



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:23 PM UTC

PDB ID : 1YH3 / pdb_00001yh3
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

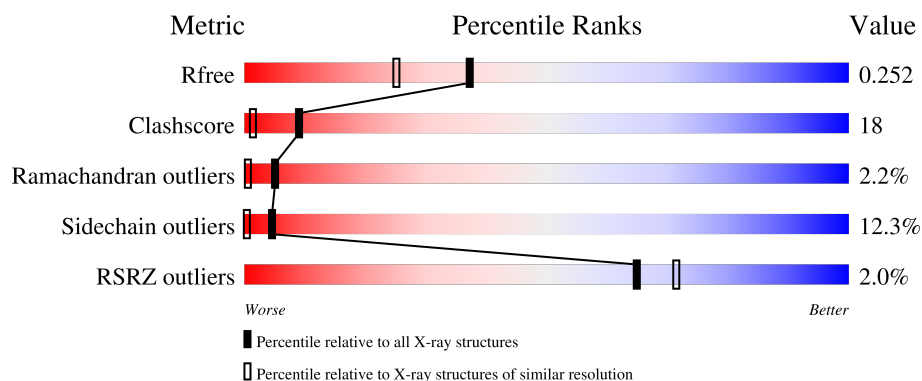
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 62% 28% 7% ..
1	B	256	3% 61% 28% 9% ..

2 Entry composition

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 mutation	UNP P28907
A	164	ALA	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
B	49	THR	GLN	SEE REMARK 999	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ALA	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907

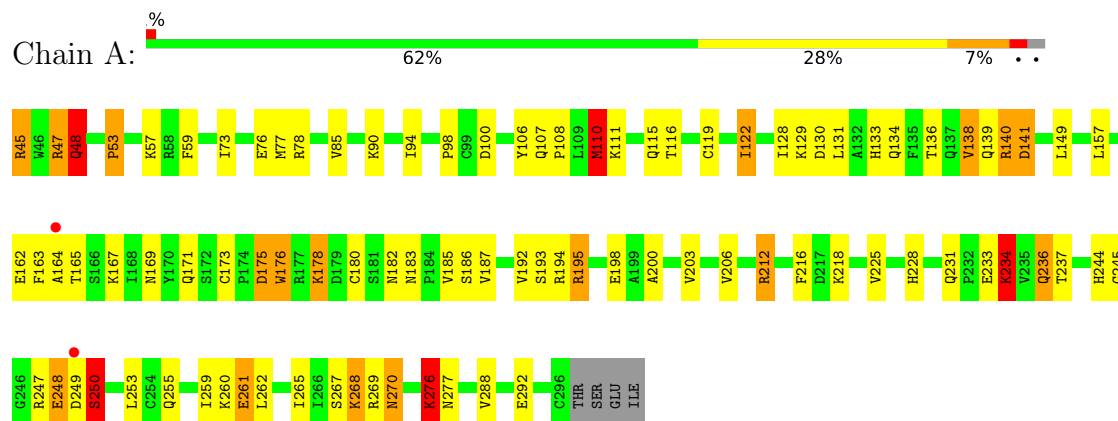
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	194	Total	O	0	0
			194	194		
2	B	130	Total	O	0	0
			130	130		

