Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:25 PM GMT

PDB ID	:	1OY8
Title	:	Structural Basis of Multiple Drug Binding Capacity of the AcrB Multidrug Efflux Pump
Authors	:	Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on	:	2003-04-03
Resolution	:	3.63 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:

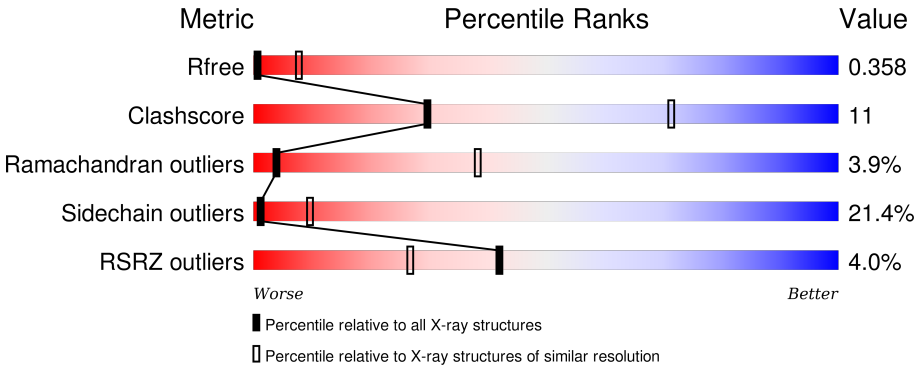
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.63 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	1014 (3.80-3.48)
Clashscore	102246	1130 (3.80-3.48)
Ramachandran outliers	100387	1084 (3.80-3.48)
Sidechain outliers	100360	1083 (3.80-3.48)
RSRZ outliers	91569	1021 (3.80-3.48)

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	4% 59% 30% 6%

2 Entry composition

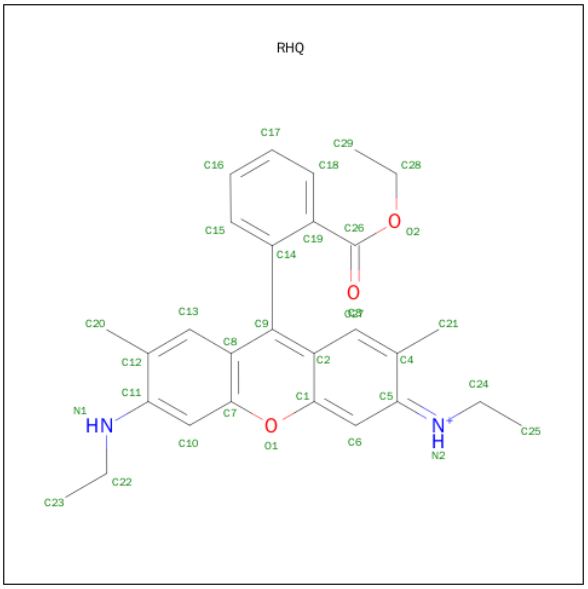
There are 2 unique types of molecules in this entry. The entry contains 7672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	1006	7639	4916	1262	1419	42	0	0	0

- Molecule 2 is RHODAMINE 6G (three-letter code: RHQ) (formula: $C_{28}H_{31}N_2O_3$).



