Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:25 PM GMT

PDB ID	:	1OYD
Title	:	Structural Basis of Multiple Binding Capacity of the AcrB multidrug Efflux Pump
Authors	:	Yu, E.W.; MeDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on	:	2003-04-03
Resolution	:	3.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

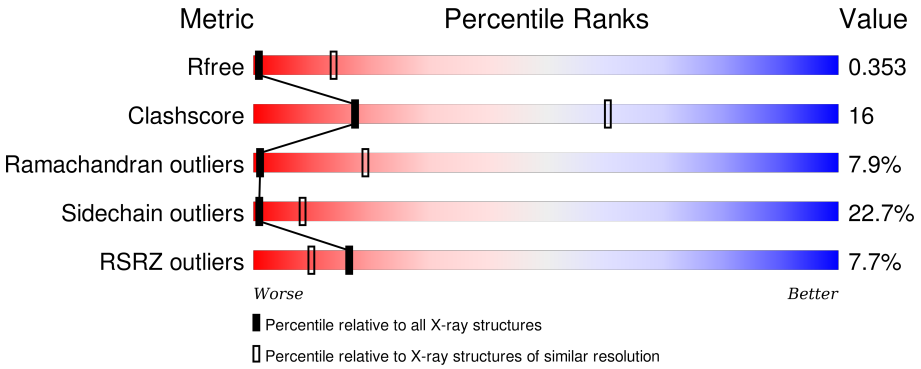
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	7% 54% 33% 8%

2 Entry composition

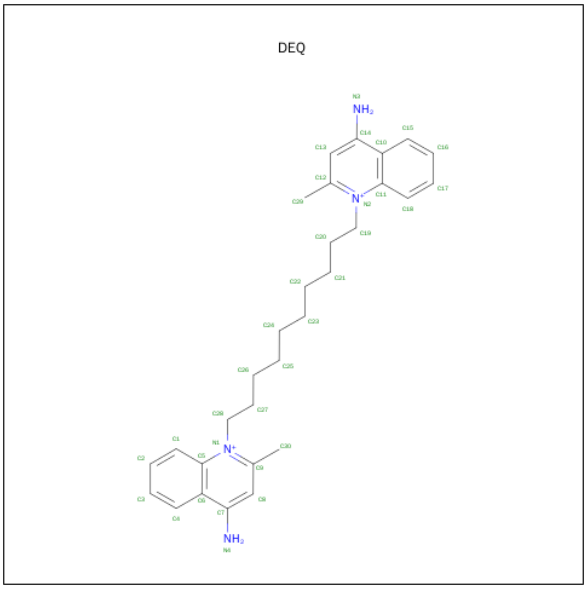
There are 2 unique types of molecules in this entry. The entry contains 7673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0	0
			7639	4916	1262	1419	42			

- Molecule 2 is DEQUALINIUM (three-letter code: DEQ) (formula: $C_{30}H_{40}N_4$).



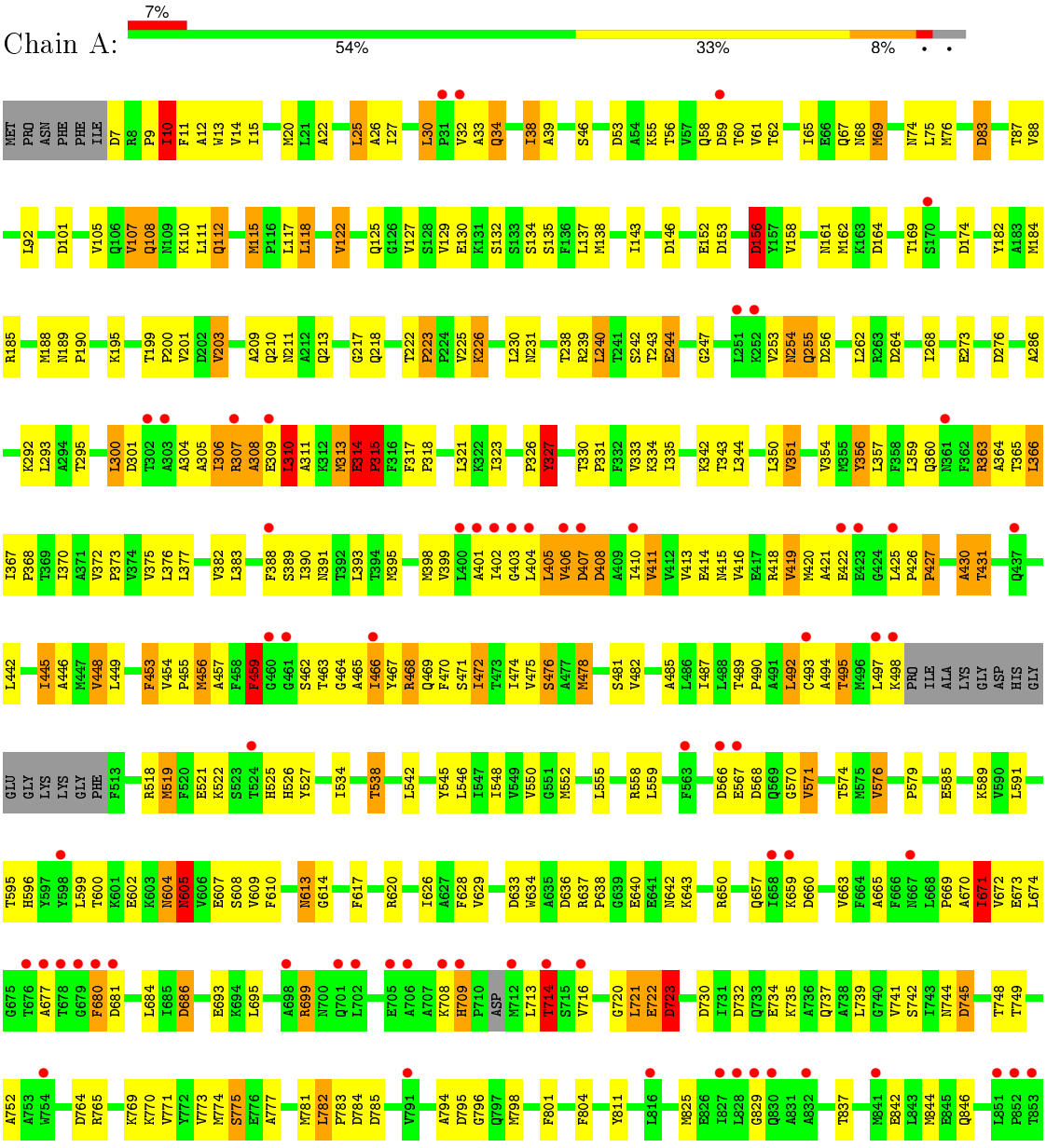
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			34	30	4		