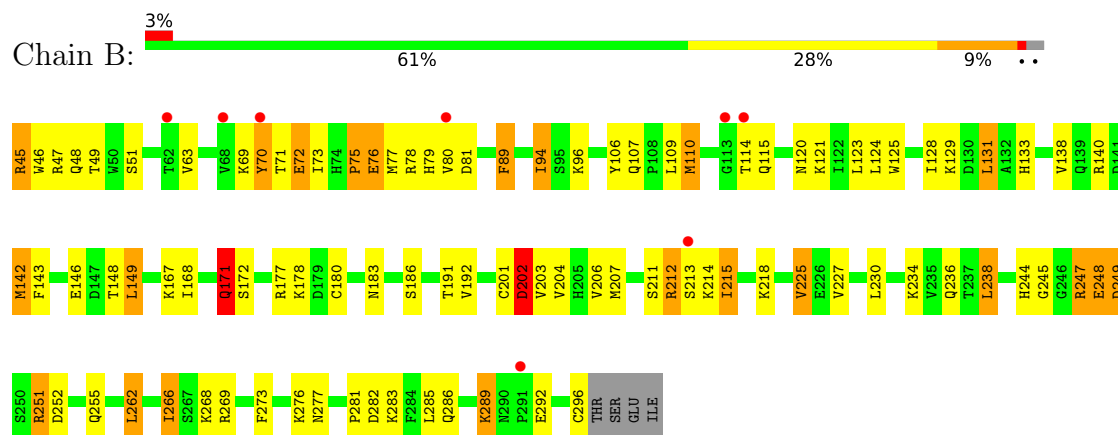
3 Residue-property plots [i](#)

