W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:43 PM GMT

PDB ID	:	1YH3
Title	:	Crystal structure of human CD38 extracellular domain
Authors	:	Liu, Q.; Kriksunov, I.A.; Graeff, R.; Munshi, C.; Lee, H.C.; Hao, Q.
Deposited on	:	2005-01-06
Resolution	:	1.91 Å(reported)

The following versions of software and data (see references (i)) 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
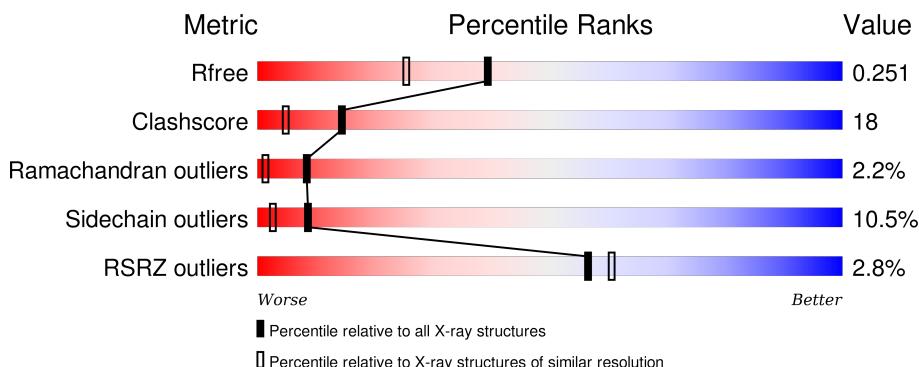
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
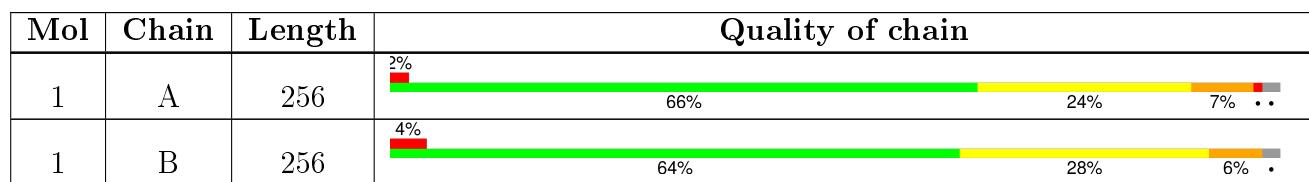
The reported resolution of this entry is 1.91 Å.

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		0.251
Clashscore		18
Ramachandran outliers		2.2%
Sidechain outliers		10.5%
RSRZ outliers		2.8%

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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	256	2% — 66% — 24% — 7% · ·
1	B	256	4% — 64% — 28% — 6% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4310 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 ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2000	1262	350	372	16			
1	B	252	Total	C	N	O	S	0	0	0
			1986	1254	347	369	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	THR	GLN	SEE REMARK 999	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ALA	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	UNP P28907
B	49	THR	GLN	SEE REMARK 999	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ALA	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	UNP P28907
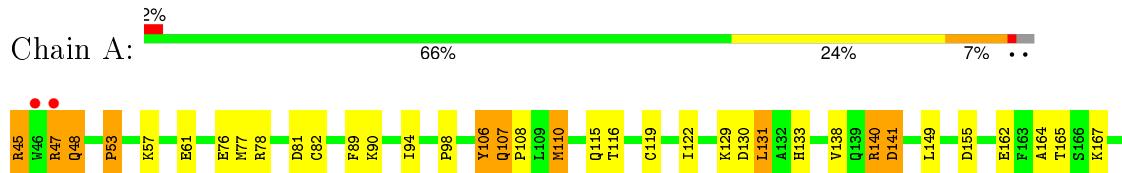
- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	194	Total	O	0	0
			194	194		
2	B	130	Total	O	0	0
			130	130		
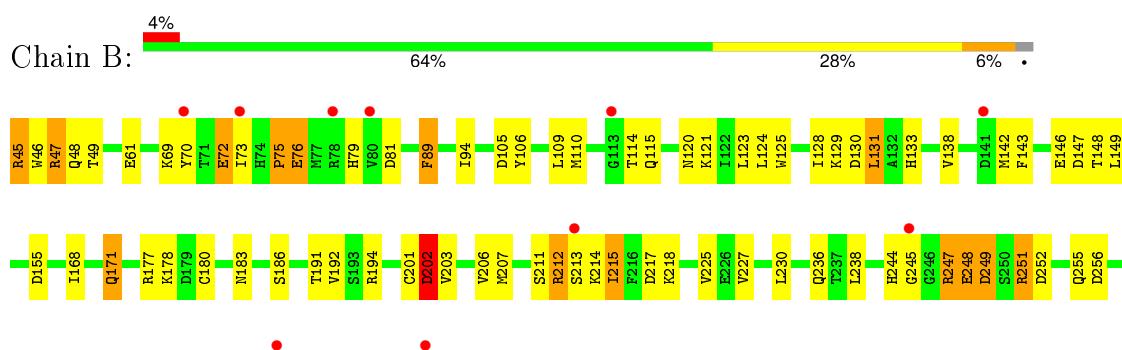
3 Residue-property plots ⓘ