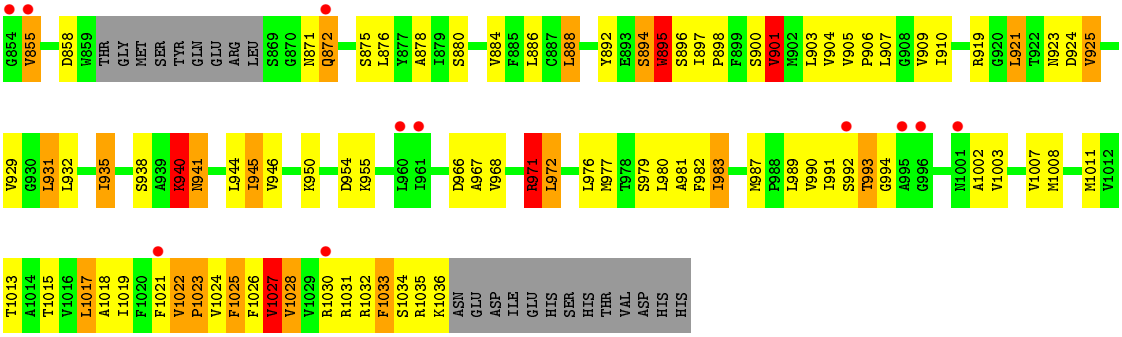
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Acriflavine resistance protein B

Chain A:




G854 V855 D858 W859 THR GLY MET SER TYR GLN GLU ARG LEU S869 G870 N871 Q872 S875 L876 Y877 A878 I879 S880 V884 F885 L886 C887 L888 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 N902 L903 V904 V905 P906 L907 G908 V909 I910 R919 G920 L921 T922 N923 D924 V925
V929 G930 I931 L932 I935 S938 A939 K940 N941 L944 I945 V946 K950 D954 K955 L960 I961 D966 A967 V968 R971 L972 L976 N977 Y978 S979 L980 A981 F982 I983 N987 P988 L989 V990 I991 S992 T993 G994 A995 G996 M1001 A1002 V1003 V1007 M1008 M1011 V1012
T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 R1031 R1032 F1033 S1034 R1035 K1036 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	144.77Å 144.77Å 517.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.80 46.61 – 3.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.80) 99.4 (46.61-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.284 , 0.338 0.375 , 0.353	Depositor DCC
R_{free} test set	1060 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	156.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 92.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 21326 reflections	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DEQ

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	0.36	0/7779	0.75	35/10563 (0.3%)

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
1	A	2	0

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	310	LEU	CA-CB-CG	9.04	136.09	115.30
1	A	315	PRO	N-CA-C	6.82	129.84	112.10
1	A	795	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	568	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	407	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	59	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	723	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	470	PHE	N-CA-C	5.94	127.03	111.00
1	A	858	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	174	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	924	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	680	PHE	N-CA-C	5.47	125.77	111.00
1	A	146	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	730	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	276	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	7	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	566	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	660	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	408	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	784	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	83	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	745	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	764	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	53	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	636	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	966	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	785	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	633	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	101	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	264	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	954	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	156	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	681	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	153	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	732	ASP	CB-CG-OD2	5.01	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	PHE	CA
1	A	680	PHE	CA

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	7639	0	7800	229	1
2	A	34	0	36	20	0
All	All	7673	0	7836	249	1

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 16.

