



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:01 AM GMT

PDB ID : 2Z6K
Title : Crystal structure of full-length human RPA14/32 heterodimer
Authors : Deng, X.; Habel, J.E.; Kabaleeswaran, V.; Borgstahl, G.E.
Deposited on : 2007-08-03
Resolution : 3.00 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 ⓘ](#)) 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

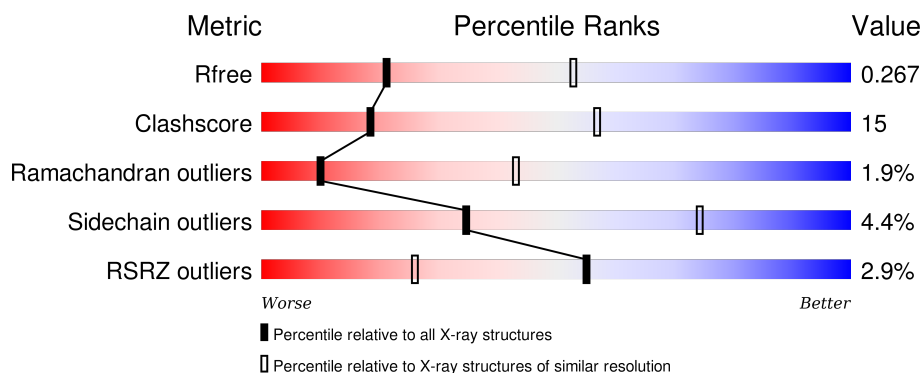
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	270	<div> <div> <div></div> <div>32%</div> <div>13%</div> <div>•</div> <div>53%</div> </div> </div>
1	B	270	<div> <div>4%</div> <div> <div></div> <div>27%</div> <div>19%</div> <div>•</div> <div>53%</div> </div> </div>
2	C	142	<div> <div>63%</div> <div>18%</div> <div>•</div> <div>18%</div> </div>
2	D	142	<div> <div>53%</div> <div>27%</div> <div>••</div> <div>18%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3818 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 Replication protein A 32 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			998	635	173	184	6			
1	B	126	Total	C	N	O	S	0	0	0
			990	631	171	182	6			

- Molecule 2 is a protein called Replication protein A 14 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	117	Total	C	N	O	S	0	0	0
			915	590	148	170	7			
2	D	117	Total	C	N	O	S	0	0	0
			915	590	148	170	7			

There are 42 discrepancies between the modelled and reference sequences:

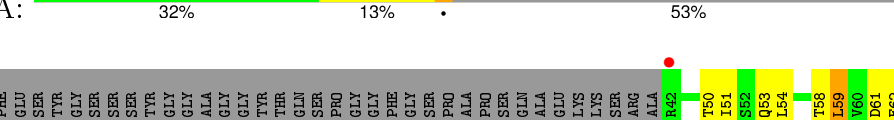
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	EXPRESSION TAG	UNP P35244
C	-19	GLY	-	EXPRESSION TAG	UNP P35244
C	-18	HIS	-	EXPRESSION TAG	UNP P35244
C	-17	HIS	-	EXPRESSION TAG	UNP P35244
C	-16	HIS	-	EXPRESSION TAG	UNP P35244
C	-15	HIS	-	EXPRESSION TAG	UNP P35244
C	-14	HIS	-	EXPRESSION TAG	UNP P35244
C	-13	HIS	-	EXPRESSION TAG	UNP P35244
C	-12	HIS	-	EXPRESSION TAG	UNP P35244
C	-11	HIS	-	EXPRESSION TAG	UNP P35244
C	-10	HIS	-	EXPRESSION TAG	UNP P35244
C	-9	HIS	-	EXPRESSION TAG	UNP P35244
C	-8	SER	-	EXPRESSION TAG	UNP P35244
C	-7	SER	-	EXPRESSION TAG	UNP P35244
C	-6	GLY	-	EXPRESSION TAG	UNP P35244
C	-5	HIS	-	EXPRESSION TAG	UNP P35244