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: ADP-ribosyl cyclase 1

- Molecule 1: ADP-ribosyl cyclase 1

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.84Å 51.49Å 66.44Å 108.27° 90.47° 97.29°	Depositor
Resolution (Å)	10.00 – 1.91 63.01 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.1 (10.00-1.91) 87.7 (63.01-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.253 0.188 , 0.251	Depositor DCC
R_{free} test set	1992 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 48721 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4310	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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)

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	1.44	14/2050 (0.7%)	1.28	15/2774 (0.5%)
1	B	1.14	2/2036 (0.1%)	1.09	9/2754 (0.3%)
All	All	1.30	16/4086 (0.4%)	1.19	24/5528 (0.4%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLN	CB-CG	9.32	1.77	1.52
1	B	61	GLU	CD-OE1	7.27	1.33	1.25
1	A	276	LYS	CD-CE	6.96	1.68	1.51
1	A	196	PHE	CG-CD2	6.53	1.48	1.38
1	A	106	TYR	CE2-CZ	6.47	1.47	1.38
1	A	276	LYS	CE-NZ	6.33	1.64	1.49
1	A	170	TYR	CD1-CE1	6.01	1.48	1.39
1	A	263	GLU	CD-OE1	5.81	1.32	1.25
1	A	255	GLN	CD-OE1	5.79	1.36	1.24
1	A	61	GLU	CG-CD	5.71	1.60	1.51
1	A	203	VAL	CB-CG2	5.64	1.64	1.52
1	B	75	PRO	C-O	5.63	1.34	1.23
1	A	189	TRP	CE3-CZ3	5.13	1.47	1.38
1	A	235	VAL	CB-CG2	5.07	1.63	1.52
1	A	107	GLN	CG-CD	5.04	1.62	1.51
1	A	200	ALA	CA-CB	5.04	1.63	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD2	9.95	127.26	118.30
1	A	219	ASP	CB-CG-OD2	9.40	126.76	118.30
1	A	141	ASP	CB-CG-OD1	-9.39	109.85	118.30
1	A	81	ASP	CB-CG-OD2	8.27	125.75	118.30
1	A	179	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	164	ALA	N-CA-CB	-7.25	99.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	B	155	ASP	CB-CG-OD2	6.77	124.39	118.30
1	B	194	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	202	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	61	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	A	53	PRO	N-CD-CG	-6.13	94.01	103.20
1	A	82	CYS	CA-CB-SG	-6.00	103.20	114.00
1	A	78	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	81	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	175	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	147	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	131	LEU	CB-CG-CD2	5.60	120.52	111.00
1	B	105	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	130	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	256	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	269	ARG	CG-CD-NE	-5.08	101.13	111.80
1	B	217	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	155	ASP	CB-CG-OD2	5.04	122.83	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	2000	0	1913	63	0
1	B	1986	0	1893	79	0
2	A	194	0	0	23	0
2	B	130	0	0	14	0
All	All	4310	0	3806	140	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 18.