All (249) 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:4001:DEQ:C21	2:A:4001:DEQ:C20	1.80	1.57
2:A:4001:DEQ:C23	2:A:4001:DEQ:C22	1.83	1.52
2:A:4001:DEQ:C28	2:A:4001:DEQ:C27	1.84	1.51
1:A:313:MET:C	1:A:315:PRO:HD3	1.82	0.99
2:A:4001:DEQ:C20	2:A:4001:DEQ:C22	2.51	0.89
1:A:314:GLU:N	1:A:315:PRO:HD3	1.93	0.81
1:A:880:SER:O	1:A:884:VAL:HG23	1.80	0.81
1:A:300:LEU:HD22	1:A:333:VAL:HG11	1.62	0.80
2:A:4001:DEQ:C28	2:A:4001:DEQ:C26	2.61	0.78
2:A:4001:DEQ:C24	2:A:4001:DEQ:C22	2.67	0.72
1:A:941:ASN:HD21	1:A:1015:THR:HG22	1.51	0.72
1:A:613:ASN:C	1:A:613:ASN:HD22	1.89	0.72
1:A:393:LEU:HD11	1:A:466:ILE:HA	1.71	0.72
1:A:613:ASN:HD22	1:A:614:GLY:N	1.89	0.71
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.72	0.70
1:A:670:ALA:O	1:A:671:ILE:O	2.10	0.70
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.75	0.68
1:A:300:LEU:O	1:A:300:LEU:HG	1.93	0.68
1:A:112:GLN:O	1:A:112:GLN:HG2	1.95	0.67
1:A:910:ILE:HG23	1:A:1013:THR:HG21	1.78	0.66
1:A:613:ASN:C	1:A:613:ASN:ND2	2.49	0.65
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.79	0.65
2:A:4001:DEQ:C1	2:A:4001:DEQ:H272	2.26	0.65
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.80	0.64
1:A:709:HIS:O	1:A:709:HIS:CG	2.51	0.64
2:A:4001:DEQ:H11	2:A:4001:DEQ:H272	1.78	0.64
1:A:306:ILE:HA	1:A:308:ALA:C	2.17	0.63
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.81	0.63
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.81	0.63
1:A:407:ASP:OD1	1:A:940:LYS:HG2	1.98	0.63
1:A:308:ALA:O	1:A:311:ALA:HB2	1.99	0.62
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.82	0.62
2:A:4001:DEQ:C27	2:A:4001:DEQ:H11	2.30	0.62
1:A:309:GLU:CG	1:A:310:LEU:HD13	2.30	0.62
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.83	0.61
1:A:10:ILE:HG12	1:A:11:PHE:CD2	2.35	0.61
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.36	0.60
1:A:305:ALA:HA	1:A:306:ILE:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:O	1:A:370:ILE:HG22	2.01	0.60
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.67	0.60
1:A:344:LEU:HD21	1:A:376:LEU:HD11	1.84	0.59
1:A:359:LEU:HD13	1:A:364:ALA:HB1	1.83	0.59
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.84	0.59
1:A:721:LEU:O	1:A:723:ASP:N	2.36	0.59
1:A:453:PHE:HE2	1:A:474:ILE:HB	1.66	0.59
1:A:1026:PHE:O	1:A:1030:ARG:HG2	2.03	0.59
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.38	0.59
1:A:309:GLU:HG2	1:A:310:LEU:HD13	1.84	0.59
1:A:310:LEU:HB2	1:A:313:MET:HB2	1.85	0.58
1:A:454:VAL:N	1:A:455:PRO:HD2	2.18	0.58
1:A:448:VAL:HG11	1:A:888:LEU:HD23	1.84	0.58
1:A:308:ALA:HB1	1:A:309:GLU:HA	1.85	0.58
1:A:457:ALA:HB2	1:A:471:SER:CB	2.34	0.58
1:A:306:ILE:HG23	1:A:308:ALA:O	2.05	0.57
1:A:306:ILE:CG2	1:A:307:ARG:HA	2.34	0.57
1:A:306:ILE:CA	1:A:308:ALA:HB3	2.35	0.57
1:A:314:GLU:N	1:A:315:PRO:CD	2.67	0.56
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.88	0.56
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.87	0.56
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.88	0.56
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.88	0.55
1:A:454:VAL:HG22	1:A:475:VAL:HG21	1.89	0.55
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.60	0.55
1:A:967:ALA:O	1:A:971:ARG:HG3	2.06	0.55
1:A:709:HIS:O	1:A:709:HIS:CD2	2.60	0.55
1:A:304:ALA:O	1:A:306:ILE:HB	2.07	0.55
2:A:4001:DEQ:C21	2:A:4001:DEQ:H201	2.21	0.54
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.90	0.54
1:A:466:ILE:HG23	1:A:925:VAL:HG21	1.89	0.54
1:A:419:VAL:CG1	1:A:430:ALA:HB1	2.38	0.54
2:A:4001:DEQ:C22	2:A:4001:DEQ:H202	2.38	0.54
1:A:716:VAL:HG12	1:A:829:GLY:HA3	1.90	0.54
1:A:308:ALA:HB1	1:A:309:GLU:C	2.28	0.54
1:A:468:ARG:O	1:A:472:ILE:HG22	2.08	0.54
1:A:372:VAL:N	1:A:373:PRO:HD2	2.23	0.54
1:A:306:ILE:C	1:A:308:ALA:HB3	2.28	0.53
1:A:576:VAL:HG13	1:A:663:VAL:HG22	1.88	0.53
1:A:907:LEU:O	1:A:1013:THR:HG22	2.09	0.53
2:A:4001:DEQ:C18	2:A:4001:DEQ:H201	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG22	1:A:748:THR:HG23	1.89	0.53
