



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 01:42 PM EDT

PDB ID : 2EG9
Title : Crystal structure of the truncated extracellular domain of mouse CD38
Authors : Kukimoto-Niino, M.; Mishima, C.; Wakiyama, M.; Terada, T.; Shirouzu, M.; Hara-Yokoyama, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-28
Resolution : 2.80 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

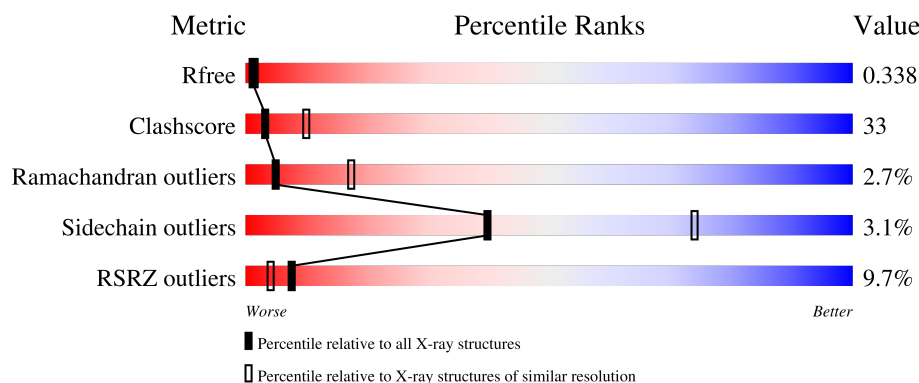
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	253	<div> <div>5%</div> <div>41%</div> <div>42%</div> <div>•</div> <div>16%</div> </div>
1	B	253	<div> <div>11%</div> <div>38%</div> <div>42%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3412 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	213	Total	C	N	O	S	0	0	0
			1696	1082	277	320	17			
1	B	211	Total	C	N	O	S	0	0	0
			1693	1082	277	317	17			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ARG	-	expression tag	UNP P56528
A	37	ALA	-	expression tag	UNP P56528
A	38	MET	-	expression tag	UNP P56528
A	39	ASP	-	expression tag	UNP P56528
A	40	TYR	-	expression tag	UNP P56528
A	41	LYS	-	expression tag	UNP P56528
A	42	ASP	-	expression tag	UNP P56528
A	43	ASP	-	expression tag	UNP P56528
A	44	ASP	-	expression tag	UNP P56528
A	45	ASP	-	expression tag	UNP P56528
A	46	LYS	-	expression tag	UNP P56528
A	47	LEU	-	expression tag	UNP P56528
A	104	ASP	ASN	engineered mutation	UNP P56528
A	124	ASP	ASN	engineered mutation	UNP P56528
A	191	MET	VAL	conflict	UNP P56528
A	213	ASP	ASN	engineered mutation	UNP P56528
A	223	ASP	ASN	engineered mutation	UNP P56528
B	36	ARG	-	expression tag	UNP P56528
B	37	ALA	-	expression tag	UNP P56528
B	38	MET	-	expression tag	UNP P56528
B	39	ASP	-	expression tag	UNP P56528
B	40	TYR	-	expression tag	UNP P56528
B	41	LYS	-	expression tag	UNP P56528
B	42	ASP	-	expression tag	UNP P56528
B	43	ASP	-	expression tag	UNP P56528

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	ASP	-	expression tag	UNP P56528
B	45	ASP	-	expression tag	UNP P56528
B	46	LYS	-	expression tag	UNP P56528
B	47	LEU	-	expression tag	UNP P56528
B	104	ASP	ASN	engineered mutation	UNP P56528
B	124	ASP	ASN	engineered mutation	UNP P56528
B	191	MET	VAL	conflict	UNP P56528
B	213	ASP	ASN	engineered mutation	UNP P56528
B	223	ASP	ASN	engineered mutation	UNP P56528

