Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID	:	3B8Q
Title	:	Crystal structure of the VEGFR2 kinase domain in complex with a naphthamide inhibitor
Authors	:	Whittington, D.A.; Long, A.M.; Gu, Y.; Zhao, H.
Deposited on	:	2007-11-01
Resolution	:	2.75 Å(reported)

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 (i)

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

The reported resolution of this entry is 2.75 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		11
Ramachandran outliers		0.7%
Sidechain outliers		1.8%
RSRZ outliers		4.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
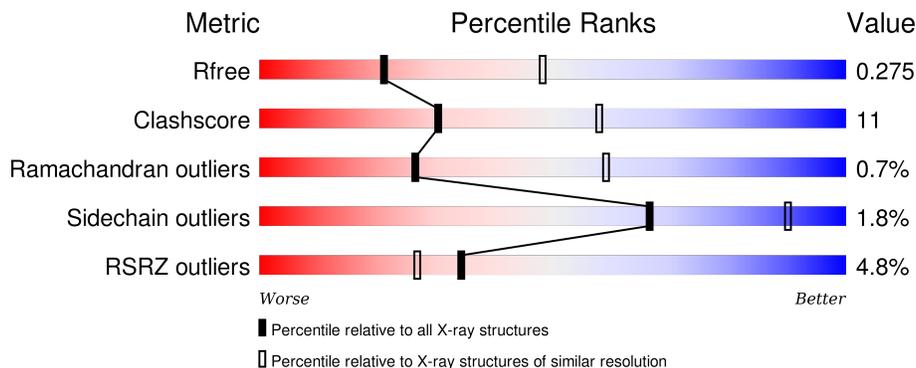
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	314	4% 73% 19% • 7%
1	B	314	5% 63% 23% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4662 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 Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2360	1512	416	416	16			
1	B	271	Total	C	N	O	S	0	0	0
			2167	1394	374	383	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	ALA	CYS	ENGINEERED	UNP P35968
A	916	THR	VAL	ENGINEERED	UNP P35968
A	990	VAL	GLU	ENGINEERED	UNP P35968
A	1172	ARG	-	EXPRESSION TAG	UNP P35968
A	1173	HIS	-	EXPRESSION TAG	UNP P35968
A	1174	HIS	-	EXPRESSION TAG	UNP P35968
A	1175	HIS	-	EXPRESSION TAG	UNP P35968
A	1176	HIS	-	EXPRESSION TAG	UNP P35968
A	1177	HIS	-	EXPRESSION TAG	UNP P35968
A	1178	HIS	-	EXPRESSION TAG	UNP P35968
B	817	ALA	CYS	ENGINEERED	UNP P35968
B	916	THR	VAL	ENGINEERED	UNP P35968
B	990	VAL	GLU	ENGINEERED	UNP P35968
B	1172	ARG	-	EXPRESSION TAG	UNP P35968
B	1173	HIS	-	EXPRESSION TAG	UNP P35968
B	1174	HIS	-	EXPRESSION TAG	UNP P35968
B	1175	HIS	-	EXPRESSION TAG	UNP P35968
B	1176	HIS	-	EXPRESSION TAG	UNP P35968
B	1177	HIS	-	EXPRESSION TAG	UNP P35968
B	1178	HIS	-	EXPRESSION TAG	UNP P35968