1:A:309:GLU:HB3	1:A:310:LEU:HD22	1.90	0.53
1:A:901:VAL:O	1:A:904:VAL:HG22	2.09	0.53
1:A:745:ASP:O	1:A:749:THR:OG1	2.24	0.53
1:A:752:ALA:O	1:A:774:MET:HA	2.09	0.52
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.09	0.52
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.92	0.52
1:A:92:LEU:HD13	1:A:107:VAL:HG21	1.92	0.52
2:A:4001:DEQ:C27	2:A:4001:DEQ:N1	2.68	0.52
1:A:308:ALA:HB1	1:A:309:GLU:CA	2.40	0.52
1:A:425:LEU:C	1:A:427:PRO:HD2	2.30	0.52
1:A:39:ALA:HB2	1:A:672:VAL:HG11	1.92	0.52
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.91	0.52
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.40	0.51
1:A:442:LEU:HA	1:A:445:ILE:HD11	1.92	0.51
1:A:534:ILE:HD12	1:A:1026:PHE:HE1	1.75	0.51
1:A:401:ALA:HB2	1:A:474:ILE:HG23	1.92	0.51
1:A:570:GLY:O	1:A:571:VAL:HG23	2.11	0.51
1:A:774:MET:O	1:A:775:SER:CB	2.58	0.51
1:A:546:LEU:O	1:A:550:VAL:HG23	2.10	0.50
1:A:310:LEU:O	1:A:310:LEU:CD2	2.59	0.50
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.93	0.50
1:A:356:TYR:CD1	1:A:365:THR:HG21	2.46	0.50
1:A:326:PRO:O	1:A:327:TYR:C	2.48	0.50
1:A:405:LEU:HD23	1:A:481:SER:HB3	1.92	0.50
1:A:10:ILE:N	1:A:10:ILE:HD13	2.27	0.50
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.93	0.50
1:A:313:MET:CA	1:A:315:PRO:HD3	2.41	0.50
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.40	0.50
2:A:4001:DEQ:H222	2:A:4001:DEQ:H202	1.93	0.49
1:A:306:ILE:HG22	1:A:307:ARG:HA	1.93	0.49
1:A:38:ILE:HG23	1:A:466:ILE:HD11	1.93	0.49
1:A:897:ILE:N	1:A:898:PRO:CD	2.76	0.49
1:A:774:MET:O	1:A:775:SER:HB3	2.12	0.49
1:A:308:ALA:HA	1:A:311:ALA:H	1.77	0.49
1:A:427:PRO:O	1:A:430:ALA:HB3	2.13	0.49
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.92	0.49
1:A:684:LEU:HD23	1:A:699:ARG:HB2	1.95	0.49
2:A:4001:DEQ:C26	2:A:4001:DEQ:H11	2.43	0.49
1:A:402:ILE:HA	1:A:405:LEU:HD12	1.94	0.49
1:A:118:LEU:HD13	1:A:122:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4001:DEQ:H222	2:A:4001:DEQ:C20	2.43	0.49
1:A:38:ILE:HB	1:A:672:VAL:HG21	1.95	0.48
1:A:905:VAL:HG13	1:A:935:ILE:HG12	1.94	0.48
1:A:367:ILE:HG23	1:A:492:LEU:CD1	2.44	0.48
1:A:903:LEU:O	1:A:906:PRO:HD2	2.13	0.48
1:A:637:ARG:HG2	1:A:642:ASN:HB3	1.95	0.48
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.94	0.48
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.14	0.48
1:A:445:ILE:O	1:A:449:LEU:HG	2.13	0.48
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.48
1:A:310:LEU:HD23	1:A:310:LEU:O	2.13	0.48
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.28	0.48
1:A:118:LEU:HD13	1:A:122:VAL:HG11	1.94	0.48
1:A:466:ILE:HD12	1:A:466:ILE:H	1.78	0.48
1:A:713:LEU:O	1:A:714:THR:HG23	2.13	0.48
1:A:979:SER:O	1:A:983:ILE:HG13	2.13	0.48
1:A:112:GLN:O	1:A:112:GLN:CG	2.62	0.48
1:A:25:LEU:C	1:A:25:LEU:HD13	2.34	0.48
1:A:475:VAL:HG22	1:A:478:MET:CE	2.44	0.48
1:A:744:ASN:O	1:A:748:THR:HG22	2.14	0.48
2:A:4001:DEQ:H282	2:A:4001:DEQ:C25	2.44	0.47
1:A:34:GLN:O	1:A:391:ASN:HA	2.13	0.47
1:A:390:ILE:HG22	1:A:390:ILE:O	2.14	0.47
1:A:200:PRO:CD	1:A:749:THR:HG23	2.45	0.47
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.49	0.47
1:A:407:ASP:O	1:A:411:VAL:HG23	2.15	0.47
1:A:604:ASN:O	1:A:605:ASN:ND2	2.47	0.47
2:A:4001:DEQ:C28	2:A:4001:DEQ:C25	2.93	0.47
1:A:403:GLY:HA3	1:A:982:PHE:HD1	1.78	0.47
1:A:695:LEU:HD22	1:A:825:MET:SD	2.55	0.47
1:A:115:MET:O	1:A:118:LEU:HB2	2.15	0.46
1:A:449:LEU:HB2	1:A:478:MET:SD	2.55	0.46
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.97	0.46
1:A:158:VAL:HG22	1:A:162:MET:CE	2.46	0.46
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.98	0.46
1:A:875:SER:O	1:A:878:ALA:HB3	2.16	0.46
1:A:1033:PHE:O	1:A:1034:SER:OG	2.27	0.46
1:A:637:ARG:HG2	1:A:642:ASN:HD22	1.81	0.46
1:A:485:ALA:HA	1:A:489:THR:HB	1.98	0.46
1:A:972:LEU:C	1:A:972:LEU:HD13	2.35	0.46
1:A:390:ILE:HG23	1:A:395:MET:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:HIS:O	1:A:527:TYR:N	2.49	0.46
1:A:931:LEU:O	1:A:935:ILE:HD12	2.15	0.45