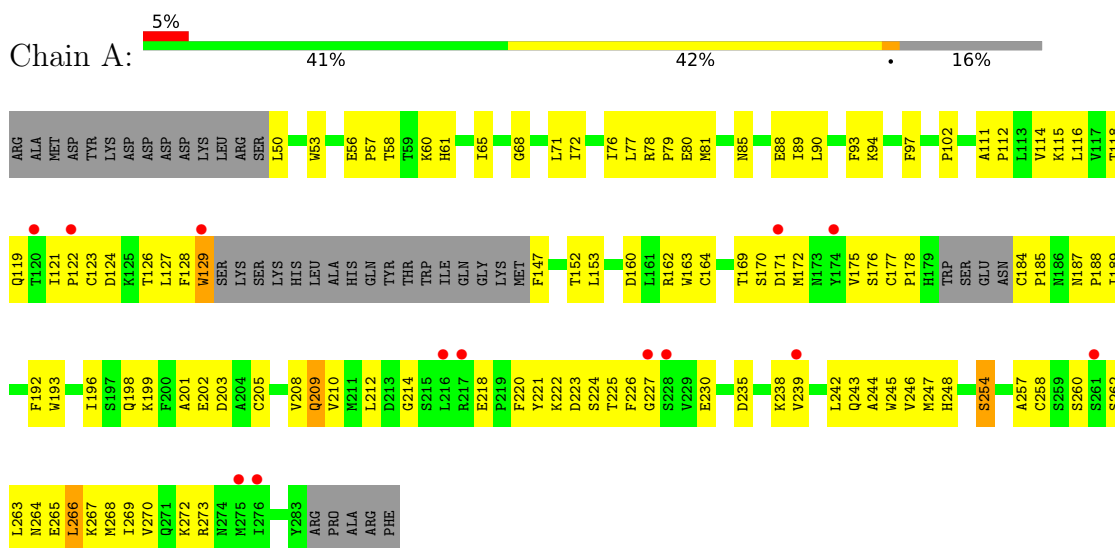
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	10	Total O 10 10	0	0

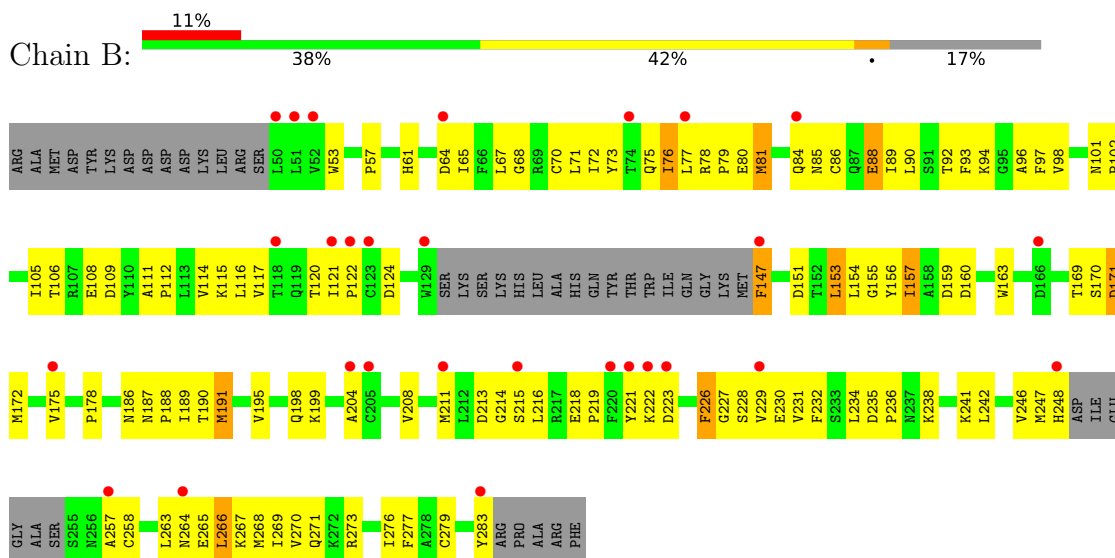
3 Residue-property plots

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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	59.07Å 176.81Å 44.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.80 49.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.12-2.80) 97.9 (49.12-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.58 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.340 0.264 , 0.338	Depositor DCC
R_{free} test set	1225 reflections (10.31%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	1.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3412	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% 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	0.35	0/1736	0.55	0/2355
1	B	0.33	0/1735	0.54	0/2355
All	All	0.34	0/3471	0.55	0/4710

There are no bond length outliers.

There are no bond angle outliers.

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	1696	0	1643	99	0
1	B	1693	0	1636	127	0
2	A	13	0	0	1	0
2	B	10	0	0	0	0
All	All	3412	0	3279	222	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 33.

