



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:35 PM EDT

PDB ID : 3BU8 / pdb_00003bu8
Title : Crystal Structure of TRF2 TRFH domain and TIN2 peptide complex
Authors : Chen, Y.; Yang, Y.; van Overbeek, M.; Donigian, J.R.; Baciú, P.; de Lange, T.; Lei, M.
Deposited on : 2008-01-02
Resolution : 2.15 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

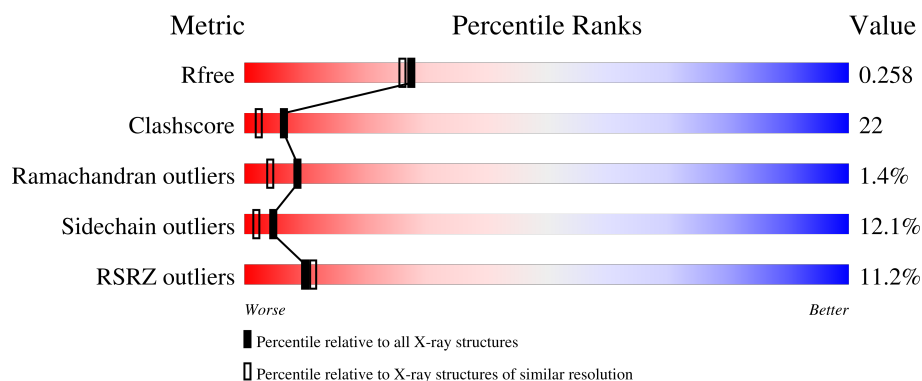
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	235	
1	B	235	
2	C	19	
2	D	19	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3760 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 Telomeric repeat-binding factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1667	1058	293	306	10			
1	B	207	Total	C	N	O	S	0	0	0
			1683	1067	296	310	10			

- Molecule 2 is a protein called TERF1-interacting nuclear factor 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	0
			121	74	27	20			
2	D	10	Total	C	N	O	0	0	0
			79	50	17	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	257	SER	-	SEE REMARK 999	UNP Q9BSI4
D	257	SER	-	SEE REMARK 999	UNP Q9BSI4

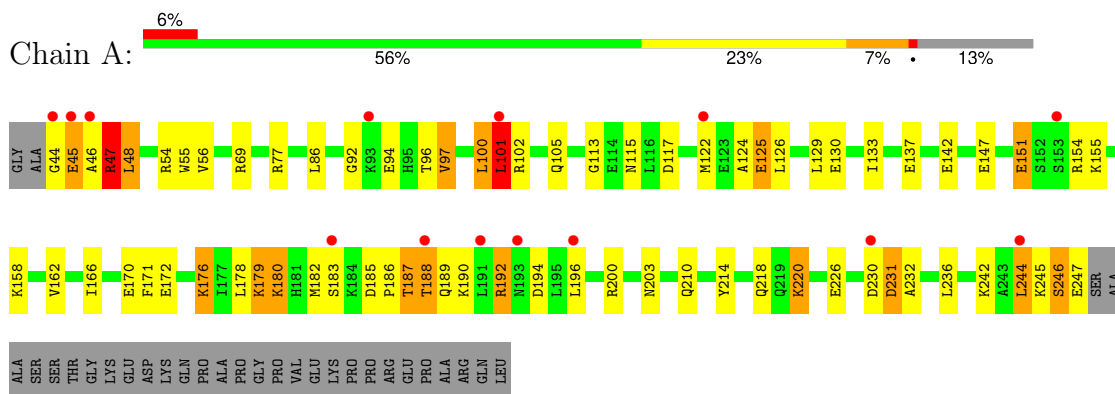
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	90	Total	O	0	0
			90	90		
3	C	10	Total	O	0	0
			10	10		
3	D	5	Total	O	0	0
			5	5		