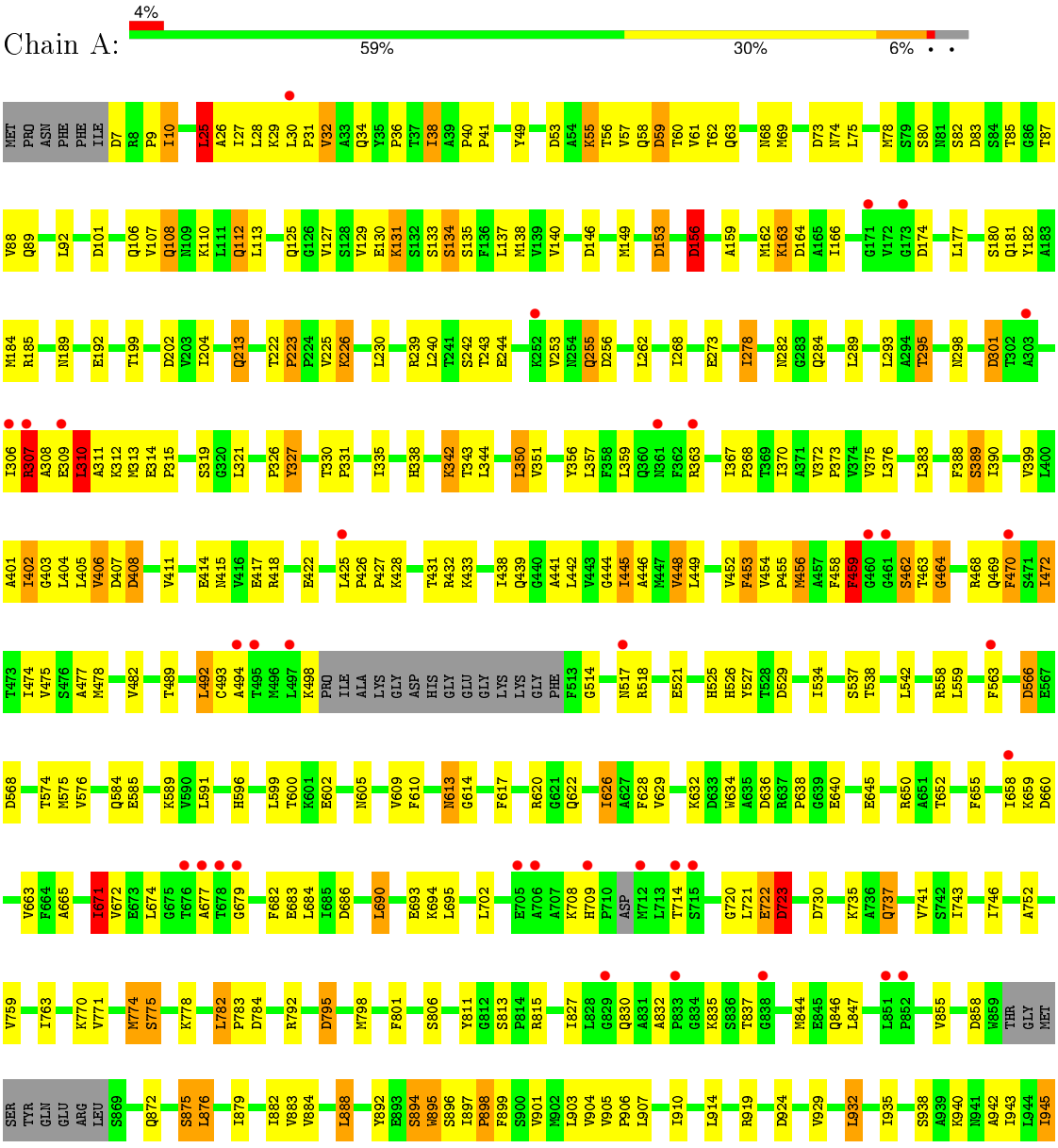
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	28	2	3	0	0

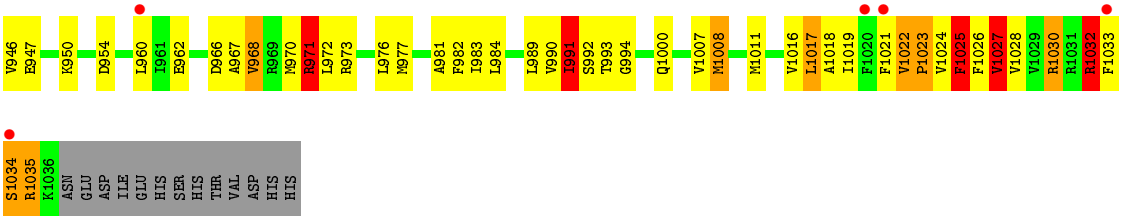
3 Residue-property plots (i)

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:




V946
E947
K950
D954
L960
I961
E962
D966
A967
V968
R969
M970
R971
L972
R973
L976
M977
A981
F982
I983
L984
L989
V990
I991
S992
T993
G994
Q1000
V1007
M1008
M1011
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	144.80Å 144.80Å 518.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.63 46.62 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.63) 99.1 (46.62-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.245 , 0.322 0.361 , 0.358	Depositor DCC
R_{free} test set	1230 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	130.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 24586 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: RHQ