All (222) 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:84:GLN:HE22	1:B:117:VAL:HA	1.15	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:HG3	1:A:262:SER:HB3	1.36	1.06
1:B:246:VAL:HG11	1:B:257:ALA:HB3	1.41	1.01
1:B:121:ILE:HG23	1:B:147:PHE:HZ	1.37	0.88
1:A:119:GLN:HE22	1:A:153:LEU:H	1.24	0.83
1:B:222:LYS:HA	1:B:227:GLY:HA3	1.59	0.83
1:B:105:ILE:HG13	1:B:188:PRO:HG3	1.62	0.81
1:A:72:ILE:HG23	1:A:76:ILE:HD11	1.62	0.80
1:A:258:CYS:HA	1:A:263:LEU:HD13	1.63	0.80
1:B:121:ILE:HG23	1:B:147:PHE:CZ	2.16	0.79
1:B:114:VAL:HG21	1:B:195:VAL:HG12	1.65	0.77
1:B:73:TYR:CD2	1:B:153:LEU:HD23	2.20	0.76
1:A:235:ASP:OD2	1:A:238:LYS:HG3	1.88	0.73
1:B:111:ALA:HB3	1:B:112:PRO:HD3	1.71	0.72
1:B:258:CYS:HA	1:B:263:LEU:HD13	1.72	0.72
1:A:248:HIS:ND1	1:A:254:SER:HB3	2.04	0.72
1:A:119:GLN:HE21	1:A:152:THR:HB	1.55	0.72
1:B:221:TYR:CE2	1:B:223:ASP:HB3	2.26	0.70
1:A:56:GLU:HB2	1:A:162:ARG:NE	2.06	0.69
1:B:97:PHE:HE1	1:B:172:MET:HG2	1.58	0.69
1:B:266:LEU:HD13	1:B:277:PHE:CE1	2.29	0.68
1:A:119:GLN:NE2	1:A:153:LEU:H	1.92	0.68
1:B:94:LYS:HE3	1:B:172:MET:HG3	1.76	0.67
1:B:67:LEU:HD21	1:B:90:LEU:HD22	1.74	0.67
1:A:257:ALA:O	1:A:263:LEU:HD12	1.94	0.66
1:B:73:TYR:HA	1:B:77:LEU:HD22	1.78	0.66
1:B:72:ILE:O	1:B:76:ILE:HG23	1.96	0.66
1:A:242:LEU:HD23	1:A:270:VAL:HG21	1.77	0.65
1:A:198:GLN:O	1:A:202:GLU:HG3	1.95	0.65
1:A:220:PHE:CD2	1:A:266:LEU:HB2	2.32	0.65
1:B:85:ASN:HB3	1:B:88:GLU:HB2	1.77	0.65
1:B:258:CYS:HA	1:B:263:LEU:CD1	2.26	0.64
1:A:243:GLN:HE21	1:A:245:TRP:HE1	1.43	0.64
1:B:57:PRO:HG3	1:B:175:VAL:O	1.98	0.64
1:A:111:ALA:HB3	1:A:112:PRO:HD3	1.80	0.63
1:B:102:PRO:O	1:B:187:ASN:HA	2.00	0.62
1:B:169:THR:HG22	1:B:171:ASP:H	1.63	0.62
1:A:121:ILE:HD13	1:A:147:PHE:CE2	2.35	0.62
1:A:221:TYR:CE1	1:A:224:SER:HB2	2.34	0.62
1:B:264:ASN:O	1:B:268:MET:HE2	1.99	0.62
1:A:60:LYS:O	1:A:61:HIS:HB2	2.00	0.61
1:B:191:MET:O	1:B:195:VAL:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:HG22	1:A:170:SER:N	2.15	0.61
1:B:70:CYS:SG	1:B:89:ILE:HD11	2.41	0.61
1:B:84:GLN:NE2	1:B:117:VAL:HA	2.00	0.60
1:A:126:THR:HB	2:A:289:HOH:O	2.02	0.60
1:A:226:PHE:HA	1:A:230:GLU:HB2	1.82	0.60
1:B:211:MET:HB3	1:B:247:MET:HE2	1.83	0.60
1:A:268:MET:O	1:A:272:LYS:HG2	2.02	0.59
1:B:84:GLN:OE1	1:B:117:VAL:HG13	2.02	0.59
1:A:246:VAL:HG11	1:A:257:ALA:HB3	1.84	0.59
1:A:121:ILE:HD13	1:A:147:PHE:HE2	1.66	0.59
1:A:127:LEU:HD13	1:A:209:GLN:HB2	1.85	0.59
1:B:242:LEU:HD23	1:B:270:VAL:HG21	1.84	0.59
1:A:184:CYS:N	1:A:185:PRO:HD3	2.18	0.59
1:A:225:THR:O	1:A:230:GLU:HG3	2.03	0.59