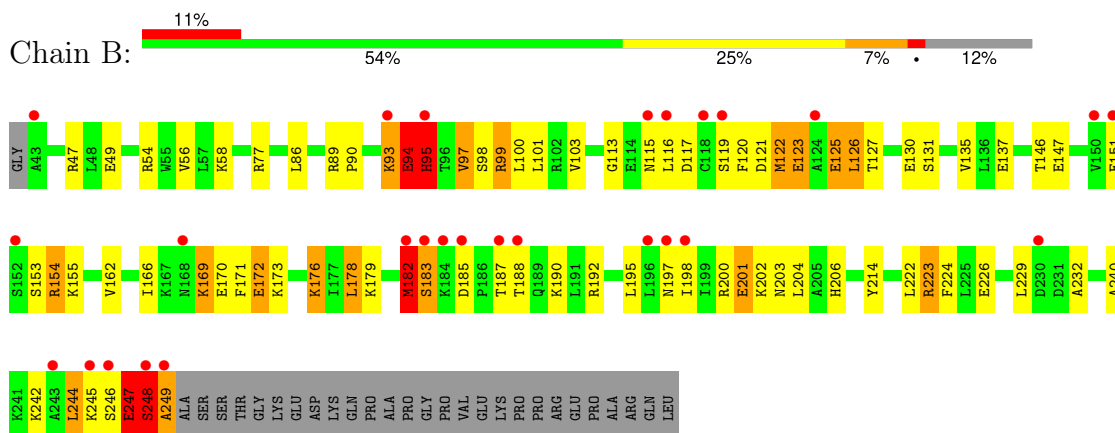
3 Residue-property plots [i](#)

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.

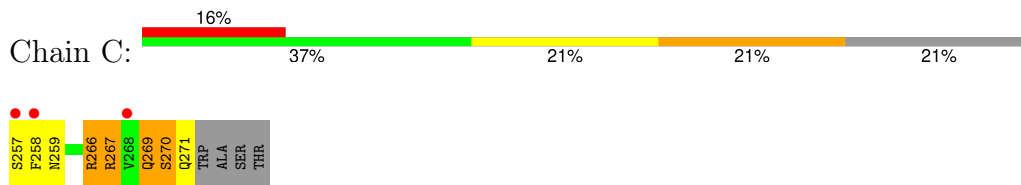
• Molecule 1: Telomeric repeat-binding factor 2



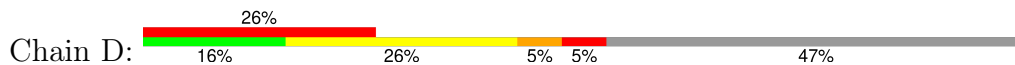
• Molecule 1: Telomeric repeat-binding factor 2



