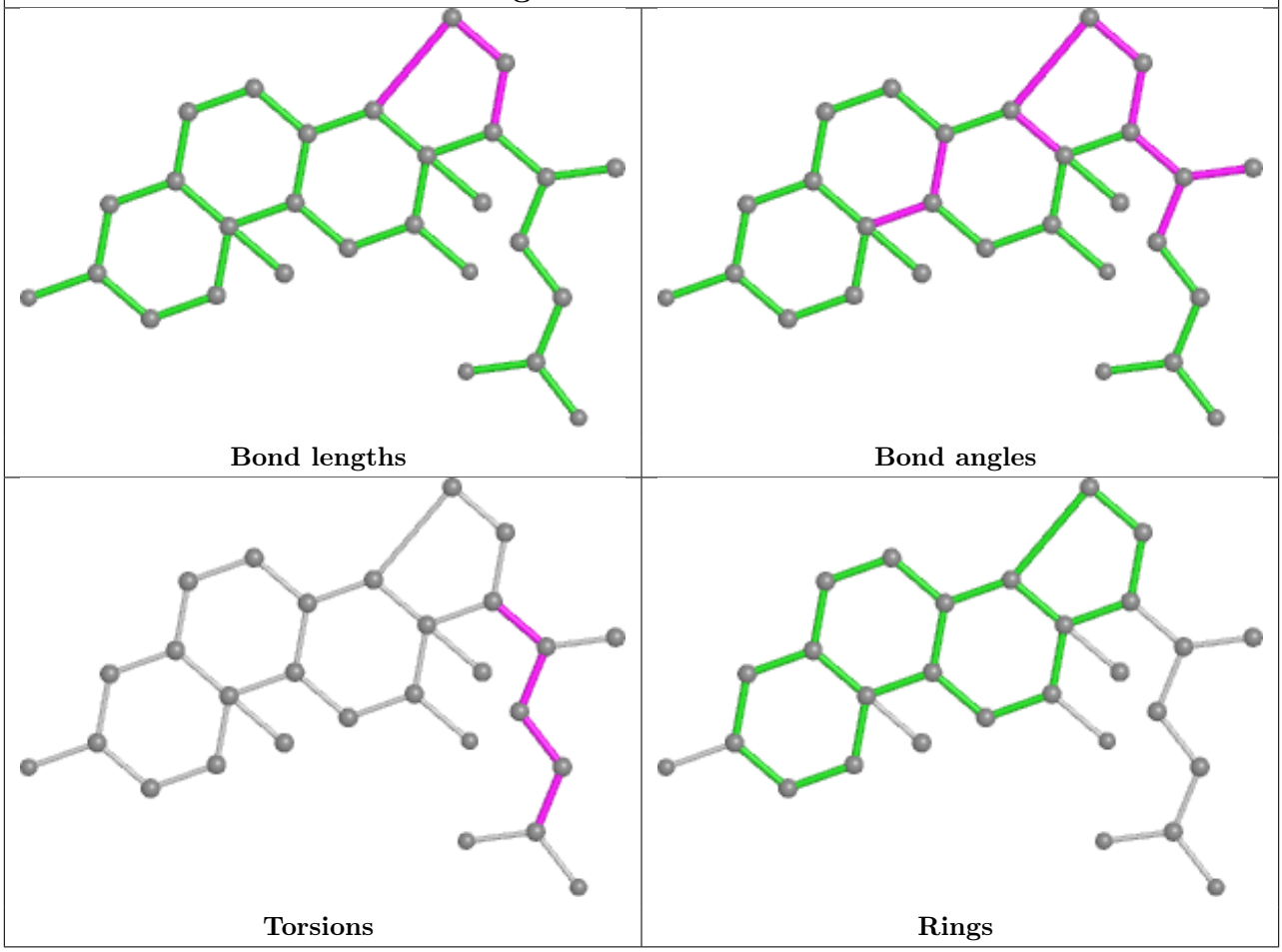
There are no ring outliers.