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ILE	-	EXPRESSION TAG	UNP P35244
C	-3	GLU	-	EXPRESSION TAG	UNP P35244
C	-2	GLY	-	EXPRESSION TAG	UNP P35244
C	-1	ARG	-	EXPRESSION TAG	UNP P35244
C	0	HIS	-	EXPRESSION TAG	UNP P35244
D	-20	MET	-	EXPRESSION TAG	UNP P35244
D	-19	GLY	-	EXPRESSION TAG	UNP P35244
D	-18	HIS	-	EXPRESSION TAG	UNP P35244
D	-17	HIS	-	EXPRESSION TAG	UNP P35244
D	-16	HIS	-	EXPRESSION TAG	UNP P35244
D	-15	HIS	-	EXPRESSION TAG	UNP P35244
D	-14	HIS	-	EXPRESSION TAG	UNP P35244
D	-13	HIS	-	EXPRESSION TAG	UNP P35244
D	-12	HIS	-	EXPRESSION TAG	UNP P35244
D	-11	HIS	-	EXPRESSION TAG	UNP P35244
D	-10	HIS	-	EXPRESSION TAG	UNP P35244
D	-9	HIS	-	EXPRESSION TAG	UNP P35244
D	-8	SER	-	EXPRESSION TAG	UNP P35244
D	-7	SER	-	EXPRESSION TAG	UNP P35244
D	-6	GLY	-	EXPRESSION TAG	UNP P35244
D	-5	HIS	-	EXPRESSION TAG	UNP P35244
D	-4	ILE	-	EXPRESSION TAG	UNP P35244
D	-3	GLU	-	EXPRESSION TAG	UNP P35244
D	-2	GLY	-	EXPRESSION TAG	UNP P35244
D	-1	ARG	-	EXPRESSION TAG	UNP P35244
D	0	HIS	-	EXPRESSION TAG	UNP P35244

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 

- Chain B:
-
- 4% 27% 19% 53%
- MET TRP ASN SER GLY PHE GLU SER TYR GLY GLY ALA GLY GLY TYR TYR GLN SER PRO GLY GLY PHE GLY SER PRO ALA SER GLN ALA GLU LYS SER ARG ALA R42 146 750 151 457 758 159 760 761 765 768 770 774
- S72 Q73 T75 R81 E84 R85 A86 R87 T88 R89 R90 D95 D96 R97 R98 P101 H102 D103 V104 R105 Q106 W107 V108 D109 THR ASP ASP THR SER SER SER ASN T118 V119 P122 E123 V126 A129 R133 S134 F135 Q136 H137 K138 K139 V142 K145 T146
- N153 T157 H158 I159 V162 A163 N164 M167 V168 K171 S174 Q175 PRO SER SER ALA GLY VAL ARG ALA PRO ILE LYS SER ASN PRO GLY MET SER GLU ASN GLY ASN HIS ILE TYR SER THR VAL ASP ASP ASP HIS PHE LEU SER THR VAL ALA GLU

- Chain C: 



● Molecule 2: Replication protein A 14 kDa subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	97.46 Å 97.46 Å 125.64 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 31.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.00) 99.9 (31.76-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.269 0.232 , 0.267	Depositor DCC
R_{free} test set	1168 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.5	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28891 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3818	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, 0.375 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	0.61	0/1015	0.72	0/1379
1	B	0.52	0/1007	0.64	0/1368
2	C	0.57	0/934	0.67	0/1262
2	D	0.48	0/934	0.68	0/1262
All	All	0.55	0/3890	0.68	0/5271

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	1
1	B	1	0
2	D	0	1
All	All	5	2

There are no bond length outliers.

There are no bond angle outliers.

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	88	THR	CB
1	A	97	MET	CA
1	A	156	THR	CB
1	A	175	GLN	CA
1	B	97	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	MET	Peptide

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Mol	Chain	Res	Type	Group
2	D	59	LEU	Peptide

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	998	0	1022	35	0
1	B	990	0	1016	37	0
2	C	915	0	921	24	0
2	D	915	0	921	29	0
All	All	3818	0	3880	119	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 15.