• Molecule 2: TERF1-interacting nuclear factor 2



• Molecule 2: TERF1-interacting nuclear factor 2



S257	F258	N259	L263	G264	R265	R266	ARG	VAL	GLN	SER	GLN	TRP	ALA	SER	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.23Å 75.23Å 181.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.15 69.51 – 2.16	Depositor EDS
% Data completeness (in resolution range)	93.2 (500.00-2.15) 94.0 (69.51-2.16)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.71 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.256 0.241 , 0.258	Depositor DCC
R_{free} test set	2856 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3760	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [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	0.44	0/1692	1.04	11/2269 (0.5%)
1	B	0.49	0/1708	1.20	23/2291 (1.0%)
2	C	0.45	0/122	1.32	1/162 (0.6%)
2	D	1.26	1/80 (1.2%)	2.62	8/106 (7.5%)
All	All	0.49	1/3602 (0.0%)	1.18	43/4828 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	265	ARG	CA-C	5.16	1.59	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	SER	N-CA-C	-15.15	91.69	111.24
1	B	183	SER	N-CA-C	13.05	129.31	112.34
1	B	93	LYS	N-CA-C	11.54	128.35	114.04
1	A	47	ARG	N-CA-C	-10.82	98.70	114.39
2	D	259	ASN	N-CA-C	10.62	125.93	110.10
1	A	189	GLN	N-CA-C	10.30	122.19	110.97
2	D	265	ARG	N-CA-C	9.37	130.76	110.80
2	D	258	PHE	N-CA-C	-9.16	94.96	107.88
2	C	258	PHE	N-CA-C	-8.97	98.89	111.81
1	B	247	GLU	N-CA-C	8.53	121.33	110.24
1	B	170	GLU	N-CA-C	-8.41	100.05	110.65
2	D	264	GLY	N-CA-C	-7.71	101.97	111.45
1	B	249	ALA	N-CA-C	7.68	132.51	111.00
1	A	151	GLU	N-CA-C	7.67	120.61	111.33
1	B	121	ASP	N-CA-C	7.66	121.61	109.50
1	A	101	LEU	CA-CB-CG	7.57	142.81	116.30
1	B	95	HIS	N-CA-C	-7.38	104.16	113.01
2	D	265	ARG	N-CA-CB	-7.18	98.35	110.49
1	B	93	LYS	CB-CA-C	-7.01	96.67	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	N-CA-C	-6.66	103.95	111.14
1	A	102	ARG	N-CA-C	-6.63	103.97	111.14
1	B	126	LEU	N-CA-C	6.54	119.71	109.96
1	B	232	ALA	N-CA-C	6.44	118.87	110.43
2	D	263	LEU	CA-C-N	5.89	126.87	121.86
2	D	263	LEU	C-N-CA	5.89	126.87	121.86
1	A	232	ALA	N-CA-C	5.86	118.51	110.24
1	A	48	LEU	N-CA-C	-5.78	104.95	112.23
1	B	185	ASP	N-CA-C	-5.72	101.72	110.01
1	B	127	THR	N-CA-C	-5.63	101.95	110.39
1	B	182	MET	CA-C-N	5.61	129.67	120.63
1	B	182	MET	C-N-CA	5.61	129.67	120.63
1	B	130	GLU	N-CA-C	-5.52	105.26	111.28
1	B	248	SER	N-CA-C	5.41	122.33	110.80
1	A	92	GLY	N-CA-C	-5.38	99.32	112.44
1	B	182	MET	N-CA-C	5.32	118.03	110.10
1	B	202	LYS	N-CA-C	-5.31	104.57	111.74
1	B	179	LYS	N-CA-C	5.29	117.04	111.28
1	B	99	ARG	N-CA-C	-5.25	105.45	111.07
2	D	258	PHE	CB-CA-C	-5.24	101.42	111.78
1	A	130	GLU	N-CA-C	-5.23	105.66	111.36
1	A	142	GLU	N-CA-C	5.17	117.81	111.82
1	A	171	PHE	N-CA-C	5.16	116.59	111.07
1	B	120	PHE	N-CA-C	-5.00	106.77	112.92

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	1667	0	1716	69	0
1	B	1683	0	1731	70	0
2	C	121	0	125	14	0
2	D	79	0	82	14	0
3	A	105	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	90	0	0	6	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
All	All	3760	0	3654	157	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 22.