1:A:739:LEU:HD23	1:A:739:LEU:N	2.31	0.45
1:A:313:MET:O	1:A:317:PHE:CZ	2.69	0.45
1:A:855:VAL:HG12	1:A:855:VAL:O	2.16	0.45
1:A:383:LEU:HB3	1:A:388:PHE:HB2	1.98	0.45
1:A:493:CYS:SG	1:A:497:LEU:HD22	2.56	0.45
1:A:188:MET:N	1:A:775:SER:HA	2.32	0.45
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.98	0.45
1:A:390:ILE:HG23	1:A:395:MET:SD	2.56	0.45
1:A:222:THR:HB	1:A:223:PRO:HD3	1.98	0.45
1:A:111:LEU:HD23	1:A:111:LEU:C	2.37	0.45
1:A:343:THR:CG2	1:A:989:LEU:HD21	2.47	0.45
1:A:309:GLU:HB3	1:A:310:LEU:HD13	1.99	0.45
1:A:398:MET:O	1:A:402:ILE:HG13	2.17	0.45
1:A:300:LEU:CD2	1:A:333:VAL:HG11	2.39	0.44
1:A:38:ILE:HD13	1:A:672:VAL:HG22	1.99	0.44
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.99	0.44
1:A:25:LEU:HD13	1:A:26:ALA:N	2.33	0.44
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.49	0.44
1:A:993:THR:HB	1:A:994:GLY:CA	2.47	0.44
1:A:892:TYR:HB3	1:A:897:ILE:HG21	2.00	0.44
1:A:367:ILE:HG12	1:A:492:LEU:HD13	1.98	0.44
1:A:465:ALA:HB1	1:A:469:GLN:CG	2.48	0.44
1:A:343:THR:OG1	1:A:989:LEU:HD21	2.18	0.44
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	2.00	0.43
1:A:65:ILE:O	1:A:69:MET:HB2	2.17	0.43
1:A:905:VAL:O	1:A:909:VAL:HG23	2.18	0.43
1:A:10:ILE:N	1:A:10:ILE:CD1	2.81	0.43
1:A:10:ILE:O	1:A:14:VAL:HG23	2.18	0.43
1:A:465:ALA:HB1	1:A:469:GLN:HG3	2.00	0.43
1:A:894:SER:O	1:A:895:TRP:HB2	2.18	0.43
2:A:4001:DEQ:C27	2:A:4001:DEQ:C1	2.93	0.43
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.99	0.43
1:A:686:ASP:CB	1:A:695:LEU:HD12	2.49	0.43
1:A:60:THR:HG23	1:A:61:VAL:HG23	2.01	0.43
1:A:1027:VAL:O	1:A:1030:ARG:N	2.51	0.43
1:A:373:PRO:O	1:A:377:LEU:HG	2.18	0.43
1:A:777:ALA:O	1:A:781:MET:HG2	2.19	0.43
1:A:721:LEU:HD22	1:A:825:MET:CE	2.49	0.43
1:A:426:PRO:N	1:A:427:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:HG2	1:A:469:GLN:N	2.34	0.43
1:A:672:VAL:HG12	1:A:673:GLU:N	2.34	0.43
1:A:399:VAL:O	1:A:402:ILE:HB	2.19	0.43
1:A:453:PHE:HE1	1:A:932:LEU:HB2	1.83	0.43
1:A:367:ILE:HG21	1:A:413:VAL:HG22	2.00	0.43
1:A:306:ILE:HG22	1:A:307:ARG:HD3	2.00	0.42
1:A:203:VAL:CG1	1:A:262:LEU:HD13	2.48	0.42
1:A:466:ILE:HD12	1:A:466:ILE:N	2.35	0.42
1:A:1003:VAL:O	1:A:1007:VAL:HG23	2.20	0.42
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.49	0.42
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.02	0.42
1:A:465:ALA:O	1:A:466:ILE:C	2.58	0.42
1:A:410:ILE:HG22	1:A:411:VAL:N	2.35	0.42
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.68	0.42
1:A:684:LEU:CD1	1:A:855:VAL:HG13	2.50	0.42
1:A:463:THR:HG23	1:A:466:ILE:HG21	2.02	0.41
1:A:929:VAL:HA	1:A:932:LEU:HD12	2.02	0.41
1:A:33:ALA:O	1:A:34:GLN:O	2.38	0.41
1:A:211:ASN:HA	1:A:240:LEU:HD23	2.02	0.41
1:A:468:ARG:CG	1:A:469:GLN:N	2.83	0.41
1:A:376:LEU:O	1:A:398:MET:HE1	2.20	0.41
1:A:456:MET:HA	1:A:876:LEU:HB3	2.02	0.41
1:A:12:ALA:HB1	1:A:487:ILE:HG22	2.02	0.41
1:A:367:ILE:HG23	1:A:492:LEU:HD12	2.02	0.41
1:A:416:VAL:O	1:A:420:MET:HG3	2.21	0.41
1:A:344:LEU:HD21	1:A:376:LEU:CD1	2.49	0.41
1:A:494:ALA:O	1:A:495:THR:C	2.59	0.41
1:A:247:GLY:HA2	1:A:268:ILE:HD12	2.02	0.41
1:A:559:LEU:HD22	1:A:923:ASN:HB2	2.02	0.41
1:A:459:PHE:CD1	1:A:459:PHE:N	2.88	0.41
1:A:38:ILE:HD13	1:A:672:VAL:CG2	2.51	0.41
1:A:921:LEU:CD1	1:A:1002:ALA:HA	2.50	0.41
1:A:453:PHE:CD2	1:A:471:SER:HA	2.56	0.41
1:A:254:ASN:O	1:A:256:ASP:N	2.54	0.41
1:A:782:LEU:CB	1:A:783:PRO:HD2	2.51	0.41
1:A:610:PHE:HB3	1:A:628:PHE:HB2	2.03	0.41
1:A:545:TYR:HA	1:A:548:ILE:HD12	2.03	0.41
1:A:370:ILE:O	1:A:370:ILE:CG2	2.69	0.40
1:A:354:VAL:HG13	1:A:980:LEU:HD23	2.03	0.40
2:A:4001:DEQ:C21	2:A:4001:DEQ:H202	2.21	0.40
1:A:467:TYR:CE2	1:A:925:VAL:HG22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:CD2	1:A:390:ILE:HG13	2.51	0.40
1:A:330:THR:HB	1:A:331:PRO:HD3	2.03	0.40
1:A:896:SER:N	1:A:898:PRO:HD2	2.37	0.40
1:A:534:ILE:HD12	1:A:1026:PHE:CE1	2.56	0.40
1:A:111:LEU:HD23	1:A:111:LEU:O	2.20	0.40
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:O	1:A:596:HIS:NE2[16_445]	1.90	0.30