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	1/7779 (0.0%)	0.67	28/10563 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1032	ARG	CZ-NH1	6.24	1.41	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1032	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	723	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	407	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	858	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	25	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	568	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	795	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	310	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	146	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	966	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	59	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	174	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	7	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	153	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	156	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	202	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	53	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	636	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	83	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	730	ASP	CB-CG-OD2	5.22	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	660	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	924	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	566	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	784	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	256	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	101	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	408	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	954	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7639	0	7800	168	0
2	A	33	0	31	6	0
All	All	7672	0	7831	174	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 11.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:O	1:A:307:ARG:HB2	1.74	0.87
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.57	0.85
1:A:308:ALA:HB1	1:A:309:GLU:HA	1.59	0.82
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.62	0.81
1:A:222:THR:HB	1:A:223:PRO:HD3	1.64	0.80
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.62	0.80
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.46	0.79
2:A:2001:RHQ:C24	2:A:2001:RHQ:H211	2.13	0.79
1:A:112:GLN:HG2	1:A:112:GLN:O	1.84	0.76
2:A:2001:RHQ:H241	2:A:2001:RHQ:H211	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HB3	1:A:295:THR:H	1.52	0.74
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.71	0.72
1:A:403:GLY:HA3	1:A:982:PHE:HD1	1.55	0.71
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.26	0.71
1:A:306:ILE:HG23	1:A:307:ARG:H	1.56	0.70
2:A:2001:RHQ:H222	2:A:2001:RHQ:H202	1.73	0.70
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.74	0.70
1:A:372:VAL:N	1:A:373:PRO:HD2	2.07	0.70
1:A:894:SER:O	1:A:895:TRP:HB2	1.92	0.70
1:A:901:VAL:O	1:A:904:VAL:HG22	1.92	0.68
1:A:31:PRO:HG2	1:A:389:SER:HB3	1.78	0.66
1:A:373:PRO:HA	1:A:376:LEU:HD12	1.78	0.65
1:A:159:ALA:HA	1:A:163:LYS:HB3	1.78	0.64
1:A:449:LEU:HB2	1:A:478:MET:SD	2.39	0.63
1:A:929:VAL:HA	1:A:932:LEU:HD12	1.80	0.62
1:A:306:ILE:HG23	1:A:307:ARG:N	2.16	0.60
1:A:610:PHE:HB3	1:A:628:PHE:HB2	1.82	0.60
1:A:456:MET:HA	1:A:876:LEU:HB3	1.81	0.60
1:A:306:ILE:CG2	1:A:307:ARG:N	2.64	0.60