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

• Molecule 1: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



4 Data and refinement statistics

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 10.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.1 (10.00-1.91) 97.4 (10.00-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.253 0.189 , 0.252	Depositor DCC
R_{free} test set	2029 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.70	25/2050 (1.2%)	1.49	20/2774 (0.7%)
1	B	1.40	12/2036 (0.6%)	1.36	7/2754 (0.3%)
All	All	1.56	37/4086 (0.9%)	1.43	27/5528 (0.5%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLN	CB-CG	8.42	1.77	1.52
1	A	110	MET	SD-CE	-8.23	1.58	1.79
1	A	187	VAL	CA-CB	7.59	1.64	1.54
1	B	75	PRO	C-O	7.24	1.34	1.24
1	A	259	ILE	CA-CB	6.98	1.63	1.54
1	A	255	GLN	CD-OE1	6.92	1.36	1.23
1	A	206	VAL	CA-CB	6.91	1.63	1.54
1	A	193	SER	CA-C	6.63	1.61	1.52
1	B	63	VAL	C-O	6.47	1.31	1.24
1	A	128	ILE	CA-C	6.46	1.60	1.52
1	B	172	SER	C-O	6.38	1.31	1.23
1	A	141	ASP	CG-OD2	6.02	1.36	1.25
1	A	182	ASN	N-CA	5.88	1.54	1.46
1	A	200	ALA	CA-CB	5.84	1.63	1.53
1	A	85	VAL	N-CA	5.75	1.53	1.46
1	A	237	THR	CA-CB	5.72	1.64	1.53
1	B	171	GLN	C-O	-5.69	1.17	1.23
1	B	78	ARG	C-O	5.65	1.31	1.24
1	A	59	PHE	CA-CB	5.61	1.60	1.53
1	A	134	GLN	CA-C	-5.58	1.45	1.52
1	B	81	ASP	CA-C	5.56	1.60	1.52
1	A	175	ASP	CA-C	5.54	1.59	1.52
1	A	185	VAL	CA-CB	5.47	1.60	1.54
1	A	261	GLU	N-CA	-5.43	1.39	1.46
1	A	276	LYS	CD-CE	5.40	1.68	1.52
1	B	142	MET	SD-CE	5.38	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	LYS	C-O	5.37	1.30	1.23
1	A	122	ILE	CB-CG1	5.35	1.64	1.53
1	B	78	ARG	C-N	5.34	1.39	1.33
1	B	71	THR	N-CA	5.20	1.52	1.46
1	A	276	LYS	CE-NZ	5.17	1.64	1.49
1	A	169	ASN	CA-CB	5.15	1.59	1.52
1	A	253	LEU	C-O	-5.12	1.17	1.24
1	A	265	ILE	C-O	5.12	1.29	1.24
1	B	70	TYR	CA-CB	5.09	1.61	1.53
1	A	267	SER	C-O	-5.08	1.18	1.24
1	B	70	TYR	N-CA	5.05	1.52	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	VAL	N-CA-C	10.70	120.69	110.42
1	B	225	VAL	CB-CA-C	8.09	118.25	111.05
1	A	236	GLN	CB-CG-CD	-8.01	98.99	112.60
1	B	281	PRO	N-CA-C	6.94	123.64	114.27
1	A	164	ALA	N-CA-CB	-6.92	99.95	110.33
1	A	212	ARG	N-CA-C	6.67	121.26	113.18
1	A	249	ASP	N-CA-C	-6.66	104.18	112.90
1	A	270	ASN	N-CA-C	6.60	120.69	112.24
1	B	110	MET	N-CA-C	-6.56	103.97	112.23
1	A	73	ILE	N-CA-C	6.38	117.17	110.72
1	A	53	PRO	N-CD-CG	-6.13	94.01	103.20
1	B	51	SER	CA-CB-OG	-6.10	98.91	111.10
1	A	138	VAL	CB-CA-C	-6.05	104.23	111.97
1	A	195	ARG	CA-CB-CG	-5.77	102.56	114.10
1	B	140	ARG	N-CA-C	5.66	119.70	112.34
1	B	204	VAL	N-CA-C	-5.62	100.38	108.53
1	A	194	ARG	N-CA-C	-5.55	105.13	111.07
1	A	236	GLN	N-CA-C	-5.36	105.00	112.45
1	A	163	PHE	CA-C-N	5.36	131.37	121.52
1	A	163	PHE	C-N-CA	5.36	131.37	121.52
1	A	136	THR	N-CA-C	5.25	117.00	111.28
1	A	157	LEU	CD1-CG-CD2	-5.18	99.40	110.80
1	A	234	LYS	CB-CA-C	-5.17	100.65	109.03
1	A	111	LYS	CB-CA-C	-5.14	102.81	110.88
1	B	89	PHE	N-CA-C	-5.07	105.21	111.40
1	A	265	ILE	N-CA-C	5.05	115.27	110.42
1	A	100	ASP	N-CA-CB	-5.02	104.00	111.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2000	0	1913	64	0
1	B	1986	0	1893	81	0
2	A	194	0	0	23	0
2	B	130	0	0	14	0
All	All	4310	0	3806	143	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 (143) 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:CB	1:A:236:GLN:CG	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:236:GLN:CB	1:A:236:GLN:CD	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:110:MET:HE1	1:A:192:VAL:HG12	1.61	0.80
1:B:70:TYR:CD2	1:B:149:LEU:HB2	2.16	0.80
1:A:45:ARG:HB2	1:A:45:ARG:HH11	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:CD2	1:B:79:HIS:O	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:CB	1:A:236:GLN:OE1	2.35	0.73
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.70	0.73
1:B:70:TYR:OH	1:B:148:THR:C	2.32	0.72
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:TYR:CZ	1:B:148:THR:C	2.82	0.57
1:B:183:ASN:ND2	1:B:186:SER:H	2.02	0.57
1:A:276:LYS:NZ	2:A:485:HOH:O	2.36	0.56
1:B:45:ARG:HG2	1:B:46:TRP:H	1.69	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: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:A:47:ARG:O	1:A:48:GLN:HB2	2.08	0.54
1:B:70:TYR:OH	1:B:148:THR:CA	2.56	0.54
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:A:90:LYS:CG	1:A:94:ILE:HG13	2.39	0.52
1:A:183:ASN:HD21	1:A:186:SER:H	1.54	0.52
1:B:106:TYR:O	1:B:110:MET:CG	2.57	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:HB2	1:A:45:ARG:NH1	2.23	0.50
1:B:79:HIS:O	1:B:79:HIS:CG	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH11	1:A:45:ARG:CB	2.19	0.49
1:B:211:SER:HG	1:B:245:GLY:HA3	1.73	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:201:CYS:O	1:B:202:ASP:CB	2.62	0.48
1:B:251:ARG:HG3	2:B:419:HOH:O	2.13	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:247:ARG:C	1:B:248:GLU:O	2.56	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:106:TYR:O	1:A:110:MET:CG	2.61	0.46
1:A:236:GLN:OE1	1:A:236:GLN:HB2	2.13	0.46
1:B:244:HIS:HD2	1:B:249:ASP:O	1.98	0.46
1:B:72:GLU:CD	2:B:323:HOH:O	2.59	0.45
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:77:MET:C	1:B:79:HIS:H	2.25	0.45
1:B:266:ILE:H	1:B:266:ILE:HG12	1.46	0.44
1:A:260:LYS:HA	1:A:260:LYS:HE2	1.98	0.44
1:A:76:GLU:HG2	1:A:77:MET:HG2	2.00	0.44
1:A:178:LYS:HE2	2:A:394:HOH:O	2.18	0.44
1:A:216:PHE:CE2	1:A:261:GLU:OE2	2.65	0.44
1:A:110:MET:HB3	1:A:110:MET:HE2	1.62	0.44
1:B:76:GLU:H	1:B:76:GLU:HG3	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:139:GLN:C	1:A:140:ARG:HG2	2.38	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: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:B:70:TYR:CE1	1:B:148:THR:C	2.98	0.41
1:A:119:CYS:HB3	2:A:488:HOH:O	2.20	0.41
1:B:215:ILE:H	1:B:215:ILE:HG12	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:H	1:B:251:ARG:HG2	1.55	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%)	6	1
1	B	250/256 (98%)	234 (94%)	10 (4%)	6 (2%)	4	0
All	All	500/512 (98%)	469 (94%)	20 (4%)	11 (2%)	5	0