1:A:77:LEU:C	1:A:79:PRO:HD3	2.24	0.58
1:B:102:PRO:O	1:B:188:PRO:HD3	2.04	0.57
1:B:266:LEU:HD13	1:B:277:PHE:HE1	1.68	0.57
1:A:169:THR:HG22	1:A:170:SER:H	1.70	0.57
1:B:90:LEU:O	1:B:93:PHE:HB3	2.04	0.57
1:A:119:GLN:HE22	1:A:153:LEU:N	2.00	0.57
1:A:225:THR:HG22	1:A:230:GLU:HG3	1.85	0.57
1:B:53:TRP:CD2	1:B:178:PRO:HG3	2.40	0.57
1:A:85:ASN:O	1:A:89:ILE:HG13	2.03	0.56
1:A:212:LEU:HD12	1:A:263:LEU:HD21	1.87	0.56
1:B:246:VAL:CG2	1:B:263:LEU:HD11	2.36	0.56
1:A:243:GLN:NE2	1:A:245:TRP:HE1	2.02	0.56
1:A:169:THR:HG22	1:A:171:ASP:H	1.70	0.55
1:A:193:TRP:CE3	1:A:196:ILE:HD11	2.42	0.55
1:A:72:ILE:HD11	1:B:67:LEU:HD12	1.87	0.55
1:B:111:ALA:O	1:B:115:LYS:HG3	2.07	0.55
1:B:94:LYS:HG2	1:B:98:VAL:HG21	1.89	0.55
1:B:111:ALA:HB1	1:B:115:LYS:HE3	1.88	0.54
1:B:147:PHE:HB2	1:B:151:ASP:CB	2.37	0.54
1:A:111:ALA:C	1:A:115:LYS:HE3	2.27	0.54
1:B:226:PHE:O	1:B:230:GLU:HB2	2.07	0.54
1:B:80:GLU:HG3	1:B:81:MET:H	1.73	0.53
1:A:210:VAL:HG13	1:A:244:ALA:HA	1.90	0.53
1:B:72:ILE:HD11	1:B:156:TYR:OH	2.08	0.53
1:B:94:LYS:HA	1:B:97:PHE:CZ	2.44	0.53
1:A:53:TRP:CZ2	1:A:102:PRO:HG2	2.44	0.53
1:A:192:PHE:CE2	1:A:196:ILE:HD13	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LYS:HA	1:B:227:GLY:CA	2.34	0.53
1:B:89:ILE:HG13	1:B:90:LEU:N	2.24	0.53
1:B:222:LYS:HE3	1:B:265:GLU:CD	2.29	0.52
1:B:218:GLU:HG3	1:B:218:GLU:O	2.08	0.52
1:A:222:LYS:HE3	1:A:265:GLU:OE2	2.10	0.52
1:A:78:ARG:HG3	1:A:80:GLU:CD	2.30	0.52
1:B:77:LEU:O	1:B:79:PRO:HD3	2.10	0.52
1:B:78:ARG:HH21	1:B:120:THR:HG22	1.74	0.52
1:A:121:ILE:HG13	1:A:203:ASP:HB3	1.92	0.52
1:B:73:TYR:HA	1:B:77:LEU:HB2	1.91	0.51
1:B:153:LEU:HD13	1:B:154:LEU:N	2.25	0.51
1:A:102:PRO:HB2	1:A:178:PRO:HG2	1.93	0.51
1:B:86:CYS:HA	1:B:89:ILE:HG12	1.93	0.51
1:A:58:THR:HG23	1:A:163:TRP:HA	1.93	0.51
1:A:266:LEU:O	1:A:266:LEU:HD22	2.10	0.51
1:B:231:VAL:HG13	1:B:232:PHE:CD1	2.46	0.51
1:A:56:GLU:O	1:A:177:CYS:HB2	2.11	0.51
1:A:71:LEU:HD13	1:B:71:LEU:HB2	1.93	0.51
1:B:121:ILE:CG2	1:B:147:PHE:HZ	2.14	0.50
1:B:106:THR:O	1:B:109:ASP:HB2	2.11	0.50
1:B:235:ASP:OD2	1:B:238:LYS:HG3	2.11	0.50
1:A:72:ILE:O	1:A:76:ILE:HG12	2.10	0.50
1:A:269:ILE:O	1:A:273:ARG:HG3	2.12	0.50
1:B:187:ASN:ND2	1:B:190:THR:H	2.10	0.50
1:A:127:LEU:CD1	1:A:209:GLN:HB2	2.42	0.50
1:A:126:THR:O	1:A:209:GLN:HG2	2.11	0.50
1:B:121:ILE:HG22	1:B:122:PRO:O	2.13	0.49
1:A:122:PRO:HD2	1:A:147:PHE:CD2	2.47	0.49
1:A:129:TRP:N	1:A:129:TRP:CD1	2.80	0.49
1:B:246:VAL:HG21	1:B:263:LEU:HD11	1.94	0.49
1:A:119:GLN:HE21	1:A:152:THR:CB	2.24	0.49
1:B:230:GLU:CD	1:B:230:GLU:H	2.16	0.49