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

Ligand DXC A 2034



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1032/1049 (98%)	-0.14	30 (2%) 51 40	48, 74, 98, 106	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	714	THR	3.9
1	A	866	GLU	3.8
1	A	833	PRO	3.6
1	A	423	GLU	3.3
1	A	425	LEU	3.2
1	A	709	HIS	3.2
1	A	708	LYS	3.1
1	A	835	LYS	3.1
1	A	852	PRO	3.0
1	A	712	MET	2.9
1	A	843	LEU	2.9
1	A	701	GLN	2.9
1	A	500	ILE	2.6
1	A	834	GLY	2.6
1	A	865	GLN	2.6
1	A	420	MET	2.5
1	A	460	GLY	2.4
1	A	840	ALA	2.4
1	A	841	MET	2.3
1	A	832	ALA	2.3
1	A	842	GLU	2.2
1	A	408	ASP	2.2
1	A	448	VAL	2.2
1	A	851	LEU	2.2
1	A	870	GLY	2.1
1	A	702	LEU	2.1
1	A	956	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	303	ALA	2.1
1	A	711	ASP	2.1
1	A	831	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

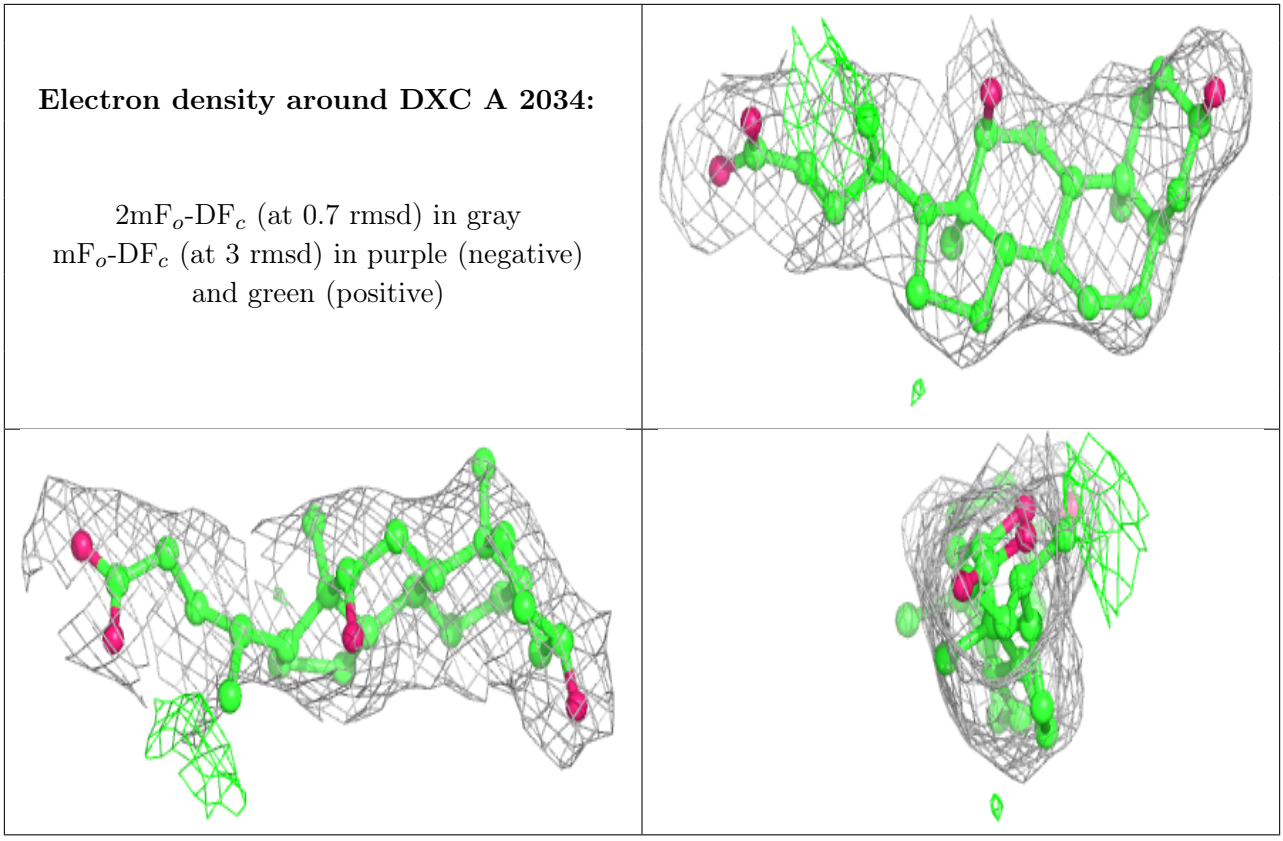
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DXC	A	2034	28/28	0.87	0.26	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.

Electron density around DXC A 2034:

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



6.5 Other polymers (i)

There are no such residues in this entry.