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.82	0.60
1:A:330:THR:HB	1:A:331:PRO:HD3	1.83	0.60
1:A:454:VAL:N	1:A:455:PRO:HD2	2.17	0.60
1:A:1030:ARG:HA	1:A:1034:SER:HB3	1.84	0.60
1:A:298:ASN:HB2	1:A:301:ASP:HB2	1.84	0.59
1:A:463:THR:HG23	1:A:563:PHE:HE1	1.67	0.59
2:A:2001:RHQ:H222	2:A:2001:RHQ:C20	2.32	0.59
1:A:453:PHE:HE2	1:A:474:ILE:HB	1.68	0.57
1:A:472:ILE:HA	1:A:475:VAL:HB	1.86	0.57
1:A:383:LEU:HB3	1:A:388:PHE:HB2	1.85	0.57
1:A:110:LYS:HD3	1:A:113:LEU:HD12	1.85	0.56
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.88	0.55
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.21	0.55
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.89	0.55
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.89	0.55
1:A:470:PHE:HD1	1:A:929:VAL:HG21	1.71	0.54
1:A:709:HIS:O	1:A:709:HIS:CG	2.60	0.54
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.89	0.54
1:A:575:MET:HB3	1:A:626:ILE:HD12	1.91	0.53
1:A:458:PHE:O	1:A:459:PHE:O	2.26	0.53
1:A:10:ILE:HD13	1:A:10:ILE:N	2.25	0.52
1:A:613:ASN:HD22	1:A:613:ASN:C	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG22	1:A:390:ILE:O	2.10	0.51
1:A:993:THR:HB	1:A:994:GLY:CA	2.40	0.51
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.93	0.51
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.93	0.51
1:A:445:ILE:O	1:A:449:LEU:HG	2.10	0.51
1:A:156:ASP:HA	1:A:181:GLN:HA	1.92	0.51
1:A:584:GLN:H	1:A:622:GLN:HE21	1.59	0.51
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.92	0.51
1:A:983:ILE:HG23	1:A:1008:MET:HG2	1.93	0.51
1:A:204:ILE:HG23	1:A:759:VAL:HG13	1.93	0.50
1:A:55:LYS:HE3	1:A:813:SER:H	1.76	0.50
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.94	0.49
1:A:425:LEU:C	1:A:427:PRO:HD2	2.31	0.49
1:A:453:PHE:CE2	1:A:474:ILE:HB	2.47	0.49
1:A:904:VAL:HG11	1:A:942:ALA:HB2	1.93	0.49
1:A:468:ARG:O	1:A:472:ILE:HG22	2.13	0.49
1:A:426:PRO:N	1:A:427:PRO:HD2	2.28	0.49
1:A:75:LEU:HD21	1:A:92:LEU:HD23	1.94	0.49
1:A:576:VAL:HG13	1:A:663:VAL:HG22	1.93	0.49
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.94	0.49
2:A:2001:RHQ:H242	2:A:2001:RHQ:H211	1.95	0.48
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.95	0.48
1:A:879:ILE:HA	1:A:882:ILE:HD12	1.96	0.48
1:A:282:ASN:HD22	1:A:599:LEU:HD21	1.79	0.48
1:A:307:ARG:H	1:A:308:ALA:C	2.17	0.48
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.95	0.48
1:A:671:ILE:H	1:A:671:ILE:HG13	1.40	0.48
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.96	0.48
1:A:456:MET:O	1:A:876:LEU:HD13	2.14	0.47
1:A:306:ILE:C	1:A:308:ALA:HB3	2.35	0.47
1:A:428:LYS:HG2	1:A:494:ALA:HB1	1.96	0.47
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.14	0.47
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.97	0.47
1:A:401:ALA:O	1:A:405:LEU:HG	2.15	0.47
1:A:613:ASN:HD22	1:A:614:GLY:N	2.13	0.47
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.97	0.47
1:A:993:THR:HB	1:A:994:GLY:HA2	1.97	0.47
1:A:993:THR:CB	1:A:994:GLY:HA2	2.44	0.46
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.96	0.46
1:A:721:LEU:O	1:A:723:ASP:N	2.48	0.46
1:A:59:ASP:HA	1:A:63:GLN:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:N	1:A:373:PRO:CD	2.77	0.46
1:A:991:ILE:O	1:A:993:THR:N	2.49	0.46
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.96	0.46
1:A:73:ASP:H	1:A:106:GLN:HE22	1.64	0.46
1:A:879:ILE:O	1:A:883:VAL:HG23	2.16	0.46
1:A:350:LEU:HD12	1:A:984:LEU:HB3	1.98	0.46
1:A:905:VAL:HB	1:A:906:PRO:CD	2.38	0.46