1:A:111:ALA:O	1:A:115:LYS:HG3	2.12	0.49
1:A:171:ASP:OD1	1:A:172:MET:N	2.44	0.49
1:B:114:VAL:HG13	1:B:199:LYS:HG2	1.95	0.49
1:A:220:PHE:CG	1:A:266:LEU:HB2	2.48	0.48
1:B:153:LEU:CD2	1:B:157:ILE:HD11	2.43	0.48
1:B:213:ASP:OD1	1:B:215:SER:N	2.46	0.48
1:A:214:GLY:N	1:A:247:MET:O	2.47	0.48
1:A:260:SER:O	1:A:264:ASN:ND2	2.46	0.48
1:A:264:ASN:O	1:A:268:MET:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG11	1:B:170:SER:O	2.13	0.48
1:B:257:ALA:O	1:B:263:LEU:HD12	2.13	0.48
1:B:102:PRO:HB2	1:B:178:PRO:HG2	1.95	0.48
1:B:94:LYS:HA	1:B:97:PHE:CE2	2.49	0.47
1:B:248:HIS:HB2	1:B:283:TYR:CD1	2.49	0.47
1:A:214:GLY:HA3	1:A:247:MET:O	2.14	0.47
1:B:71:LEU:O	1:B:75:GLN:HG3	2.14	0.47
1:B:120:THR:O	1:B:121:ILE:HG13	2.14	0.47
1:B:67:LEU:CD2	1:B:90:LEU:HD22	2.44	0.47
1:A:90:LEU:O	1:A:93:PHE:HB3	2.15	0.47
1:A:119:GLN:NE2	1:A:152:THR:HB	2.27	0.47
1:A:164:CYS:HA	1:A:188:PRO:HG2	1.97	0.47
1:A:61:HIS:O	1:A:65:ILE:HG13	2.15	0.47
1:A:266:LEU:O	1:A:270:VAL:HG23	2.15	0.47
1:B:222:LYS:CA	1:B:227:GLY:HA3	2.38	0.47
1:A:56:GLU:HB2	1:A:162:ARG:CD	2.45	0.46
1:B:211:MET:SD	1:B:247:MET:HE1	2.55	0.46
1:B:89:ILE:O	1:B:93:PHE:N	2.47	0.46
1:B:213:ASP:HB3	1:B:216:LEU:CD1	2.45	0.46
1:B:263:LEU:HD13	1:B:279:CYS:SG	2.55	0.46
1:B:92:THR:OG1	1:B:116:LEU:HD11	2.15	0.46
1:B:155:GLY:O	1:B:159:ASP:HB2	2.15	0.46
1:B:70:CYS:SG	1:B:89:ILE:CD1	3.03	0.46
1:A:68:GLY:HA3	1:B:64:ASP:O	2.16	0.46
1:B:108:GLU:O	1:B:112:PRO:HD3	2.17	0.45
1:A:114:VAL:HG13	1:A:199:LYS:HD3	1.97	0.45
1:B:76:ILE:HG12	1:B:77:LEU:N	2.30	0.45
1:B:213:ASP:HB3	1:B:216:LEU:HD12	1.98	0.45
1:A:81:MET:HE3	1:A:118:THR:O	2.17	0.45
1:A:169:THR:HG22	1:A:171:ASP:N	2.31	0.45
1:A:76:ILE:HG13	1:A:77:LEU:N	2.32	0.45
1:A:102:PRO:O	1:A:187:ASN:HA	2.16	0.45
1:B:153:LEU:HD21	1:B:157:ILE:HD11	1.98	0.45
1:B:72:ILE:O	1:B:77:LEU:HD13	2.16	0.45
1:B:273:ARG:HB3	1:B:273:ARG:HH11	1.80	0.45
1:A:121:ILE:CD1	1:A:147:PHE:HE2	2.30	0.45
1:B:61:HIS:O	1:B:65:ILE:HG13	2.17	0.45
1:B:219:PRO:HG2	1:B:257:ALA:HB1	1.99	0.45
1:A:208:VAL:HG23	1:A:239:VAL:CG1	2.47	0.45
1:B:211:MET:HB3	1:B:247:MET:CE	2.47	0.45
1:B:147:PHE:HB2	1:B:151:ASP:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LYS:HB2	1:B:277:PHE:CE2	2.52	0.44
1:A:71:LEU:HD12	1:B:68:GLY:HA2	1.99	0.44
1:B:80:GLU:OE2	1:B:120:THR:HB	2.18	0.44
1:B:214:GLY:N	1:B:247:MET:O	2.50	0.44
1:B:121:ILE:HG12	1:B:147:PHE:CZ	2.51	0.44
1:A:114:VAL:CG1	1:A:199:LYS:HD3	2.47	0.44
1:A:208:VAL:HG23	1:A:239:VAL:HG13	1.99	0.44
1:B:114:VAL:CG2	1:B:195:VAL:HG12	2.41	0.44