- Molecule 2 is N-(4-CHLOROPHENYL)-6-[(6,7-DIMETHOXYQUINOLIN-4-YL)OXY]NAP HTHALENE-1-CARBOXAMIDE (three-letter code: 900) (formula: $C_{28}H_{21}ClN_2O_4$).
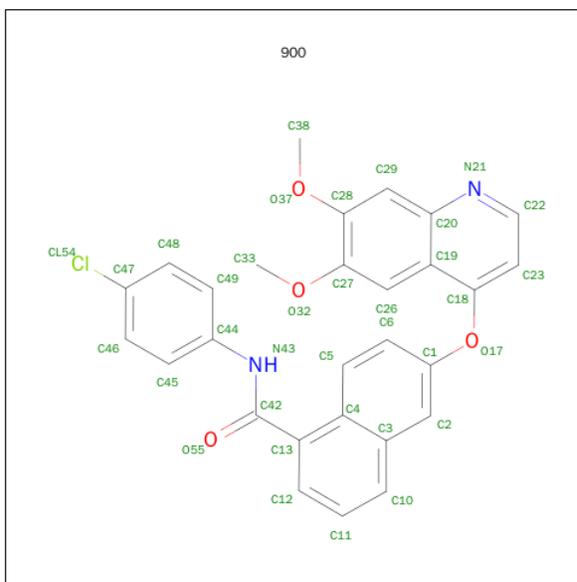
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			35	28	1	2	4		
2	B	1	Total	C	Cl	N	O	0	0
			35	28	1	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	16	Total	O	0	0
			16	16		

3 Residue-property plots ⓘ

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: Vascular endothelial growth factor receptor 2
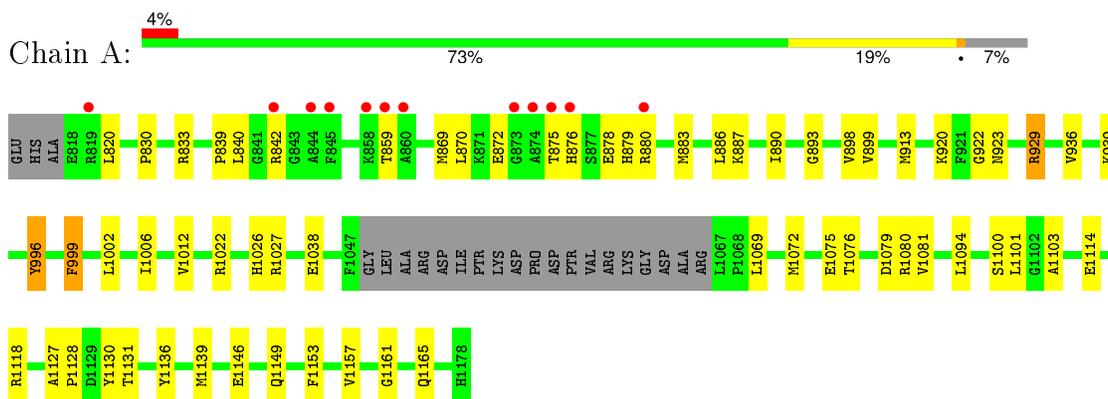
- Molecule 1: Vascular endothelial growth factor receptor 2
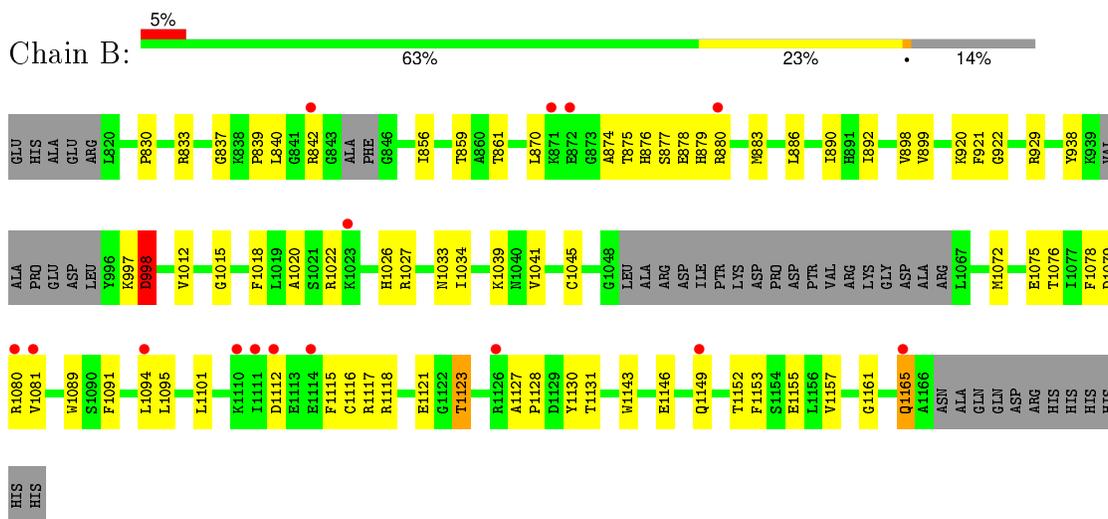
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.12Å 67.78Å 88.09Å 90.00° 92.14° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 29.34 – 2.74	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.75) 93.9 (29.34-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.66 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.276 0.215 , 0.275	Depositor DCC
R_{free} test set	1261 reflections (7.84%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.8	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 16152 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4662	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 900