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	998/1049 (95%)	759 (76%)	160 (16%)	79 (8%)	1 19

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	10	ILE
1	A	34	GLN
1	A	135	SER
1	A	255	GLN
1	A	306	ILE
1	A	308	ALA
1	A	315	PRO
1	A	411	VAL
1	A	431	THR

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Mol	Chain	Res	Type
1	A	459	PHE
1	A	466	ILE
1	A	495	THR
1	A	521	GLU
1	A	522	LYS
1	A	526	HIS
1	A	604	ASN
1	A	671	ILE
1	A	714	THR
1	A	722	GLU
1	A	723	ASP
1	A	775	SER
1	A	794	ALA
1	A	901	VAL
1	A	940	LYS
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	152	GLU
1	A	161	ASN
1	A	209	ALA
1	A	217	GLY
1	A	295	THR
1	A	301	ASP
1	A	327	TYR
1	A	421	ALA
1	A	464	GLY
1	A	552	MET
1	A	605	ASN
1	A	720	GLY
1	A	796	GLY
1	A	872	GLN
1	A	894	SER
1	A	900	SER
1	A	941	ASN
1	A	955	LYS
1	A	971	ARG
1	A	1027	VAL
1	A	74	ASN
1	A	105	VAL
1	A	134	SER

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	571	VAL
1	A	427	PRO
1	A	430	ALA
1	A	472	ILE
1	A	519	MET
1	A	538	THR
1	A	665	ALA
1	A	895	TRP
1	A	75	LEU
1	A	244	GLU
1	A	300	LEU
1	A	363	ARG
1	A	405	LEU
1	A	677	ALA
1	A	837	THR
1	A	22	ALA
1	A	223	PRO
1	A	1033	PHE
1	A	314	GLU
1	A	638	PRO
1	A	490	PRO
1	A	626	ILE
1	A	318	PRO
1	A	579	PRO
1	A	669	PRO
1	A	1028	VAL

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	818/855 (96%)	632 (77%)	186 (23%)	1 8