1:B:234:LEU:O	1:B:236:PRO:HD3	2.18	0.44
1:A:128:PHE:HZ	1:A:201:ALA:HA	1.83	0.43
1:B:204:ALA:HB1	1:B:208:VAL:CG2	2.48	0.43
1:A:187:ASN:HD21	1:A:189:ILE:HB	1.83	0.43
1:B:186:ASN:HA	1:B:191:MET:SD	2.59	0.43
1:A:78:ARG:HG3	1:A:80:GLU:OE2	2.19	0.43
1:A:171:ASP:CG	1:A:172:MET:H	2.21	0.43
1:A:94:LYS:HA	1:A:97:PHE:CE2	2.53	0.43
1:A:222:LYS:HA	1:A:227:GLY:HA3	2.00	0.43
1:A:122:PRO:HD2	1:A:147:PHE:CE2	2.54	0.43
1:A:112:PRO:HA	1:A:115:LYS:HD2	2.01	0.42
1:B:105:ILE:HG13	1:B:188:PRO:CG	2.40	0.42
1:B:121:ILE:HA	1:B:122:PRO:HD3	1.92	0.42
1:B:73:TYR:HD2	1:B:153:LEU:HD23	1.79	0.42
1:B:163:TRP:CZ2	1:B:189:ILE:HA	2.55	0.42
1:B:236:PRO:HG3	1:B:273:ARG:HH12	1.85	0.42
1:B:86:CYS:O	1:B:89:ILE:HG12	2.19	0.42
1:B:273:ARG:HB3	1:B:273:ARG:NH1	2.34	0.42
1:B:226:PHE:HA	1:B:230:GLU:HG2	2.02	0.42
1:A:225:THR:HG22	1:A:230:GLU:CG	2.49	0.42
1:B:112:PRO:O	1:B:116:LEU:HG	2.20	0.42
1:B:222:LYS:HE3	1:B:265:GLU:OE1	2.19	0.42
1:A:57:PRO:HB3	1:A:175:VAL:C	2.40	0.42
1:A:220:PHE:HB3	1:A:262:SER:HB2	2.03	0.41
1:A:263:LEU:O	1:A:267:LYS:HB2	2.20	0.41
1:B:80:GLU:OE2	1:B:120:THR:CB	2.68	0.41
1:B:97:PHE:CE1	1:B:172:MET:HG2	2.45	0.41
1:B:198:GLN:HB3	1:B:229:VAL:HG21	2.02	0.41
1:B:269:ILE:O	1:B:273:ARG:HG3	2.20	0.41
1:B:147:PHE:N	1:B:147:PHE:CD2	2.88	0.41
1:B:72:ILE:C	1:B:77:LEU:HD13	2.41	0.41
1:B:199:LYS:HA	1:B:199:LYS:HD2	1.71	0.41
1:A:119:GLN:NE2	1:A:152:THR:CB	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG11	1:B:170:SER:C	2.41	0.41
1:B:122:PRO:HD2	1:B:147:PHE:CZ	2.55	0.41
1:A:53:TRP:HB2	1:A:176:SER:OG	2.21	0.41
1:A:218:GLU:HG2	1:A:220:PHE:O	2.21	0.41
1:B:267:LYS:O	1:B:271:GLN:HG3	2.21	0.41
1:A:222:LYS:HE2	1:A:269:ILE:HD11	2.02	0.41
1:B:241:LYS:HB2	1:B:276:ILE:HB	2.03	0.41
1:B:101:ASN:HA	1:B:102:PRO:HD2	1.88	0.41
1:A:264:ASN:O	1:A:267:LYS:HB3	2.21	0.40
1:B:72:ILE:HG13	1:B:73:TYR:N	2.36	0.40
1:A:222:LYS:C	1:A:224:SER:H	2.25	0.40
1:B:108:GLU:HA	1:B:111:ALA:HB2	2.03	0.40
1:A:88:GLU:HG2	1:A:116:LEU:HD21	2.04	0.40
1:B:160:ASP:O	1:B:160:ASP:OD1	2.39	0.40
1:B:85:ASN:CB	1:B:88:GLU:HB2	2.47	0.40
1:B:163:TRP:H	1:B:189:ILE:HD11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	207/253 (82%)	187 (90%)	16 (8%)	4 (2%)	8	26
1	B	205/253 (81%)	177 (86%)	21 (10%)	7 (3%)	3	13
All	All	412/506 (81%)	364 (88%)	37 (9%)	11 (3%)	5	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	81	MET
1	B	228	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	CYS
1	B	226	PHE
1	A	124	ASP
1	A	254	SER
1	B	153	LEU
1	B	124	ASP
1	A	223	ASP
1	B	96	ALA
1	B	157	ILE

