Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:41 AM GMT

PDB ID	:	3BU8
Title	:	Crystal Structure of TRF2 TRFH domain and TIN2 peptide complex
Authors	:	Chen, Y.; Yang, Y.; van Overbeek, M.; Donigian, J.R.; Baciu, 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

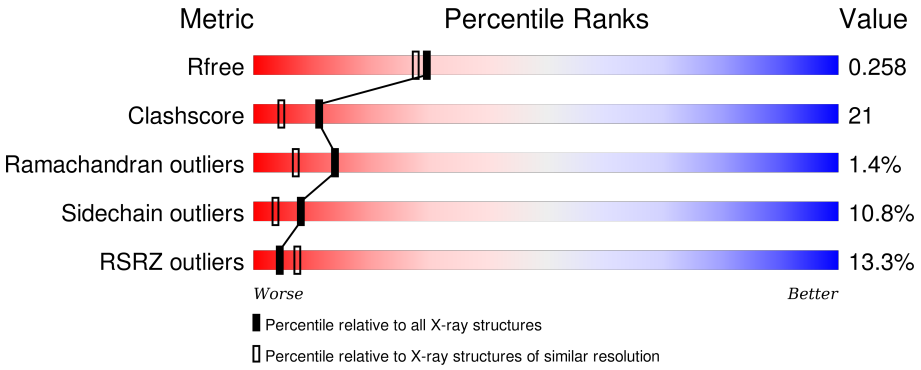
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 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	235	10% 60% 20% 7% 13%
1	B	235	9% 58% 23% 7% 12%
2	C	19	42% 42% 21% 16% 21%
2	D	19	32% 26% 16% 5% 5% 47%

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.

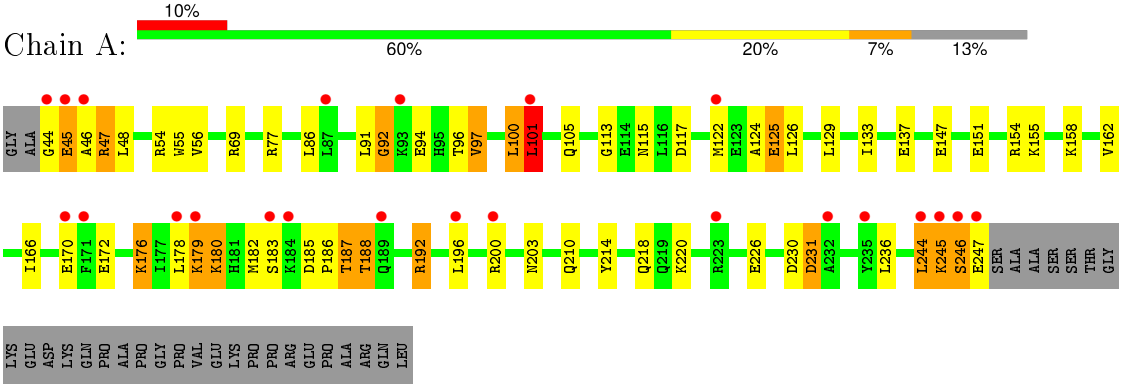
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	90	Total	O	0	0
			90	90		
3	C	10	Total	O	0	0
			10	10		
3	D	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

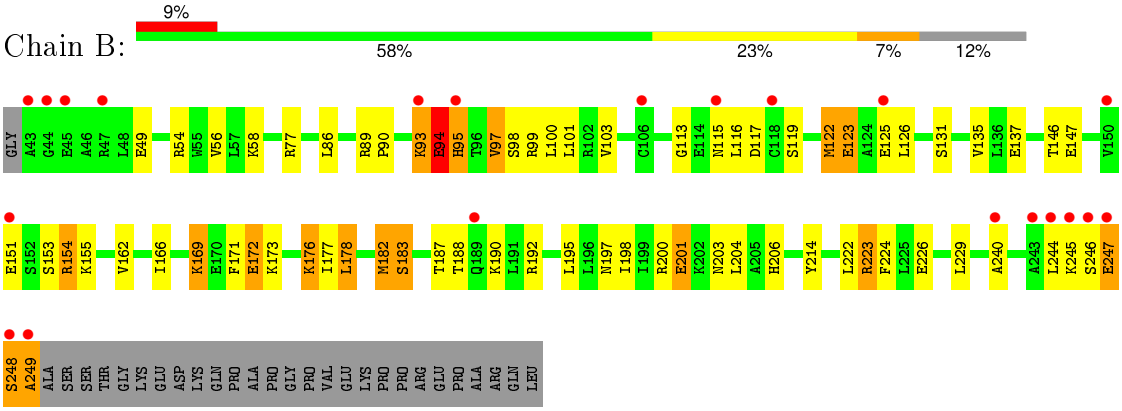
- Molecule 1: Telomeric repeat-binding factor 2