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	0.40	0/2422	0.65	0/3273
1	B	0.38	0/2218	0.67	3/2992 (0.1%)
All	All	0.39	0/4640	0.66	3/6265 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	998	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	998	ASP	N-CA-C	5.55	126.00	111.00
1	B	998	ASP	CB-CG-OD1	5.12	122.91	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	2360	0	2346	46	0
1	B	2167	0	2179	53	0
2	A	35	0	21	6	0
2	B	35	0	21	5	0
3	A	49	0	0	1	0
3	B	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4662	0	4567	101	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 (101) 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:B:875:THR:HG22	1:B:877:SER:H	1.24	1.01
1:B:997:LYS:O	1:B:998:ASP:HB2	1.66	0.93
2:A:501:900:H382	2:A:501:900:H333	1.48	0.92
1:B:1128:PRO:HG2	1:B:1131:THR:HB	1.62	0.82
1:B:1078:PHE:CZ	1:B:1116:CYS:HB3	2.20	0.76
1:B:874:ALA:HB1	1:B:878:GLU:OE1	1.86	0.75
1:A:1161:GLY:O	1:A:1165:GLN:HG3	1.89	0.72
1:B:1078:PHE:HZ	1:B:1116:CYS:HB3	1.56	0.70
1:B:870:LEU:HD11	1:B:879:HIS:HA	1.74	0.69
1:A:872:GLU:H	1:A:872:GLU:CD	1.97	0.67
1:A:875:THR:HB	1:A:878:GLU:HG3	1.76	0.67
1:A:922:GLY:HA2	2:A:501:900:H383	1.79	0.64
1:B:1127:ALA:HB1	1:B:1131:THR:HG21	1.77	0.64
1:B:1079:ASP:O	1:B:1080:ARG:HB2	1.97	0.64
1:A:1079:ASP:O	1:A:1080:ARG:HB2	1.98	0.63
1:A:922:GLY:CA	2:A:501:900:H383	2.28	0.63
1:A:870:LEU:HD11	1:A:879:HIS:HA	1.80	0.63
1:A:996:TYR:O	1:A:999:PHE:HB2	1.98	0.63
1:B:1075:GLU:HG2	1:B:1076:THR:N	2.14	0.62
1:A:1128:PRO:HG2	1:A:1131:THR:HB	1.80	0.62
1:A:936:VAL:HG22	1:A:999:PHE:HD2	1.65	0.61
1:A:1153:PHE:O	1:A:1157:VAL:HG23	2.00	0.61
1:A:939:LYS:HE2	1:A:996:TYR:HB2	1.82	0.61
1:B:1045:CYS:HB2	2:B:502:900:H5	1.83	0.60
1:A:1079:ASP:HB2	1:A:1081:VAL:HG23	1.83	0.60
1:B:1153:PHE:O	1:B:1157:VAL:HG23	2.02	0.60