All (119) 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)
2:D:4:MET:HE1	2:D:82:THR:HG21	1.26	1.12
1:A:88:THR:HG23	1:A:89:ASN:N	1.75	1.01
1:A:61:ASP:OD1	1:A:62:GLU:OE1	1.77	1.01
1:A:88:THR:HG23	1:A:89:ASN:H	1.26	0.99
1:B:86:ALA:HB3	1:B:89:ASN:OD1	1.63	0.98
1:A:108:VAL:HG12	1:A:109:ASP:N	1.79	0.98
1:A:96:ASP:O	1:A:97:MET:HB3	1.73	0.89
2:D:4:MET:CE	2:D:82:THR:HG21	2.02	0.89
2:D:4:MET:HE1	2:D:82:THR:CG2	2.05	0.86
2:C:2:VAL:HA	2:C:3:ASP:O	1.78	0.82
1:A:88:THR:CG2	1:A:89:ASN:H	1.92	0.82
2:D:6:ASP:OD1	2:D:7:LEU:HG	1.80	0.81
1:A:108:VAL:CG1	1:A:109:ASP:H	1.93	0.81
1:B:86:ALA:HB1	1:B:87:PRO:HD2	1.62	0.80
1:A:122:PRO:O	1:A:123:GLU:HB2	1.79	0.80
2:C:28:VAL:HG22	2:C:68:GLU:HG3	1.63	0.80
1:A:150:GLU:OE1	1:A:150:GLU:HA	1.82	0.79
1:A:108:VAL:CG1	1:A:109:ASP:N	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:CG2	1:A:89:ASN:N	2.46	0.79
1:A:108:VAL:HG12	1:A:109:ASP:H	1.43	0.79
1:A:153:ASN:HD21	2:C:95:ASP:H	1.31	0.78
2:C:35:HIS:HD2	2:C:37:THR:OG1	1.66	0.78
1:B:89:ASN:HD22	1:B:105:ARG:HH12	1.31	0.78
2:D:28:VAL:HG22	2:D:68:GLU:HG3	1.66	0.77
2:D:31:LEU:CD2	2:D:63:ILE:O	2.33	0.77
2:C:2:VAL:HA	2:C:3:ASP:C	2.06	0.73
1:B:89:ASN:HB3	1:B:107:TRP:HD1	1.54	0.72
1:B:101:PRO:HD3	2:D:5:MET:O	1.89	0.72
2:C:56:MET:CE	2:C:56:MET:HA	2.20	0.70
1:B:118:THR:HG22	1:B:119:VAL:N	2.06	0.68
2:D:31:LEU:HD23	2:D:64:SER:HA	1.75	0.68
2:D:60:ASP:HB2	2:D:61:GLU:HB2	1.75	0.68
1:B:118:THR:HG22	1:B:119:VAL:H	1.59	0.67
1:B:89:ASN:ND2	1:B:105:ARG:HH12	1.92	0.67
1:B:86:ALA:CB	1:B:89:ASN:OD1	2.41	0.65
2:C:35:HIS:CD2	2:C:37:THR:OG1	2.50	0.64
2:D:61:GLU:OE1	2:D:86:GLN:NE2	2.31	0.63
1:B:134:SER:HB2	1:B:139:LYS:HD3	1.82	0.61
2:C:35:HIS:HB2	2:C:40:MET:SD	2.41	0.61
1:A:50:THR:HB	1:A:98:THR:HG21	1.83	0.61
1:B:65:ARG:NH1	1:B:70:GLU:HG2	2.18	0.59
1:B:167:MET:O	1:B:171:LYS:HG3	2.03	0.58
1:A:54:LEU:HD12	1:A:102:MET:HE1	1.84	0.58
1:B:103:ASP:OD2	1:B:138:LYS:HE2	2.04	0.58
1:A:122:PRO:O	1:A:123:GLU:CB	2.50	0.57
1:B:89:ASN:HD22	1:B:105:ARG:NH1	2.01	0.57
1:B:164:ASN:O	1:B:168:VAL:HG23	2.04	0.57
1:B:89:ASN:HB3	1:B:107:TRP:CD1	2.38	0.56
2:D:55:LEU:HD22	2:D:59:LEU:CD1	2.36	0.56
1:A:167:MET:HG3	2:C:112:PHE:CE1	2.41	0.56
2:D:53:ILE:HD12	2:D:69:VAL:HG11	1.87	0.55