All (157) 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:201:GLU:HG2	1:B:203:ASN:HB2	1.36	1.02
1:A:170:GLU:HA	2:C:269:GLN:HE22	1.27	0.99
1:B:182:MET:HE1	1:B:195:LEU:HD12	1.41	0.99
1:A:178:LEU:HD13	1:A:182:MET:HE3	1.45	0.96
2:D:257:SER:O	2:D:258:PHE:HD1	1.48	0.96
2:D:265:ARG:HH11	2:D:265:ARG:HG3	1.33	0.93
2:D:257:SER:O	2:D:258:PHE:CD1	2.26	0.88
1:A:178:LEU:HD11	1:A:192:ARG:HB2	1.57	0.87
1:A:45:GLU:HA	1:A:48:LEU:HD12	1.57	0.85
1:A:170:GLU:HA	2:C:269:GLN:NE2	1.91	0.85
1:A:179:LYS:HZ1	1:A:192:ARG:HH22	1.20	0.84
2:C:269:GLN:HE21	2:C:269:GLN:C	1.86	0.84
1:A:231:ASP:HB2	3:A:315:HOH:O	1.79	0.83
2:D:265:ARG:HH11	2:D:265:ARG:CG	1.92	0.82
1:B:58:LYS:NZ	1:B:94:GLU:OE1	2.13	0.81
1:A:44:GLY:C	1:A:46:ALA:H	1.87	0.80
2:D:265:ARG:C	2:D:265:ARG:HD3	2.07	0.80
1:A:100:LEU:HD23	1:A:101:LEU:N	1.98	0.79
2:D:265:ARG:CG	2:D:265:ARG:NH1	2.47	0.78
2:D:265:ARG:HD3	2:D:265:ARG:O	1.84	0.78
1:B:123:GLU:HG3	3:B:306:HOH:O	1.85	0.77
2:C:271:GLN:O	2:C:271:GLN:HG3	1.85	0.76
1:B:223:ARG:HA	1:B:223:ARG:NE	2.01	0.74
1:A:220:LYS:HD3	3:A:352:HOH:O	1.87	0.73
1:B:122:MET:HG2	1:B:123:GLU:H	1.54	0.72
1:B:201:GLU:O	1:B:201:GLU:HG3	1.89	0.71
1:A:180:LYS:HE3	3:A:357:HOH:O	1.90	0.70
1:A:124:ALA:O	2:C:266:ARG:HG2	1.92	0.69
1:A:188:THR:O	1:A:188:THR:HG23	1.93	0.68
1:B:222:LEU:O	1:B:226:GLU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD12	1:A:182:MET:HB2	1.75	0.68
1:B:166:ILE:O	1:B:204:LEU:HD21	1.94	0.68
1:A:176:LYS:HD2	3:A:338:HOH:O	1.93	0.67
1:B:178:LEU:CD2	1:B:182:MET:HE2	2.25	0.66
1:B:182:MET:HE1	1:B:195:LEU:CD1	2.22	0.66
1:A:179:LYS:NZ	1:A:192:ARG:HH22	1.94	0.66
1:A:69:ARG:NH2	1:A:226:GLU:OE2	2.28	0.65
1:A:97:VAL:O	1:A:101:LEU:HD13	1.96	0.65
1:B:197:ASN:ND2	1:B:200:ARG:CZ	2.60	0.65
1:A:44:GLY:C	1:A:46:ALA:N	2.55	0.65
1:A:124:ALA:O	2:C:266:ARG:CG	2.45	0.65
1:A:178:LEU:CD1	1:A:182:MET:HE3	2.25	0.64
1:B:155:LYS:HE3	1:B:188:THR:HG21	1.80	0.64
1:B:155:LYS:HE3	1:B:188:THR:CG2	2.29	0.63
1:B:169:LYS:HB3	1:B:171:PHE:CE1	2.33	0.63
2:C:269:GLN:NE2	2:C:269:GLN:C	2.57	0.62
1:A:55:TRP:HB3	1:A:236:LEU:HD13	1.79	0.62
1:B:197:ASN:HD21	1:B:200:ARG:CZ	2.12	0.62
1:B:190:LYS:NZ	3:B:331:HOH:O	2.35	0.59
1:A:125:GLU:O	2:C:266:ARG:NH1	2.36	0.58
1:A:155:LYS:NZ	1:A:187:THR:HG21	2.18	0.58
1:A:183:SER:HB3	1:A:192:ARG:HH12	1.67	0.58
1:A:179:LYS:HZ3	1:A:192:ARG:HH12	1.51	0.58
1:B:173:LYS:NZ	1:B:176:LYS:NZ	2.52	0.58
1:A:179:LYS:HZ1	1:A:192:ARG:NH2	1.97	0.58
1:B:223:ARG:HA	1:B:223:ARG:HE	1.69	0.58
1:B:137:GLU:OE2	1:B:154:ARG:NE	2.32	0.57
1:A:77:ARG:HD2	3:A:371:HOH:O	2.04	0.57
1:B:178:LEU:C	1:B:178:LEU:HD13	2.30	0.57
1:B:248:SER:O	1:B:249:ALA:HB3	2.05	0.57
1:B:113:GLY:HA3	1:B:214:TYR:OH	2.05	0.56
1:A:54:ARG:NH2	3:A:368:HOH:O	2.38	0.56
1:B:103:VAL:HG21	1:B:229:LEU:HD21	1.86	0.56
1:A:101:LEU:O	1:A:105:GLN:HG3	2.06	0.55
1:A:214:TYR:O	1:A:218:GLN:HG3	2.06	0.55
1:A:179:LYS:NZ	1:A:192:ARG:HH12	2.04	0.55
1:A:94:GLU:HB3	1:A:97:VAL:HG13	1.89	0.55
1:A:178:LEU:HD21	1:A:196:LEU:HG	1.89	0.55
1:B:95:HIS:O	1:B:99:ARG:HG3	2.06	0.55
1:B:125:GLU:HG3	1:B:173:LYS:HZ3	1.71	0.55
2:D:265:ARG:NH1	2:D:265:ARG:HG2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:OE1	1:A:154:ARG:NH2	2.40	0.54
1:B:93:LYS:O	1:B:94:GLU:C	2.51	0.54
1:B:122:MET:HG2	1:B:123:GLU:N	2.23	0.53
1:A:126:LEU:HD21	1:B:146:THR:HG21	1.91	0.53
1:A:154:ARG:HG2	1:A:158:LYS:HE3	1.90	0.52
1:A:183:SER:HB3	1:A:192:ARG:NH1	2.24	0.52
1:A:247:GLU:O	1:A:247:GLU:CD	2.53	0.52
1:B:178:LEU:HD21	1:B:192:ARG:HG3	1.92	0.52
1:A:155:LYS:HZ3	1:A:187:THR:HG21	1.74	0.52
1:A:230:ASP:OD1	1:A:231:ASP:N	2.43	0.52
1:A:246:SER:O	1:A:247:GLU:C	2.52	0.52
1:B:54:ARG:HB2	1:B:54:ARG:HH11	1.75	0.52
2:C:269:GLN:HE21	2:C:270:SER:N	2.08	0.52
1:B:115:ASN:ND2	3:B:335:HOH:O	2.42	0.51