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	GLU
1	B	247	ARG
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%)	200 (90%)	21 (10%)	8	1
1	B	218/236 (92%)	185 (85%)	33 (15%)	3	0
All	All	439/472 (93%)	385 (88%)	54 (12%)	4	0

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	47	ARG
1	A	48	GLN
1	A	57	LYS
1	A	78	ARG
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	212	ARG
1	A	225	VAL
1	A	234	LYS
1	A	250	SER
1	A	262	LEU
1	A	268	LYS
1	A	276	LYS
1	B	45	ARG
1	B	69	LYS
1	B	72	GLU
1	B	76	GLU
1	B	80	VAL
1	B	94	ILE
1	B	107	GLN
1	B	128	ILE
1	B	131	LEU
1	B	142	MET
1	B	149	LEU
1	B	167	LYS

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Mol	Chain	Res	Type
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	234	LYS
1	B	238	LEU
1	B	251	ARG
1	B	262	LEU
1	B	266	ILE
1	B	268	LYS
1	B	276	LYS
1	B	283	LYS
1	B	285	LEU
1	B	286	GLN
1	B	289	LYS
1	B	296	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	83	GLN
1	A	115	GLN
1	A	133	HIS
1	A	137	GLN
1	A	171	GLN
1	A	183	ASN
1	A	244	HIS
1	A	286	GLN
1	B	79	HIS
1	B	83	GLN
1	B	115	GLN
1	B	133	HIS
1	B	183	ASN
1	B	231	GLN
1	B	244	HIS
1	B	255	GLN

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Mol	Chain	Res	Type
1	B	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	-0.41	2 (0%) 82 88	5, 17, 49, 76	0
1	B	252/256 (98%)	0.14	8 (3%) 50 55	8, 34, 56, 62	0
All	All	504/512 (98%)	-0.14	10 (1%) 65 71	5, 24, 53, 76	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	TYR	8.4
1	B	80	VAL	4.0
1	B	213	SER	2.5
1	B	291	PRO	2.5
1	B	113	GLY	2.2
1	B	62	THR	2.2
1	B	68	VAL	2.2
1	A	249	ASP	2.1
1	B	114	THR	2.1
1	A	164	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.