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.98	0.46
1:A:25:LEU:HA	1:A:28:LEU:HD12	1.99	0.45
1:A:166:ILE:HG13	1:A:289:LEU:HD13	1.98	0.45
1:A:414:GLU:O	1:A:417:GLU:HB2	2.16	0.45
1:A:596:HIS:O	1:A:600:THR:HG22	2.16	0.45
1:A:896:SER:HB2	1:A:1032:ARG:HA	1.98	0.45
1:A:489:THR:O	1:A:493:CYS:HB2	2.17	0.45
1:A:897:ILE:C	1:A:899:PHE:H	2.20	0.45
1:A:441:ALA:HB2	1:A:947:GLU:HG2	1.99	0.44
1:A:527:TYR:OH	1:A:1019:ILE:HG13	2.17	0.44
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.98	0.44
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.99	0.44
1:A:213:GLN:HG2	1:A:239:ARG:H	1.82	0.44
1:A:972:LEU:HD23	1:A:1019:ILE:HG12	1.99	0.44
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.99	0.44
1:A:438:ILE:HG22	1:A:442:LEU:HG	1.99	0.44
2:A:2001:RHQ:C20	2:A:2001:RHQ:C22	2.96	0.44
1:A:370:ILE:HG22	1:A:370:ILE:O	2.18	0.44
1:A:307:ARG:N	1:A:308:ALA:C	2.71	0.43
1:A:945:ILE:HG21	1:A:1024:VAL:O	2.18	0.43
1:A:884:VAL:O	1:A:888:LEU:HB2	2.18	0.43
1:A:782:LEU:HB3	1:A:783:PRO:HD2	2.00	0.43
1:A:36:PRO:O	1:A:38:ILE:HG13	2.18	0.43
1:A:967:ALA:HB1	1:A:971:ARG:NH1	2.33	0.43
1:A:56:THR:O	1:A:60:THR:HG22	2.18	0.43
1:A:306:ILE:HG12	1:A:309:GLU:H	1.83	0.43
1:A:32:VAL:HA	1:A:390:ILE:HB	1.99	0.43
1:A:743:ILE:HA	1:A:746:ILE:HD12	1.99	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.51	0.43
1:A:737:GLN:HG2	1:A:737:GLN:H	1.64	0.43
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:945:ILE:HD11	1:A:1019:ILE:HD12	2.01	0.43
1:A:112:GLN:CG	1:A:112:GLN:O	2.61	0.43
1:A:454:VAL:HG22	1:A:475:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:N	1:A:10:ILE:CD1	2.81	0.43
1:A:388:PHE:CE1	1:A:469:GLN:HG2	2.55	0.42
1:A:367:ILE:HG12	1:A:492:LEU:HD22	2.00	0.42
1:A:57:VAL:HG23	1:A:82:SER:HB3	2.01	0.42
1:A:514:GLY:HA2	1:A:517:ASN:HD22	1.84	0.42
1:A:444:GLY:O	1:A:448:VAL:HG23	2.19	0.42
1:A:905:VAL:HG13	1:A:935:ILE:HG12	2.02	0.42
1:A:402:ILE:O	1:A:406:VAL:HG23	2.20	0.42
1:A:534:ILE:HD12	1:A:1026:PHE:HE1	1.85	0.42
1:A:967:ALA:O	1:A:971:ARG:HG3	2.18	0.42
1:A:690:LEU:HB3	1:A:694:LYS:HD2	2.01	0.42
1:A:426:PRO:N	1:A:427:PRO:CD	2.83	0.42
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.91	0.42
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.55	0.42
1:A:517:ASN:O	1:A:521:GLU:HB2	2.20	0.42
1:A:314:GLU:N	1:A:315:PRO:CD	2.83	0.42
1:A:26:ALA:O	1:A:30:LEU:HB2	2.20	0.42
1:A:832:ALA:HB3	1:A:835:LYS:H	1.84	0.42
1:A:162:MET:O	1:A:166:ILE:HG12	2.20	0.41
1:A:405:LEU:HD21	1:A:477:ALA:HB1	2.03	0.41
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	2.02	0.41
1:A:326:PRO:O	1:A:327:TYR:C	2.58	0.41
1:A:752:ALA:O	1:A:774:MET:HA	2.19	0.41
1:A:774:MET:HB3	1:A:775:SER:H	1.62	0.41
1:A:1026:PHE:O	1:A:1030:ARG:HG3	2.21	0.41
1:A:709:HIS:HE1	1:A:847:LEU:HD21	1.85	0.41
1:A:311:ALA:O	1:A:315:PRO:HD3	2.20	0.41
1:A:470:PHE:HA	1:A:470:PHE:HD2	1.68	0.41
1:A:671:ILE:HB	1:A:672:VAL:H	1.48	0.41
1:A:652:THR:HG23	1:A:665:ALA:HB3	2.03	0.41
1:A:312:LYS:HD2	1:A:312:LYS:HA	1.77	0.41
1:A:459:PHE:HB2	1:A:464:GLY:HA2	2.03	0.41
1:A:30:LEU:HA	1:A:31:PRO:HD2	1.94	0.40
1:A:441:ALA:O	1:A:445:ILE:HG13	2.21	0.40
1:A:897:ILE:N	1:A:898:PRO:CD	2.84	0.40
1:A:462:SER:C	1:A:464:GLY:H	2.25	0.40
1:A:133:SER:O	1:A:135:SER:N	2.50	0.40
1:A:602:GLU:HG3	1:A:605:ASN:HB2	2.02	0.40
1:A:338:HIS:O	1:A:342:LYS:HB2	2.21	0.40
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.21	0.40
1:A:679:GLY:HA2	1:A:830:GLN:HA	2.04	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	998/1049 (95%)	858 (86%)	101 (10%)	39 (4%)	4 38