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	13	TRP
1	A	15	ILE
1	A	20	MET
1	A	25	LEU
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	46	SER
1	A	55	LYS
1	A	58	GLN
1	A	67	GLN
1	A	68	ASN
1	A	69	MET
1	A	76	MET
1	A	83	ASP
1	A	87	THR
1	A	107	VAL
1	A	108	GLN
1	A	110	LYS
1	A	112	GLN
1	A	115	MET
1	A	117	LEU
1	A	118	LEU
1	A	122	VAL
1	A	125	GLN
1	A	127	VAL
1	A	130	GLU
1	A	132	SER
1	A	137	LEU
1	A	138	MET
1	A	156	ASP
1	A	164	ASP
1	A	169	THR
1	A	182	TYR
1	A	185	ARG
1	A	195	LYS
1	A	199	THR
1	A	203	VAL
1	A	210	GLN
1	A	213	GLN
1	A	225	VAL

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Mol	Chain	Res	Type
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	239	ARG
1	A	240	LEU
1	A	242	SER
1	A	243	THR
1	A	244	GLU
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	273	GLU
1	A	292	LYS
1	A	293	LEU
1	A	307	ARG
1	A	310	LEU
1	A	313	MET
1	A	314	GLU
1	A	321	LEU
1	A	323	ILE
1	A	327	TYR
1	A	334	LYS
1	A	335	ILE
1	A	342	LYS
1	A	350	LEU
1	A	351	VAL
1	A	356	TYR
1	A	357	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	408	ASP
1	A	414	GLU
1	A	415	ASN
1	A	418	ARG
1	A	419	VAL
1	A	422	GLU
1	A	431	THR
1	A	445	ILE

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Mol	Chain	Res	Type
1	A	448	VAL
1	A	453	PHE
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	468	ARG
1	A	476	SER
1	A	478	MET
1	A	492	LEU
1	A	498	LYS
1	A	518	ARG
1	A	519	MET
1	A	538	THR
1	A	542	LEU
1	A	555	LEU
1	A	558	ARG
1	A	567	GLU
1	A	574	THR
1	A	576	VAL
1	A	585	GLU
1	A	589	LYS
1	A	591	LEU
1	A	600	THR
1	A	602	GLU
1	A	605	ASN
1	A	607	GLU
1	A	608	SER
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	620	ARG
1	A	629	VAL
1	A	634	TRP
1	A	640	GLU
1	A	643	LYS
1	A	650	ARG
1	A	657	GLN
1	A	659	LYS
1	A	671	ILE
1	A	674	LEU
1	A	680	PHE
1	A	686	ASP

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Mol	Chain	Res	Type
1	A	693	GLU
1	A	699	ARG
1	A	708	LYS
1	A	709	HIS
1	A	714	THR
1	A	721	LEU
1	A	722	GLU
1	A	734	GLU
1	A	735	LYS
1	A	737	GLN
1	A	741	VAL
1	A	742	SER
1	A	765	ARG
1	A	770	LYS
1	A	773	VAL
1	A	782	LEU
1	A	798	MET
1	A	801	PHE
1	A	804	PHE
1	A	811	TYR
1	A	842	GLU
1	A	844	MET
1	A	846	GLN
1	A	855	VAL
1	A	871	ASN
1	A	872	GLN
1	A	886	LEU
1	A	888	LEU
1	A	895	TRP
1	A	901	VAL
1	A	919	ARG
1	A	921	LEU
1	A	925	VAL
1	A	931	LEU
1	A	935	ILE
1	A	938	SER
1	A	940	LYS
1	A	944	LEU
1	A	945	ILE
1	A	950	LYS
1	A	971	ARG
1	A	972	LEU

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Mol	Chain	Res	Type
1	A	976	LEU
1	A	977	MET
1	A	983	ILE
1	A	987	MET
1	A	990	VAL
1	A	991	ILE
1	A	992	SER
1	A	993	THR
1	A	1008	MET
1	A	1017	LEU
1	A	1022	VAL
1	A	1027	VAL
1	A	1028	VAL
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG
1	A	1036	LYS

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	68	ASN
1	A	125	GLN
1	A	161	ASN
1	A	181	GLN
1	A	194	ASN
1	A	218	GLN
1	A	228	GLN
1	A	284	GLN
1	A	391	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	642	ASN
1	A	667	ASN
1	A	760	ASN
1	A	941	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 carbohydrates 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	DEQ	A	4001	-	37,37,37	4.79	18 (48%)	36,50,50	4.91	20 (55%)