1:B:122:PRO:O	1:B:123:GLU:HB2	2.07	0.55
2:C:63:ILE:HA	2:C:86:GLN:NE2	2.22	0.55
2:D:31:LEU:HD23	2:D:63:ILE:O	2.08	0.54
1:B:129:ALA:HB3	1:B:145:LYS:HB3	1.89	0.54
1:B:153:ASN:HD21	2:D:95:ASP:H	1.55	0.53
2:D:89:GLU:HG2	2:D:93:PRO:HA	1.90	0.53
1:B:136:GLN:C	1:B:138:LYS:H	2.11	0.53
2:C:87:PHE:O	2:C:89:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HH12	1:A:70:GLU:HG2	1.75	0.50
2:D:55:LEU:HB3	2:D:57:GLU:H	1.77	0.50
1:A:79:ILE:HG22	1:A:95:ASP:O	2.12	0.50
1:A:65:ARG:NH1	1:A:70:GLU:HG2	2.27	0.50
1:B:126:VAL:HG12	1:B:148:PRO:HA	1.93	0.49
1:B:159:ILE:HG21	2:D:106:ILE:HD11	1.94	0.49
1:A:58:THR:HG22	1:A:59:LEU:N	2.27	0.49
2:C:31:LEU:C	2:C:31:LEU:HD23	2.34	0.48
1:A:128:VAL:HG22	1:A:146:ILE:HG12	1.96	0.48
2:C:56:MET:HE2	2:C:56:MET:HA	1.95	0.48
2:C:56:MET:HA	2:C:56:MET:HE3	1.95	0.48
1:A:75:THR:HA	1:A:128:VAL:O	2.13	0.48
1:B:59:LEU:O	1:B:59:LEU:HG	2.14	0.48
2:D:42:ILE:CG2	2:D:50:ASN:HB3	2.44	0.48
2:D:60:ASP:CB	2:D:61:GLU:HB2	2.44	0.47
1:B:174:SER:HA	1:B:175:GLN:HA	1.71	0.47
1:B:57:ALA:O	1:B:139:LYS:NZ	2.42	0.46
2:C:47:GLU:HG3	2:C:100:ASN:ND2	2.30	0.46
2:D:46:GLY:HA3	2:D:100:ASN:HB2	1.98	0.46
2:D:55:LEU:HD22	2:D:59:LEU:HD11	1.97	0.46
2:C:63:ILE:HD12	2:C:67:VAL:HG21	1.98	0.46
2:C:31:LEU:HD13	2:C:64:SER:HA	1.98	0.46
1:A:53:GLN:OE1	1:A:166:HIS:NE2	2.49	0.46
1:B:51:ILE:HD12	1:B:96:ASP:H	1.81	0.46
1:A:150:GLU:OE1	1:A:150:GLU:CA	2.59	0.45
1:A:126:VAL:HG12	1:A:148:PRO:HA	1.98	0.45
2:C:2:VAL:CA	2:C:3:ASP:O	2.58	0.45
1:B:105:ARG:HH11	1:B:107:TRP:HE1	1.64	0.45
2:C:66:ILE:HG12	2:C:89:GLU:OE2	2.17	0.45
2:D:20:PHE:O	2:D:73:VAL:HB	2.17	0.45
1:A:149:LEU:HA	1:A:149:LEU:HD12	1.73	0.45
1:A:81:ARG:NH1	1:A:95:ASP:OD2	2.49	0.45
1:A:117:ASN:HD22	1:A:117:ASN:HA	1.58	0.44
1:B:85:LYS:HA	1:B:90:ILE:HD12	2.00	0.44
1:B:86:ALA:HB1	1:B:87:PRO:CD	2.41	0.44
1:A:51:ILE:HG23	1:A:102:MET:CE	2.48	0.44
2:D:98:LEU:O	2:D:101:GLU:N	2.50	0.44
2:C:35:HIS:HA	2:C:36:PRO:HD2	1.79	0.43
1:A:101:PRO:HD3	2:C:5:MET:O	2.18	0.43
2:C:53:ILE:HD12	2:C:69:VAL:HG11	2.00	0.43
1:A:117:ASN:HB3	1:A:118:THR:H	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLN:HA	1:B:175:GLN:OE1	2.19	0.43
2:C:37:THR:HB	2:C:39:LYS:HG3	2.02	0.42
1:B:81:ARG:NH1	1:B:95:