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	255	GLN
1	A	459	PHE
1	A	526	HIS
1	A	671	ILE
1	A	837	THR
1	A	1021	PHE
1	A	1023	PRO
1	A	1034	SER
1	A	307	ARG
1	A	327	TYR
1	A	722	GLU
1	A	876	LEU
1	A	894	SER
1	A	971	ARG
1	A	1017	LEU
1	A	1025	PHE
1	A	9	PRO
1	A	74	ASN
1	A	310	LEU
1	A	295	THR
1	A	525	HIS
1	A	677	ALA
1	A	723	ASP
1	A	875	SER

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Mol	Chain	Res	Type
1	A	134	SER
1	A	226	LYS
1	A	720	GLY
1	A	775	SER
1	A	992	SER
1	A	223	PRO
1	A	898	PRO
1	A	991	ILE
1	A	1027	VAL
1	A	464	GLY
1	A	638	PRO
1	A	1016	VAL
1	A	402	ILE
1	A	658	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	818/855 (96%)	643 (79%)	175 (21%)	1 10

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS
1	A	32	VAL
1	A	38	ILE
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	68	ASN
1	A	69	MET
1	A	78	MET

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Mol	Chain	Res	Type
1	A	80	SER
1	A	85	THR
1	A	87	THR
1	A	89	GLN
1	A	107	VAL
1	A	108	GLN
1	A	112	GLN
1	A	125	GLN
1	A	127	VAL
1	A	130	GLU
1	A	131	LYS
1	A	134	SER
1	A	137	LEU
1	A	138	MET
1	A	140	VAL
1	A	149	MET
1	A	153	ASP
1	A	156	ASP
1	A	163	LYS
1	A	164	ASP
1	A	177	LEU
1	A	180	SER
1	A	182	TYR
1	A	185	ARG
1	A	199	THR
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	240	LEU
1	A	242	SER
1	A	243	THR
1	A	244	GLU
1	A	253	VAL
1	A	255	GLN
1	A	273	GLU
1	A	278	ILE
1	A	284	GLN
1	A	293	LEU
1	A	301	ASP
1	A	307	ARG
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	335	ILE
1	A	342	LYS
1	A	350	LEU
1	A	356	TYR
1	A	357	LEU
1	A	359	LEU
1	A	363	ARG
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	408	ASP
1	A	411	VAL
1	A	415	ASN
1	A	418	ARG
1	A	422	GLU
1	A	431	THR
1	A	432	ARG
1	A	433	LYS
1	A	439	GLN
1	A	445	ILE
1	A	448	VAL
1	A	452	VAL
1	A	453	PHE
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	470	PHE
1	A	472	ILE
1	A	492	LEU
1	A	498	LYS
1	A	518	ARG
1	A	529	ASP
1	A	537	SER
1	A	538	THR
1	A	542	LEU
1	A	558	ARG
1	A	559	LEU
1	A	566	ASP
1	A	574	THR

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Mol	Chain	Res	Type
1	A	585	GLU
1	A	589	LYS
1	A	591	LEU
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	620	ARG
1	A	626	ILE
1	A	629	VAL
1	A	632	LYS
1	A	634	TRP
1	A	640	GLU
1	A	645	GLU
1	A	650	ARG
1	A	659	LYS
1	A	671	ILE
1	A	674	LEU
1	A	683	GLU
1	A	684	LEU
1	A	690	LEU
1	A	693	GLU
1	A	702	LEU
1	A	708	LYS
1	A	714	THR
1	A	722	GLU
1	A	723	ASP
1	A	735	LYS
1	A	737	GLN
1	A	741	VAL
1	A	763	ILE
1	A	770	LYS
1	A	774	MET
1	A	778	LYS
1	A	782	LEU
1	A	792	ARG
1	A	795	ASP
1	A	798	MET
1	A	801	PHE
1	A	806	SER
1	A	811	TYR
1	A	815	ARG
1	A	844	MET