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	DEQ	A	4001	-	-	0/13/13/13	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	DEQ	C25-C24	-3.73	1.30	1.51
2	A	4001	DEQ	C30-C9	2.02	1.54	1.49
2	A	4001	DEQ	C3-C4	2.17	1.41	1.36
2	A	4001	DEQ	C16-C15	2.20	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	DEQ	C28-N1	2.29	1.55	1.47
2	A	4001	DEQ	C2-C1	2.44	1.42	1.36
2	A	4001	DEQ	C10-C11	2.44	1.46	1.42
2	A	4001	DEQ	C17-C18	2.48	1.42	1.36
2	A	4001	DEQ	C20-C19	3.10	1.63	1.51
2	A	4001	DEQ	C19-N2	3.14	1.58	1.47
2	A	4001	DEQ	C24-C23	3.33	1.70	1.51
2	A	4001	DEQ	C21-C20	4.95	1.80	1.51
2	A	4001	DEQ	C23-C22	5.45	1.83	1.51
2	A	4001	DEQ	C27-C28	8.81	1.84	1.51
2	A	4001	DEQ	C9-N1	9.05	1.46	1.36
2	A	4001	DEQ	C5-N1	11.11	1.55	1.40
2	A	4001	DEQ	C11-N2	13.33	1.58	1.40
2	A	4001	DEQ	C12-N2	14.96	1.53	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4001	DEQ	C20-C19-N2	-16.33	98.51	112.29
2	A	4001	DEQ	C27-C28-N1	-9.82	104.00	112.29
2	A	4001	DEQ	C29-C12-C13	-3.12	114.92	121.67
2	A	4001	DEQ	C22-C21-C20	-3.11	98.46	114.53
2	A	4001	DEQ	C24-C23-C22	-3.11	98.47	114.53
2	A	4001	DEQ	C18-C11-C10	-2.94	115.60	119.40
2	A	4001	DEQ	C30-C9-C8	-2.80	115.60	121.67
2	A	4001	DEQ	C15-C10-C14	-2.74	118.83	122.87
2	A	4001	DEQ	C17-C18-C11	2.07	123.57	119.32
2	A	4001	DEQ	C26-C25-C24	2.45	127.18	114.53
2	A	4001	DEQ	C10-C14-N3	2.94	129.15	119.96
2	A	4001	DEQ	C27-C26-C25	3.02	130.10	114.53
2	A	4001	DEQ	C18-C11-N2	3.07	124.86	121.15
2	A	4001	DEQ	C30-C9-N1	3.10	125.43	119.76
2	A	4001	DEQ	C1-C5-N1	3.12	124.93	121.15
2	A	4001	DEQ	C13-C12-N2	4.65	123.34	119.51
2	A	4001	DEQ	C25-C24-C23	5.74	144.18	114.53
2	A	4001	DEQ	C28-N1-C5	7.39	126.23	119.06
2	A	4001	DEQ	C21-C20-C19	7.45	140.76	112.38
2	A	4001	DEQ	C19-N2-C11	14.44	133.07	119.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	DEQ	20	0

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	1006/1049 (95%)	0.35	77 (7%) 16 10	131, 162, 176, 194	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	PHE	5.9
1	A	497	LEU	4.9
1	A	461	GLY	4.9
1	A	679	GLY	4.6
1	A	829	GLY	4.4
1	A	680	PHE	4.3
1	A	406	VAL	4.3
1	A	403	GLY	4.2
1	A	303	ALA	4.2
1	A	678	THR	4.2
1	A	402	ILE	4.2
1	A	705	GLU	4.1
1	A	252	LYS	4.0
1	A	460	GLY	3.9
1	A	709	HIS	3.8
1	A	852	PRO	3.7
1	A	996	GLY	3.6
1	A	828	LEU	3.6
1	A	830	GLN	3.5
1	A	960	LEU	3.5
1	A	302	THR	3.4
1	A	706	ALA	3.4
1	A	307	ARG	3.3
1	A	677	ALA	3.3
1	A	1030	ARG	3.3
1	A	658	ILE	3.3
1	A	437	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	410	ILE	3.1
1	A	992	SER	3.1
1	A	708	LYS	3.1
1	A	851	LEU	3.1
1	A	855	VAL	3.1
1	A	31	PRO	3.1
1	A	388	PHE	3.1
1	A	598	TYR	3.1
1	A	423	GLU	3.1
1	A	676	THR	3.0
1	A	407	ASP	2.9
1	A	567	GLU	2.9
1	A	754	TRP	2.9
1	A	995	ALA	2.9
1	A	961	ILE	2.8
1	A	854	GLY	2.8
1	A	400	LEU	2.8
1	A	681	ASP	2.7
1	A	425	LEU	2.6
1	A	498	LYS	2.6
1	A	170	SER	2.4
1	A	698	ALA	2.4
1	A	32	VAL	2.3
1	A	1001	ASN	2.3
1	A	309	GLU	2.3
1	A	563	PHE	2.3
1	A	712	MET	2.3
1	A	832	ALA	2.3
1	A	872	GLN	2.3
1	A	566	ASP	2.2
1	A	401	ALA	2.2
1	A	422	GLU	2.2
1	A	493	CYS	2.2
1	A	716	VAL	2.2
1	A	702	LEU	2.2
1	A	816	LEU	2.1
1	A	659	LYS	2.1
1	A	466	ILE	2.1
1	A	361	ASN	2.1
1	A	714	THR	2.1
1	A	841	MET	2.1
1	A	853	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	251	LEU	2.1
1	A	404	LEU	2.1
1	A	701	GLN	2.1
1	A	524	THR	2.0
1	A	791	VAL	2.0
1	A	667	ASN	2.0
1	A	827	ILE	2.0
1	A	59	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	DEQ	A	4001	34/34	0.49	0.60	-	185,230,396,413	0

6.5 Other polymers (i)

There are no such residues in this entry.