All (140) 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:236:GLN:CG	1:A:236:GLN:CB	1.77	1.54
1:B:45:ARG:NH1	1:B:47:ARG:HD3	1.48	1.27
1:A:180:CYS:HB2	2:A:340:HOH:O	1.42	1.19
1:A:269:ARG:HG3	2:A:484:HOH:O	1.56	1.06
1:B:45:ARG:HH11	1:B:47:ARG:HD3	0.92	1.05
1:B:70:TYR:CE2	1:B:149:LEU:HB2	1.93	1.03
1:B:143:PHE:HD2	2:B:415:HOH:O	1.48	0.95
1:B:45:ARG:HH11	1:B:47:ARG:CD	1.81	0.93
1:B:70:TYR:CE1	1:B:149:LEU:HA	2.04	0.92
1:A:122:ILE:CD1	2:A:483:HOH:O	2.16	0.91
1:A:48:GLN:HE22	1:A:171:GLN:HE21	1.04	0.91
1:A:165:THR:HG23	1:A:167:LYS:H	1.34	0.91
1:B:70:TYR:CZ	1:B:149:LEU:N	2.38	0.90
1:B:211:SER:OG	1:B:245:GLY:HA3	1.75	0.87
1:A:236:GLN:CD	1:A:236:GLN:CB	2.44	0.86
1:A:122:ILE:HD11	2:A:483:HOH:O	1.74	0.84
1:B:230:LEU:O	1:B:269:ARG:NH1	2.11	0.83
1:A:268:LYS:HE2	2:A:491:HOH:O	1.78	0.82
1:B:191:THR:HG21	2:B:423:HOH:O	1.78	0.81
1:B:70:TYR:CZ	1:B:149:LEU:CA	2.62	0.81
1:A:115:GLN:HE22	1:A:149:LEU:H	1.25	0.81
1:B:45:ARG:NH1	1:B:47:ARG:CD	2.39	0.81
1:A:48:GLN:HE22	1:A:171:GLN:NE2	1.77	0.80
1:B:70:TYR:CD2	1:B:149:LEU:HB2	2.16	0.80
1:A:45:ARG:HH11	1:A:45:ARG:HB2	1.46	0.80
1:B:70:TYR:CZ	1:B:149:LEU:HA	2.18	0.79
1:A:261:GLU:HG3	2:A:427:HOH:O	1.82	0.79
1:A:106:TYR:O	1:A:110:MET:HG2	1.83	0.78
1:B:70:TYR:OH	1:B:149:LEU:N	2.17	0.78
1:B:249:ASP:CA	2:B:419:HOH:O	2.32	0.76
1:B:79:HIS:O	1:B:79:HIS:CD2	2.40	0.74
1:A:198:GLU:OE1	2:A:489:HOH:O	2.03	0.74
1:B:138:VAL:HG11	1:B:289:LYS:HA	1.70	0.74
1:B:73:ILE:O	1:B:75:PRO:HD3	1.87	0.73
1:A:236:GLN:OE1	1:A:236:GLN:CB	2.35	0.73
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.70	0.73
1:A:276:LYS:HE3	2:A:485:HOH:O	1.90	0.72
1:B:70:TYR:CE2	1:B:149:LEU:CB	2.73	0.71
1:B:106:TYR:HB2	2:B:423:HOH:O	1.92	0.69
1:B:45:ARG:HD2	2:B:418:HOH:O	1.92	0.69
1:A:48:GLN:NE2	1:A:171:GLN:HE21	1.87	0.69
1:A:110:MET:HE3	1:A:192:VAL:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLN:HE22	1:B:149:LEU:H	1.39	0.68
1:A:216:PHE:HE2	1:A:261:GLU:OE2	1.77	0.68
1:B:236:GLN:OE1	2:B:352:HOH:O	2.10	0.68
1:B:262:LEU:HD22	1:B:266:ILE:HD13	1.75	0.67
1:B:45:ARG:HH12	1:B:47:ARG:HH11	1.40	0.67
1:B:70:TYR:OH	1:B:148:THR:C	2.32	0.67
1:B:131:LEU:HB2	2:B:359:HOH:O	1.92	0.67
1:B:106:TYR:O	1:B:110:MET:HG3	1.95	0.66
1:B:94:ILE:HD11	1:B:168:ILE:HG13	1.76	0.66
1:A:48:GLN:HA	1:A:48:GLN:OE1	1.97	0.65
1:A:276:LYS:CE	2:A:485:HOH:O	2.44	0.65
1:A:218:LYS:HB3	2:A:468:HOH:O	1.98	0.63
1:A:203:VAL:HG21	1:B:171:GLN:HG2	1.80	0.63
1:B:115:GLN:NE2	1:B:149:LEU:H	1.97	0.62
1:B:238:LEU:HD23	1:B:266:ILE:HD12	1.81	0.62
1:A:268:LYS:HD2	2:A:317:HOH:O	1.99	0.62
1:A:270:ASN:HB2	2:A:438:HOH:O	2.00	0.61
1:B:48:GLN:HG3	2:B:422:HOH:O	1.99	0.61
1:A:183:ASN:ND2	1:A:186:SER:H	1.99	0.61
1:B:48:GLN:HG2	2:B:426:HOH:O	2.00	0.61
1:A:247:ARG:O	1:A:248:GLU:O	2.19	0.61
1:A:175:ASP:OD1	1:A:178:LYS:HD2	2.01	0.60
1:B:262:LEU:HD22	1:B:266:ILE:CD1	2.31	0.60
1:A:115:GLN:NE2	1:A:149:LEU:H	1.98	0.60
1:B:70:TYR:CD1	1:B:149:LEU:HA	2.37	0.59
1:B:211:SER:OG	1:B:245:GLY:CA	2.50	0.59
1:B:45:ARG:NH1	1:B:47:ARG:HH11	2.02	0.58