1:B:1022:ARG:HH21	1:B:1022:ARG:HG3	1.67	0.59
1:B:856:ILE:HG13	1:B:856:ILE:O	2.06	0.55
1:A:840:LEU:HB3	2:A:501:900:O32	2.06	0.55
1:B:1118:ARG:HA	1:B:1121:GLU:HB3	1.89	0.55
1:A:839:PRO:HG2	1:A:842:ARG:HH11	1.72	0.55
1:A:883:MET:CE	1:A:887:LYS:HE3	2.37	0.54
1:A:820:LEU:O	1:A:887:LYS:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:VAL:HG11	1:B:1094:LEU:CD2	2.39	0.53
1:A:929:ARG:HH11	1:A:929:ARG:HG2	1.73	0.53
1:A:1100:SER:OG	1:A:1103:ALA:HB3	2.08	0.53
1:B:837:GLY:HA3	3:B:1187:HOH:O	2.08	0.53
1:A:1079:ASP:CB	1:A:1081:VAL:HG23	2.38	0.52
1:B:1101:LEU:HD12	1:B:1130:TYR:CZ	2.45	0.52
1:A:886:LEU:O	1:A:890:ILE:HG13	2.10	0.51
1:A:1002:LEU:O	1:A:1006:ILE:HG13	2.09	0.51
1:B:920:LYS:HE3	1:B:921:PHE:CZ	2.45	0.51
1:A:840:LEU:HD13	2:A:501:900:C27	2.41	0.51
1:B:922:GLY:CA	2:B:502:900:H382	2.41	0.50
1:A:1127:ALA:HB1	1:A:1131:THR:HG21	1.93	0.50
1:B:1117:ARG:O	1:B:1121:GLU:N	2.45	0.50
1:B:886:LEU:O	1:B:890:ILE:HG13	2.11	0.50
1:A:1038:GLU:HA	1:A:1038:GLU:OE1	2.12	0.50
1:B:1118:ARG:HB3	1:B:1123:THR:OG1	2.12	0.49
1:B:874:ALA:CB	1:B:878:GLU:OE1	2.58	0.49
1:A:1026:HIS:O	1:A:1027:ARG:HB2	2.13	0.49
1:B:1161:GLY:O	1:B:1165:GLN:HG3	2.12	0.49
1:A:1146:GLU:HB2	1:A:1149:GLN:HG2	1.96	0.48
1:B:1112:ASP:O	1:B:1115:PHE:HB3	2.13	0.47
1:B:1079:ASP:HB2	1:B:1081:VAL:HG23	1.97	0.47
1:B:839:PRO:HG2	1:B:842:ARG:HH11	1.79	0.47
1:A:1069:LEU:HD23	1:A:1072:MET:SD	2.55	0.47
1:A:1128:PRO:O	1:A:1131:THR:HG22	2.14	0.47
1:B:1015:GLY:O	1:B:1018:PHE:HB3	2.15	0.47
1:B:1079:ASP:CB	1:B:1081:VAL:HG23	2.45	0.47
1:B:1072:MET:HE2	1:B:1076:THR:HG22	1.96	0.46
1:B:1118:ARG:HA	1:B:1121:GLU:CB	2.45	0.46
1:B:1128:PRO:CG	1:B:1131:THR:HB	2.40	0.46
1:B:1012:VAL:HG11	1:B:1094:LEU:HD21	1.96	0.46
1:B:1091:PHE:O	1:B:1095:LEU:HG	2.15	0.46
1:A:1101:LEU:HD12	1:A:1130:TYR:CZ	2.51	0.46
1:B:1146:GLU:HB2	1:B:1149:GLN:HG2	1.98	0.46