Chain A:



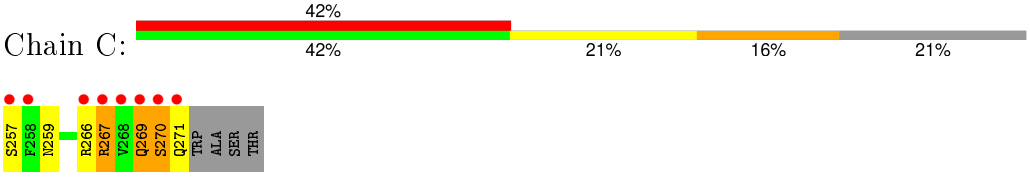
- Molecule 1: Telomeric repeat-binding factor 2

Chain B:



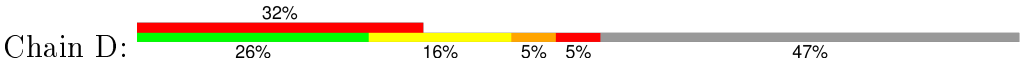
- Molecule 2: TERF1-interacting nuclear factor 2

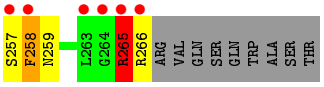
Chain C:



- Molecule 2: TERF1-interacting nuclear factor 2

Chain D:




S257
F258
N259
L263
G264
R265
R266
ARG
VAL
GLN
SER
GLN
TRP
ALA
SER
THR

4 Data and refinement statistics (i)

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 47.16 – 2.16	Depositor EDS
% Data completeness (in resolution range)	93.2 (500.00-2.15) 94.1 (47.16-2.16)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	2700 reflections (9.90%)	DCC
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 , 57.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 28753 reflections	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.*

[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

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	0.36	0/1692	0.68	2/2269 (0.1%)
1	B	0.43	1/1708 (0.1%)	0.78	5/2291 (0.2%)
2	C	0.45	0/122	0.86	0/162
2	D	1.10	0/80	1.96	5/106 (4.7%)
All	All	0.43	1/3602 (0.0%)	0.78	12/4828 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	ALA	CA-CB	-5.68	1.40	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	LEU	CA-CB-CG	11.96	142.81	115.30
1	B	249	ALA	N-CA-C	7.97	132.51	111.00
2	D	265	ARG	N-CA-C	7.32	130.76	111.00
1	B	246	SER	N-CA-C	-7.15	91.69	111.00
1	B	93	LYS	CB-CA-C	-6.86	96.67	110.40
2	D	265	ARG	N-CA-CB	-6.81	98.35	110.60
1	B	183	SER	N-CA-C	6.78	129.31	111.00
1	B	93	LYS	N-CA-C	6.42	128.35	111.00
2	D	258	PHE	N-CA-C	-5.94	94.96	111.00
2	D	259	ASN	N-CA-C	5.53	125.93	111.00
1	A	92	GLY	N-CA-C	-5.51	99.32	113.10
2	D	258	PHE	N-CA-CB	5.16	119.90	110.60

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	63	0
2	C	121	0	125	13	0
2	D	79	0	82	14	0
3	A	105	0	0	9	0
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	149	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 21.