1:B:45:ARG:HD3	1:B:47:ARG:HG2	1.85	0.58
1:B:183:ASN:ND2	1:B:186:SER:H	2.02	0.57
1:B:45:ARG:HG2	1:B:46:TRP:H	1.69	0.56
1:A:276:LYS:NZ	2:A:485:HOH:O	2.36	0.56
1:B:123:LEU:HD11	1:B:207:MET:HG3	1.87	0.56
1:A:176:TRP:HB3	2:A:424:HOH:O	2.05	0.56
1:B:211:SER:HG	1:B:245:GLY:HA3	1.71	0.56
1:B:49:THR:HG22	2:B:370:HOH:O	2.05	0.56
1:B:70:TYR:OH	1:B:148:THR:HA	2.07	0.55
1:B:201:CYS:O	1:B:202:ASP:HB2	2.08	0.54
1:A:228:HIS:HE1	2:A:348:HOH:O	1.88	0.54
1:A:108:PRO:HG3	2:A:459:HOH:O	2.07	0.54
1:B:70:TYR:OH	1:B:148:THR:CA	2.56	0.54
1:A:47:ARG:O	1:A:48:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:O	1:B:206:VAL:HA	2.07	0.54
1:B:120:ASN:ND2	1:B:121:LYS:HD2	2.23	0.53
1:A:233:GLU:HG2	2:A:450:HOH:O	2.07	0.53
1:B:183:ASN:HD21	1:B:186:SER:H	1.56	0.53
1:B:110:MET:O	1:B:114:THR:N	2.42	0.53
1:A:244:HIS:CE1	1:A:277:ASN:OD1	2.57	0.53
1:B:252:ASP:OD2	1:B:255:GLN:HG2	2.08	0.53
1:B:70:TYR:CZ	1:B:148:THR:C	2.82	0.52
1:B:106:TYR:O	1:B:110:MET:CG	2.57	0.52
1:A:183:ASN:HD21	1:A:186:SER:H	1.54	0.52
1:A:90:LYS:CG	1:A:94:ILE:HG13	2.39	0.52
1:B:212:ARG:O	1:B:214:LYS:N	2.41	0.52
1:A:140:ARG:CZ	2:A:441:HOH:O	2.57	0.52
1:A:90:LYS:HG3	1:A:94:ILE:HG13	1.92	0.52
1:B:70:TYR:CE2	1:B:149:LEU:CA	2.93	0.51
1:B:70:TYR:CE1	1:B:149:LEU:CA	2.86	0.50
1:A:98:PRO:O	1:A:183:ASN:HA	2.12	0.50
1:A:45:ARG:NH1	1:A:45:ARG:HB2	2.23	0.50
1:B:79:HIS:CG	1:B:79:HIS:O	2.65	0.49
1:A:45:ARG:HH11	1:A:45:ARG:CB	2.19	0.49
1:A:138:VAL:HG11	1:A:288:VAL:HG12	1.95	0.49
1:B:262:LEU:HD13	1:B:273:PHE:CE1	2.48	0.49
1:B:244:HIS:HE1	1:B:277:ASN:OD1	1.95	0.48
1:B:251:ARG:HG3	2:B:419:HOH:O	2.13	0.48
1:B:201:CYS:O	1:B:202:ASP:CB	2.62	0.48
1:A:107:GLN:HA	1:A:110:MET:HG3	1.96	0.47
1:A:250:SER:OG	2:A:426:HOH:O	2.20	0.47
1:B:180:CYS:HB2	2:B:380:HOH:O	2.15	0.47
1:B:133:HIS:HE1	1:B:146:GLU:OE1	1.97	0.47
1:A:195:ARG:NH1	2:A:330:HOH:O	2.47	0.46
1:B:125:TRP:CH2	1:B:129:LYS:HG3	2.51	0.46
1:B:282:ASP:OD1	1:B:282:ASP:N	2.47	0.46
1:A:236:GLN:HB2	1:A:236:GLN:OE1	2.13	0.46
1:A:106:TYR:O	1:A:110:MET:CG	2.61	0.46
1:B:244:HIS:HD2	1:B:249:ASP:O	1.98	0.46
1:A:129:LYS:HG3	1:A:133:HIS:CD2	2.52	0.45
1:A:122:ILE:HD13	2:A:483:HOH:O	2.01	0.45
1:B:266:ILE:HG12	1:B:266:ILE:H	1.46	0.44
1:A:260:LYS:HA	1:A:260:LYS:HE2	1.98	0.44
1:A:216:PHE:CE2	1:A:261:GLU:OE2	2.65	0.44
1:A:178:LYS:HE2	2:A:394:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:HG2	1:A:77:MET:HG2	2.00	0.44
1:B:76:GLU:HG3	1:B:76:GLU:H	1.24	0.44
1:A:53:PRO:O	1:A:173:CYS:HB2	2.19	0.43
1:B:110:MET:CE	1:B:192:VAL:HG12	2.48	0.43
1:A:110:MET:HE2	1:A:110:MET:CA	2.49	0.43
1:A:48:GLN:NE2	1:A:171:GLN:NE2	2.54	0.43
1:B:89:PHE:HA	1:B:109:LEU:HD22	2.01	0.42
1:B:202:ASP:HB3	1:B:203:VAL:H	1.61	0.42
1:B:247:ARG:C	1:B:248:GLU:O	2.56	0.42
1:A:203:VAL:CG2	1:B:171:GLN:HG2	2.46	0.42
1:A:231:GLN:HG3	1:A:234:LYS:HE2	2.02	0.42
1:B:236:GLN:NE2	2:B:384:HOH:O	2.53	0.41
1:A:119:CYS:HB3	2:A:488:HOH:O	2.20	0.41
1:B:251:ARG:HG2	1:B:251:ARG:H	1.55	0.41
1:B:215:ILE:H	1:B:215:ILE:HG12	1.66	0.41
1:B:72:GLU:CD	2:B:323:HOH:O	2.59	0.41