5.3.2 Protein sidechains ⓘ

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	195/231 (84%)	189 (97%)	6 (3%)	40	74
1	B	195/231 (84%)	189 (97%)	6 (3%)	40	74
All	All	390/462 (84%)	378 (97%)	12 (3%)	40	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	129	TRP
1	A	160	ASP
1	A	205	CYS
1	A	209	GLN
1	A	266	LEU
1	B	76	ILE
1	B	88	GLU
1	B	147	PHE
1	B	171	ASP
1	B	191	MET
1	B	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	209	GLN
1	B	61	HIS
1	B	84	GLN
1	B	119	GLN
1	B	187	ASN
1	B	198	GLN
1	B	243	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	213/253 (84%)	0.32	13 (6%) 21 13	18, 44, 68, 83	0
1	B	211/253 (83%)	0.74	28 (13%) 3 2	26, 55, 84, 99	0
All	All	424/506 (83%)	0.53	41 (9%) 7 4	18, 49, 79, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	LEU	6.0
1	B	215	SER	6.0
1	B	229	VAL	5.6
1	A	228	SER	5.3
1	A	120	THR	4.9
1	B	221	TYR	4.8
1	B	223	ASP	4.4
1	A	216	LEU	3.9
1	B	121	ILE	3.9
1	B	248	HIS	3.7
1	B	220	PHE	3.7
1	B	204	ALA	3.5
1	B	122	PRO	3.4
1	B	211	MET	3.4
1	B	175	VAL	3.0
1	B	264	ASN	2.8
1	B	222	LYS	2.8
1	A	217	ARG	2.8
1	B	283	TYR	2.7
1	A	275	MET	2.7
1	A	174	TYR	2.6
1	B	129	TRP	2.6
1	A	227	GLY	2.6
1	A	171	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	276	ILE	2.5
1	B	118	THR	2.4
1	B	74	THR	2.4
1	B	84	GLN	2.4
1	B	51	LEU	2.4
1	A	129	TRP	2.3
1	B	257	ALA	2.3
1	A	122	PRO	2.2
1	B	123	CYS	2.2
1	B	205	CYS	2.2
1	B	166	ASP	2.2
1	B	52	VAL	2.2
1	B	77	LEU	2.1
1	B	64	ASP	2.1
1	A	261	SER	2.1
1	B	147	PHE	2.1
1	A	239	VAL	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 monosaccharides 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.