1:B:94:GLU:HB3	1:B:97:VAL:HG13	1.92	0.51
1:A:100:LEU:HD23	1:A:100:LEU:C	2.35	0.51
1:A:183:SER:CB	1:A:192:ARG:NH1	2.74	0.51
1:B:54:ARG:HB2	1:B:54:ARG:NH1	2.27	0.50
1:B:247:GLU:O	1:B:248:SER:OG	2.18	0.50
1:A:56:VAL:HG12	1:A:86:LEU:HD11	1.93	0.49
2:D:257:SER:C	2:D:258:PHE:CD1	2.90	0.49
1:B:166:ILE:HG22	1:B:204:LEU:CD2	2.42	0.49
1:B:147:GLU:O	1:B:151:GLU:HB2	2.13	0.49
1:B:197:ASN:O	1:B:200:ARG:HB3	2.13	0.49
2:C:257:SER:N	3:C:286:HOH:O	2.45	0.49
2:C:257:SER:C	2:C:259:ASN:H	2.20	0.49
1:B:101:LEU:HD13	2:D:257:SER:HB2	1.94	0.49
2:D:266:ARG:HG2	2:D:266:ARG:HH11	1.77	0.49
1:B:126:LEU:HD12	1:B:126:LEU:N	2.28	0.49
1:B:54:ARG:HH11	1:B:54:ARG:CB	2.26	0.49
2:D:266:ARG:HG2	2:D:266:ARG:NH1	2.27	0.49
1:A:247:GLU:CD	1:A:247:GLU:C	2.82	0.48
2:C:267:ARG:C	2:C:267:ARG:HD3	2.39	0.47
1:B:245:LYS:O	1:B:245:LYS:HG3	2.13	0.47
1:A:162:VAL:HG21	1:A:182:MET:CE	2.45	0.47
1:A:44:GLY:O	1:A:46:ALA:N	2.47	0.47
1:B:173:LYS:NZ	1:B:176:LYS:HZ3	2.12	0.47
1:B:240:ALA:O	1:B:244:LEU:HB2	2.15	0.47
1:A:230:ASP:O	3:A:328:HOH:O	2.21	0.47
1:A:170:GLU:CA	2:C:269:GLN:NE2	2.72	0.46
1:A:183:SER:CB	1:A:192:ARG:HH12	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:O	2:D:266:ARG:NE	2.47	0.46
1:A:178:LEU:HD11	1:A:192:ARG:CB	2.39	0.46
1:B:77:ARG:HD3	3:B:333:HOH:O	2.16	0.45
1:A:137:GLU:CD	1:A:154:ARG:NH1	2.75	0.45
1:B:123:GLU:O	1:B:123:GLU:HG2	2.15	0.45
1:B:97:VAL:O	1:B:101:LEU:HG	2.17	0.45
1:B:172:GLU:H	1:B:172:GLU:CD	2.24	0.45
1:B:173:LYS:HZ1	1:B:176:LYS:NZ	2.15	0.45
1:B:173:LYS:HZ2	1:B:176:LYS:HZ3	1.64	0.45
1:B:89:ARG:HB3	1:B:90:PRO:HD2	1.99	0.45
1:B:131:SER:O	1:B:135:VAL:HG23	2.17	0.44
1:B:153:SER:OG	1:B:224:PHE:CG	2.70	0.44
1:A:154:ARG:CG	1:A:158:LYS:HE3	2.47	0.44
1:B:200:ARG:CD	3:B:281:HOH:O	2.66	0.44
1:A:56:VAL:CG1	1:A:86:LEU:HD11	2.47	0.44
1:A:190:LYS:O	1:A:194:ASP:CG	2.61	0.44
1:A:244:LEU:HD22	1:A:244:LEU:HA	1.69	0.44
1:A:113:GLY:HA3	1:A:214:TYR:OH	2.18	0.44
1:B:162:VAL:O	1:B:166:ILE:HG13	2.17	0.44
1:B:97:VAL:O	1:B:100:LEU:HB3	2.18	0.43
1:B:172:GLU:CD	1:B:173:LYS:H	2.26	0.43
1:A:47:ARG:NH1	3:A:343:HOH:O	2.51	0.43
2:C:257:SER:C	2:C:259:ASN:N	2.76	0.43
1:A:242:LYS:C	1:A:244:LEU:N	2.76	0.43
1:B:117:ASP:O	2:D:266:ARG:HB2	2.19	0.43
1:B:172:GLU:CD	1:B:172:GLU:N	2.77	0.43
1:A:137:GLU:OE2	1:A:154:ARG:NH1	2.51	0.43
1:B:123:GLU:HG2	1:B:126:LEU:HD13	2.00	0.43
1:A:183:SER:HA	1:A:192:ARG:HH11	1.83	0.43
1:B:173:LYS:HZ2	1:B:176:LYS:NZ	2.17	0.43
1:B:173:LYS:NZ	1:B:176:LYS:HZ2	2.17	0.42
1:B:178:LEU:C	1:B:178:LEU:CD1	2.93	0.42
1:A:115:ASN:C	1:A:117:ASP:H	2.28	0.42
1:A:179:LYS:HE2	1:A:192:ARG:NH2	2.34	0.41
1:B:100:LEU:C	1:B:100:LEU:HD23	2.45	0.41
1:A:183:SER:HA	1:A:192:ARG:NH1	2.34	0.41
1:A:115:ASN:HB3	1:A:117:ASP:OD1	2.20	0.41
1:A:129:LEU:O	1:A:133:ILE:HG13	2.21	0.41
1:B:56:VAL:CG1	1:B:86:LEU:HD11	2.51	0.41
1:B:178:LEU:HD22	1:B:182:MET:HE2	2.00	0.41
1:B:49:GLU:OE2	1:B:89:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:O	1:A:166:ILE:HG13	2.21	0.41
1:A:185:ASP:HA	1:A:186:PRO:HD2	1.93	0.40
1:B:77:ARG:CD	3:B:333:HOH:O	2.69	0.40
1:B:198:ILE:HD11	1:B:206:HIS:CG	2.56	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	202/235 (86%)	195 (96%)	4 (2%)	3 (2%)	8	4
1	B	205/235 (87%)	197 (96%)	7 (3%)	1 (0%)	24	20
2	C	13/19 (68%)	12 (92%)	0	1 (8%)	1	0
2	D	8/19 (42%)	7 (88%)	0	1 (12%)	0	0
All	All	428/508 (84%)	411 (96%)	11 (3%)	6 (1%)	9	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	LYS
2	C	270	SER
2	D	265	ARG
1	A	45	GLU
1	B	94	GLU
1	A	246	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	184/207 (89%)	163 (89%)	21 (11%)	5	2
1	B	185/207 (89%)	163 (88%)	22 (12%)	5	2
2	C	13/16 (81%)	10 (77%)	3 (23%)	1	0
2	D	8/16 (50%)	7 (88%)	1 (12%)	4	2
All	All	390/446 (87%)	343 (88%)	47 (12%)	5	2