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	250/256 (98%)	235 (94%)	10 (4%)	5 (2%)	9	2
1	B	250/256 (98%)	234 (94%)	10 (4%)	6 (2%)	7	1
All	All	500/512 (98%)	469 (94%)	20 (4%)	11 (2%)	8	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	GLU
1	B	247	ARG

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Mol	Chain	Res	Type
1	A	292	GLU
1	B	202	ASP
1	B	248	GLU
1	B	292	GLU
1	A	48	GLN
1	B	249	ASP
1	A	250	SER
1	A	245	GLY
1	B	213	SER

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	221/236 (94%)	201 (91%)	20 (9%)	12	4
1	B	218/236 (92%)	192 (88%)	26 (12%)	6	2
All	All	439/472 (93%)	393 (90%)	46 (10%)	8	2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	47	ARG
1	A	57	LYS
1	A	89	PHE
1	A	110	MET
1	A	116	THR
1	A	130	ASP
1	A	131	LEU
1	A	140	ARG
1	A	141	ASP
1	A	162	GLU
1	A	176	TRP
1	A	178	LYS
1	A	213	SER

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Mol	Chain	Res	Type
1	A	225	VAL
1	A	250	SER
1	A	262	LEU
1	A	268	LYS
1	A	270	ASN
1	A	276	LYS
1	B	45	ARG
1	B	47	ARG
1	B	69	LYS
1	B	72	GLU
1	B	76	GLU
1	B	89	PHE
1	B	128	ILE
1	B	131	LEU
1	B	142	MET
1	B	171	GLN
1	B	177	ARG
1	B	178	LYS
1	B	202	ASP
1	B	212	ARG
1	B	215	ILE
1	B	218	LYS
1	B	225	VAL
1	B	227	VAL
1	B	251	ARG
1	B	262	LEU
1	B	266	ILE
1	B	268	LYS
1	B	276	LYS
1	B	285	LEU
1	B	286	GLN
1	B	296	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	133	HIS
1	A	171	GLN
1	A	183	ASN
1	A	244	HIS
1	A	286	GLN

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Mol	Chain	Res	Type
1	B	79	HIS
1	B	115	GLN
1	B	133	HIS
1	B	171	GLN
1	B	183	ASN
1	B	244	HIS
1	B	270	ASN
1	B	286	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	252/256 (98%)	-0.14	4 (1%)	74 78	5, 17, 49, 76	0
1	B	252/256 (98%)	0.25	10 (3%)	42 46	8, 34, 56, 62	0
All	All	504/512 (98%)	0.05	14 (2%)	56 60	5, 24, 53, 76	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	TYR	7.4
1	A	249	ASP	6.4
1	B	213	SER	5.8
1	B	294	SER	5.3
1	B	80	VAL	4.0
1	B	78	ARG	3.7
1	A	46	TRP	3.5
1	A	248	GLU	2.9
1	A	47	ARG	2.5
1	B	141	ASP	2.4
1	B	284	PHE	2.3
1	B	245	GLY	2.2
1	B	73	ILE	2.0
1	B	113	GLY	2.0

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

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

6.3   Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.