All (149) 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
2:D:257:SER:O	2:D:258:PHE:HD1	1.48	0.96
2:D:265:ARG:HG3	2:D:265:ARG:HH11	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:170:GLU:HA	2:C:269:GLN:NE2	1.91	0.85
1:A:45:GLU:HA	1:A:48:LEU:HD12	1.57	0.85
1:A:179:LYS:HZ1	1:A:192:ARG:HH22	1.20	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:100:LEU:HD23	1:A:101:LEU:N	1.98	0.79
2:C:269:GLN:C	2:C:269:GLN:HE21	1.86	0.79
2:D:265:ARG:NH1	2:D:265:ARG:CG	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
1:A:44:GLY:C	1:A:46:ALA:H	1.87	0.77
2:C:271:GLN:O	2:C:271:GLN:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:ARG:HD3	2:D:265:ARG:C	2.07	0.75
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:B:182:MET:HE1	1:B:195:LEU:HD12	1.72	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:HG23	1:A:188:THR:O	1.93	0.68
1:B:222:LEU:O	1:B:226:GLU:HB2	1.93	0.68
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:178:LEU:HD13	1:A:182:MET:HE3	1.76	0.67
1:A:176:LYS:HD2	3:A:338:HOH:O	1.93	0.67
1:A:179:LYS:NZ	1:A:192:ARG:HH22	1.94	0.66
1:A:97:VAL:O	1:A:101:LEU:HD13	1.96	0.65
1:A:69:ARG:NH2	1:A:226:GLU:OE2	2.28	0.65
1:B:197:ASN:ND2	1:B:200:ARG:CZ	2.60	0.65
1:A:124:ALA:O	2:C:266:ARG:CG	2.45	0.65
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
1:B:197:ASN:HD21	1:B:200:ARG:CZ	2.12	0.62
1:A:55:TRP:HB3	1:A:236:LEU:HD13	1.79	0.62
1:A:44:GLY:C	1:A:46:ALA:N	2.55	0.60
1:B:247:GLU:O	1:B:248:SER:OG	2.18	0.60
1:B:182:MET:CE	1:B:195:LEU:HD12	2.31	0.59
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
2:C:269:GLN:NE2	2:C:269:GLN:C	2.57	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG21	1:B:229:LEU:HD21	1.86	0.56
1:A:162:VAL:HG21	1:A:182:MET:HE2	1.87	0.56
1:A:178:LEU:HD13	1:A:182:MET:CE	2.35	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:178:LEU:HD21	1:A:196:LEU:HG	1.89	0.55
1:A:94:GLU:HB3	1:A:97:VAL:HG13	1.89	0.55
1:B:95:HIS:O	1:B:99:ARG:HG3	2.06	0.55
2:D:265:ARG:HG2	2:D:265:ARG:NH1	2.21	0.55
1:A:147:GLU:OE1	1:A:154:ARG:NH2	2.40	0.54
1:B:125:GLU:HG3	1:B:173:LYS:HZ3	1.73	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:B:178:LEU:HD13	1:B:178:LEU:C	2.30	0.52
1:B:178:LEU:HD21	1:B:192:ARG:HG3	1.92	0.52
1:B:173:LYS:NZ	1:B:176:LYS:HZ2	2.07	0.52
1:A:230:ASP:OD1	1:A:231:ASP:N	2.43	0.52
2:C:269:GLN:HE21	2:C:270:SER:N	2.08	0.52
1:B:54:ARG:HB2	1:B:54:ARG:HH11	1.75	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:183:SER:CB	1:A:192:ARG:NH1	2.74	0.51
1:B:54:ARG:NH1	1:B:54:ARG:HB2	2.27	0.50
1:A:56:VAL:HG12	1:A:86:LEU:HD11	1.93	0.49
1:B:166:ILE:HG22	1:B:204:LEU:CD2	2.42	0.49
1:B:93:LYS:O	1:B:94:GLU:C	2.51	0.49
1:B:197:ASN:O	1:B:200:ARG:HB3	2.13	0.49
1:B:147:GLU:O	1:B:151:GLU:HB2	2.13	0.49
2:C:257:SER:N	3:C:286:HOH:O	2.45	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:NH1	2:D:266:ARG:HG2	2.27	0.49
1:A:246:SER:O	1:A:247:GLU:C	2.52	0.47
1:B:245:LYS:HG3	1:B:245:LYS:O	2.13	0.47
1:A:162:VAL:HG21	1:A:182:MET:CE	2.45	0.47
1:A:247:GLU:O	1:A:247:GLU:CD	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:O	1:A:46:ALA:N	2.47	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
1:A:100:LEU:C	1:A:100:LEU:HD23	2.35	0.46
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:A:155:LYS:HZ2	1:A:187:THR:HG21	1.81	0.46
1:B:77:ARG:HD3	3:B:333:HOH:O	2.16	0.45
1:B:123:GLU:HG2	1:B:123:GLU:O	2.15	0.45
1:B:173:LYS:HZ2	1:B:176:LYS:NZ	2.14	0.45
1:B:97:VAL:O	1:B:101:LEU:HG	2.17	0.45
2:C:257:SER:C	2:C:259:ASN:H	2.20	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:B:200:ARG:CD	3:B:281:HOH:O	2.66	0.44
1:A:154:ARG:CG	1:A:158:LYS:HE3	2.47	0.44
1:A:56:VAL:CG1	1:A:86:LEU:HD11	2.47	0.44
1:A:244:LEU:HA	1:A:244:LEU:HD22	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:A:47:ARG:NH1	3:A:343:HOH:O	2.51	0.43
1:B:117:ASP:O	2:D:266:ARG:HB2	2.19	0.43
1:B:123:GLU:HG2	1:B:126:LEU:HD13	2.00	0.43
1:A:137:GLU:OE2	1:A:154:ARG:NH1	2.51	0.43
1:A:183:SER:HA	1:A:192:ARG:HH11	1.83	0.43
2:C:267:ARG:HD3	2:C:267:ARG:C	2.39	0.43
1:A:188:THR:CG2	1:A:188:THR:O	2.64	0.42
1:B:173:LYS:HZ1	1:B:176:LYS:NZ	2.18	0.42
2:D:257:SER:C	2:D:258:PHE:CD1	2.90	0.41
1:A:179:LYS:HE2	1:A:192:ARG:NH2	2.34	0.41
1:A:183:SER:HA	1:A:192:ARG:NH1	2.34	0.41
1:A:245:LYS:NZ	3:A:364:HOH:O	2.42	0.41
1:A:115:ASN:HB3	1:A:117:ASP:OD1	2.20	0.41
1:B:56:VAL:CG1	1:B:86:LEU:HD11	2.51	0.41
1:A:129:LEU:O	1:A:133:ILE:HG13	2.21	0.41
1:B:176:LYS:HG3	1:B:177:ILE:N	2.33	0.41
1:A:137:GLU:CD	1:A:154:ARG:NH1	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:OE2	1:B:89:ARG:HD3	2.20	0.41
1:A:162:VAL:O	1:A:166:ILE:HG13	2.21	0.41
1:B:172:GLU:H	1:B:172:GLU:CD	2.24	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
1:A:185:ASP:HA	1:A:186:PRO:HD2	1.93	0.40
1:A:91:LEU:C	1:A:92:GLY:O	2.58	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%)	13 6
1	B	205/235 (87%)	197 (96%)	7 (3%)	1 (0%)	34 26
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%)	14 7