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	96	THR
1	A	97	VAL
1	A	100	LEU
1	A	101	LEU
1	A	122	MET
1	A	125	GLU
1	A	151	GLU
1	A	172	GLU
1	A	176	LYS
1	A	179	LYS
1	A	180	LYS
1	A	187	THR
1	A	188	THR
1	A	192	ARG
1	A	200	ARG
1	A	203	ASN
1	A	210	GLN
1	A	220	LYS
1	A	231	ASP
1	A	244	LEU
1	B	94	GLU
1	B	95	HIS
1	B	97	VAL
1	B	98	SER
1	B	119	SER
1	B	122	MET
1	B	123	GLU

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Mol	Chain	Res	Type
1	B	125	GLU
1	B	154	ARG
1	B	169	LYS
1	B	172	GLU
1	B	176	LYS
1	B	178	LEU
1	B	182	MET
1	B	183	SER
1	B	187	THR
1	B	201	GLU
1	B	223	ARG
1	B	242	LYS
1	B	244	LEU
1	B	247	GLU
1	B	248	SER
2	C	266	ARG
2	C	267	ARG
2	C	269	GLN
2	D	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	197	ASN
1	A	203	ASN
1	B	193	ASN
1	B	197	ASN
1	B	211	ASN
2	C	269	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 [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