1:B:840:LEU:HB3	2:B:502:900:O32	2.17	0.45
1:B:875:THR:HG22	1:B:876:HIS:N	2.30	0.45
1:B:883:MET:O	1:B:886:LEU:HB3	2.15	0.45
1:B:1128:PRO:O	1:B:1131:THR:HG22	2.16	0.45
1:B:1152:THR:OG1	1:B:1155:GLU:HG3	2.16	0.45
1:A:893:GLY:HA3	3:A:1208:HOH:O	2.16	0.45
1:B:922:GLY:HA2	2:B:502:900:H382	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1026:HIS:O	1:B:1027:ARG:HB2	2.17	0.45
1:A:922:GLY:HA3	2:A:501:900:H383	1.98	0.44
1:A:869:MET:HB3	1:A:913:MET:HG2	1.99	0.44
1:A:899:VAL:O	1:A:899:VAL:HG13	2.17	0.44
1:B:898:VAL:O	1:B:899:VAL:C	2.56	0.44
1:B:892:ILE:HA	1:B:1022:ARG:HD3	2.00	0.43
1:B:859:THR:O	1:B:861:THR:HG23	2.18	0.43
1:B:1039:LYS:O	1:B:1041:VAL:HG23	2.19	0.43
1:A:1114:GLU:O	1:A:1118:ARG:HG3	2.18	0.43
1:A:1022:ARG:HG3	1:A:1022:ARG:HH21	1.84	0.42
1:B:899:VAL:HG13	1:B:899:VAL:O	2.19	0.42
2:B:502:900:O55	2:B:502:900:H5	2.20	0.42
1:A:883:MET:HE3	1:A:887:LYS:HE3	2.00	0.42
1:A:830:PRO:HB2	1:A:833:ARG:HG2	2.02	0.42
1:B:1020:ALA:C	1:B:1022:ARG:H	2.22	0.41
1:A:898:VAL:O	1:A:899:VAL:C	2.59	0.41
1:A:1075:GLU:HG2	1:A:1076:THR:N	2.36	0.41
1:A:876:HIS:O	1:A:879:HIS:HB3	2.21	0.41
1:A:1079:ASP:O	1:A:1080:ARG:CB	2.63	0.41
1:A:1146:GLU:CB	1:A:1149:GLN:HG2	2.51	0.41
1:A:1136:TYR:O	1:A:1139:MET:HB2	2.20	0.41
1:B:1146:GLU:HB2	1:B:1149:GLN:CG	2.51	0.41
1:B:1033:ASN:O	1:B:1034:ILE:HD13	2.21	0.40
1:A:1012:VAL:HG11	1:A:1094:LEU:CD2	2.52	0.40
1:A:920:LYS:HE2	1:A:1038:GLU:CD	2.42	0.40
1:B:1089:TRP:CE3	1:B:1143:TRP:HA	2.56	0.40
1:B:830:PRO:HB2	1:B:833:ARG:HB2	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	288/314 (92%)	272 (94%)	15 (5%)	1 (0%)	46	77
1	B	263/314 (84%)	244 (93%)	16 (6%)	3 (1%)	17	46
All	All	551/628 (88%)	516 (94%)	31 (6%)	4 (1%)	26	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	859	THR
1	B	998	ASP
1	B	938	TYR
1	B	1165	GLN