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%)	164 (89%)	20 (11%)	8	3
1	B	185/207 (89%)	166 (90%)	19 (10%)	9	5
2	C	13/16 (81%)	11 (85%)	2 (15%)	3	1
2	D	8/16 (50%)	7 (88%)	1 (12%)	6	2
All	All	390/446 (87%)	348 (89%)	42 (11%)	8	4

All (42) 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	231	ASP
1	A	244	LEU
1	B	94	GLU
1	B	95	HIS
1	B	97	VAL
1	B	98	SER

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Mol	Chain	Res	Type
1	B	119	SER
1	B	122	MET
1	B	123	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	247	GLU
1	B	248	SER
2	C	267	ARG
2	C	269	GLN
2	D	265	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
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 (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

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, 95^{th} 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%)	0.80	23 (11%)	7	11	33, 46, 68, 87	0
1	B	207/235 (88%)	0.98	21 (10%)	9	15	36, 51, 74, 85	0
2	C	15/19 (78%)	3.14	8 (53%)	0	0	41, 67, 81, 82	0
2	D	10/19 (52%)	3.39	6 (60%)	0	0	52, 69, 80, 81	0
All	All	436/508 (85%)	1.02	58 (13%)	4	7	33, 49, 74, 87	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	257	SER	8.9
1	B	249	ALA	7.7
2	C	271	GLN	7.1
1	B	248	SER	6.8
2	C	268	VAL	6.6
1	A	45	GLU	6.6
2	C	269	GLN	5.5
2	C	270	SER	5.5
1	B	246	SER	5.4
1	A	246	SER	5.3
2	C	267	ARG	5.2
1	B	244	LEU	5.1
2	D	258	PHE	5.1
2	D	265	ARG	4.8
2	C	257	SER	4.4
2	D	264	GLY	4.4
1	A	247	GLU	4.4
2	C	258	PHE	3.9
1	B	43	ALA	3.9
1	B	247	GLU	3.6
1	B	245	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	3.5
1	A	244	LEU	3.5
1	B	95	HIS	3.4
2	C	266	ARG	3.3
1	A	101	LEU	3.2
1	A	184	LYS	3.2
2	D	266	ARG	3.1
1	B	93	LYS	2.9
1	A	232	ALA	2.9
1	B	151	GLU	2.9
2	D	263	LEU	2.9
1	A	171	PHE	2.9
1	A	200	ARG	2.9
1	A	170	GLU	2.7
1	A	93	LYS	2.7
1	A	179	LYS	2.7
1	A	245	LYS	2.6
1	A	44	GLY	2.6
1	A	196	LEU	2.6
1	B	150	VAL	2.6
1	B	243	ALA	2.6
1	B	115	ASN	2.6
1	B	47	ARG	2.5
1	B	44	GLY	2.5
1	A	223	ARG	2.4
1	A	189	GLN	2.3
1	A	87	LEU	2.3
1	B	125	GLU	2.3
1	A	178	LEU	2.3
1	A	235	TYR	2.2
1	A	122	MET	2.2
1	B	189	GLN	2.2
1	B	45	GLU	2.2
1	B	240	ALA	2.1
1	A	183	SER	2.1
1	B	118	CYS	2.1
1	B	106	CYS	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.