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Mol	Chain	Res	Type
1	A	846	GLN
1	A	855	VAL
1	A	872	GLN
1	A	875	SER
1	A	888	LEU
1	A	895	TRP
1	A	903	LEU
1	A	907	LEU
1	A	910	ILE
1	A	914	LEU
1	A	919	ARG
1	A	932	LEU
1	A	938	SER
1	A	940	LYS
1	A	943	ILE
1	A	945	ILE
1	A	950	LYS
1	A	960	LEU
1	A	962	GLU
1	A	968	VAL
1	A	970	MET
1	A	971	ARG
1	A	973	ARG
1	A	976	LEU
1	A	977	MET
1	A	990	VAL
1	A	991	ILE
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1022	VAL
1	A	1025	PHE
1	A	1027	VAL
1	A	1028	VAL
1	A	1030	ARG
1	A	1032	ARG
1	A	1035	ARG

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	67	GLN

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Mol	Chain	Res	Type
1	A	68	ASN
1	A	106	GLN
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	228	GLN
1	A	231	ASN
1	A	282	ASN
1	A	391	ASN
1	A	517	ASN
1	A	526	HIS
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	747	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	RHQ	A	2001	-	33,36,36	2.60	7 (21%)	40,51,51	1.77	10 (25%)

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	RHQ	A	2001	-	-	0/15/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	RHQ	O1-C1	2.34	1.38	1.35
2	A	2001	RHQ	C9-C8	3.84	1.50	1.43
2	A	2001	RHQ	O2-C26	5.22	1.46	1.33
2	A	2001	RHQ	C19-C14	5.50	1.50	1.40
2	A	2001	RHQ	C11-C12	5.76	1.51	1.40
2	A	2001	RHQ	C8-C7	6.34	1.49	1.41
2	A	2001	RHQ	C2-C9	7.63	1.50	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	RHQ	C2-C9-C8	-3.15	117.24	119.57
2	A	2001	RHQ	C10-C11-N1	-3.13	116.15	121.95
2	A	2001	RHQ	O2-C26-O27	-2.82	118.47	123.66
2	A	2001	RHQ	C21-C4-C3	-2.57	116.98	120.81
2	A	2001	RHQ	C3-C2-C9	-2.54	121.35	124.27
2	A	2001	RHQ	O1-C7-C10	2.58	119.46	116.18
2	A	2001	RHQ	C13-C8-C7	2.83	119.80	116.42
2	A	2001	RHQ	C24-N2-C5	2.96	126.35	120.84
2	A	2001	RHQ	O2-C26-C19	4.33	120.03	112.16
2	A	2001	RHQ	C12-C11-N1	4.49	125.02	119.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	RHQ	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.19	40 (3%) 42 27	55, 101, 129, 149	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	PHE	4.5
1	A	461	GLY	4.4
1	A	960	LEU	4.3
1	A	709	HIS	4.2
1	A	252	LYS	3.8
1	A	497	LEU	3.7
1	A	678	THR	3.6
1	A	307	ARG	3.5
1	A	676	THR	3.2
1	A	425	LEU	3.1
1	A	460	GLY	3.0
1	A	658	ILE	3.0
1	A	1033	PHE	2.9
1	A	852	PRO	2.9
1	A	494	ALA	2.9
1	A	706	ALA	2.9
1	A	712	MET	2.8
1	A	679	GLY	2.8
1	A	171	GLY	2.7
1	A	173	GLY	2.6
1	A	851	LEU	2.6
1	A	677	ALA	2.6
1	A	303	ALA	2.6
1	A	470	PHE	2.6
1	A	517	ASN	2.5
1	A	714	THR	2.5
1	A	715	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	829	GLY	2.4
1	A	563	PHE	2.4
1	A	306	ILE	2.3
1	A	838	GLY	2.2
1	A	361	ASN	2.2
1	A	705	GLU	2.2
1	A	30	LEU	2.2
1	A	495	THR	2.1
1	A	1020	PHE	2.1
1	A	1034	SER	2.1
1	A	833	PRO	2.1
1	A	363	ARG	2.0
1	A	309	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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	RHQ	A	2001	33/33	0.13	1.06	-	169,195,208,210	0

6.5 Other polymers (i)

There are no such residues in this entry.