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	204/235 (86%)	0.61	14 (6%) 23 26	33, 46, 68, 87	0
1	B	207/235 (88%)	0.80	27 (13%) 7 8	36, 51, 74, 85	0
2	C	15/19 (78%)	1.75	3 (20%) 3 3	41, 67, 81, 82	0
2	D	10/19 (52%)	2.34	5 (50%) 0 1	52, 69, 80, 80	0
All	All	436/508 (85%)	0.78	49 (11%) 10 11	33, 49, 74, 87	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	5.7
2	D	257	SER	5.1
2	C	268	VAL	4.7
2	C	258	PHE	4.6
1	B	183	SER	4.5
2	D	258	PHE	4.4
1	B	115	ASN	4.2
1	B	43	ALA	4.0
2	D	263	LEU	4.0
1	A	44	GLY	3.9
1	A	93	LYS	3.9
1	A	101	LEU	3.5
2	D	264	GLY	3.4
1	B	118	CYS	3.2
1	B	93	LYS	3.0
1	A	244	LEU	3.0
1	B	196	LEU	2.9
1	A	183	SER	2.9
1	B	246	SER	2.9
1	B	124	ALA	2.9
1	B	245	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	95	HIS	2.8
1	B	184	LYS	2.7
1	A	45	GLU	2.7
1	B	151	GLU	2.7
1	B	197	ASN	2.6
1	A	122	MET	2.6
1	B	168	ASN	2.6
1	B	185	ASP	2.5
1	B	243	ALA	2.5
1	A	188	THR	2.4
1	B	119	SER	2.4
1	B	150	VAL	2.4
1	B	152	SER	2.3
2	C	257	SER	2.3
1	A	230	ASP	2.2
1	B	116	LEU	2.2
1	B	187	THR	2.2
1	B	249	ALA	2.2
1	A	196	LEU	2.2
1	B	248	SER	2.2
1	B	230	ASP	2.2
1	B	182	MET	2.1
1	B	188	THR	2.1
2	D	266	ARG	2.1
1	A	191	LEU	2.1
1	A	193	ASN	2.1
1	B	198	ILE	2.0
1	A	153	SER	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 ⓘ

There are no such residues in this entry.