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	255/270 (94%)	250 (98%)	5 (2%)	63	89
1	B	235/270 (87%)	231 (98%)	4 (2%)	68	90
All	All	490/540 (91%)	481 (98%)	9 (2%)	66	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	880	ARG
1	A	923	ASN
1	A	929	ARG
1	A	996	TYR
1	A	999	PHE
1	B	880	ARG
1	B	929	ARG
1	B	998	ASP
1	B	1123	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	900	ASN
1	A	933	ASN
1	A	1040	ASN
1	A	1162	ASN
1	A	1165	GLN
1	B	847	GLN
1	B	879	HIS
1	B	894	HIS
1	B	900	ASN
1	B	933	ASN
1	B	1040	ASN
1	B	1162	ASN
1	B	1165	GLN

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 ⓘ

2 ligands are 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	900	A	501	-	39,39,39	1.96	13 (33%)	54,55,55	2.05	6 (11%)
2	900	B	502	-	39,39,39	1.86	15 (38%)	54,55,55	1.98	7 (12%)

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	900	A	501	-	-	0/16/16/16	0/5/5/5
2	900	B	502	-	-	0/16/16/16	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	900	C5-C4	2.02	1.46	1.42
2	B	502	900	C4-C3	2.03	1.46	1.42
2	A	501	900	C22-N21	2.13	1.36	1.32
2	B	502	900	C48-C47	2.15	1.42	1.38
2	B	502	900	C49-C44	2.18	1.42	1.39
2	B	502	900	C11-C12	2.20	1.43	1.38
2	A	501	900	O17-C18	2.26	1.42	1.38
2	A	501	900	C6-C1	2.43	1.43	1.38
2	B	502	900	C11-C10	2.50	1.42	1.36
2	B	502	900	C26-C27	2.53	1.41	1.36
2	B	502	900	C5-C6	2.55	1.42	1.36
2	A	501	900	C11-C10	2.58	1.42	1.36
2	A	501	900	O37-C28	2.58	1.41	1.37
2	B	502	900	C49-C48	2.81	1.43	1.38
2	A	501	900	C5-C6	2.84	1.42	1.36
2	A	501	900	C13-C4	2.85	1.48	1.43
2	A	501	900	C46-C47	3.02	1.43	1.38
2	B	502	900	O32-C27	3.03	1.42	1.37
2	B	502	900	C2-C1	3.06	1.42	1.37
2	B	502	900	O37-C28	3.09	1.42	1.37
2	B	502	900	C13-C4	3.10	1.48	1.43
2	B	502	900	C45-C44	3.16	1.44	1.39
2	B	502	900	C29-C28	3.17	1.42	1.36
2	A	501	900	C29-C28	3.42	1.42	1.36
2	B	502	900	C12-C13	3.48	1.43	1.37
2	A	501	900	C2-C1	3.54	1.43	1.37
2	A	501	900	C12-C13	3.73	1.44	1.37
2	A	501	900	C49-C44	4.19	1.46	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	900	O32-C27-C26	-8.68	113.61	125.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	900	O32-C27-C26	-7.91	114.65	125.25
2	A	501	900	C19-C20-N21	-5.21	117.33	122.88
2	B	502	900	C19-C20-N21	-4.64	117.95	122.88
2	B	502	900	C18-O17-C1	-2.45	113.82	118.50
2	A	501	900	C18-O17-C1	-2.37	113.97	118.50
2	A	501	900	C22-N21-C20	2.05	120.34	116.87
2	B	502	900	O37-C28-C27	2.27	118.64	115.40
2	B	502	900	C22-N21-C20	2.45	121.03	116.87
2	B	502	900	C29-C20-N21	4.57	123.00	117.95
2	A	501	900	C29-C20-N21	4.68	123.12	117.95
2	A	501	900	O32-C27-C28	7.00	125.39	115.40
2	B	502	900	O32-C27-C28	7.19	125.66	115.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	900	6	0
2	B	502	900	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	292/314 (92%)	-0.19	12 (4%)	41	34	12, 24, 67, 84	0
1	B	271/314 (86%)	0.16	15 (5%)	29	22	14, 38, 68, 79	0
All	All	563/628 (89%)	-0.02	27 (4%)	34	27	12, 31, 68, 84	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	845	PHE	6.5
1	A	819	ARG	5.2
1	A	859	THR	5.1
1	A	860	ALA	4.6
1	B	1165	GLN	4.3
1	B	1023	LYS	3.8
1	B	880	ARG	3.5
1	A	873	GLY	3.4
1	A	858	LYS	3.4
1	A	880	ARG	3.4
1	B	1111	ILE	3.3
1	A	844	ALA	3.0
1	A	842	ARG	2.9
1	B	1080	ARG	2.8
1	B	1149	GLN	2.7
1	B	1110	LYS	2.7
1	A	874	ALA	2.6
1	B	842	ARG	2.5
1	A	876	HIS	2.3
1	B	1126	ARG	2.3
1	B	871	LYS	2.2
1	B	1081	VAL	2.2
1	B	1112	ASP	2.1
1	A	875	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	872	GLU	2.1
1	B	1094	LEU	2.1
1	B	1114	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	900	A	501	35/35	0.89	0.20	1.22	25,29,36,39	0
2	900	B	502	35/35	0.88	0.19	0.70	25,30,33,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.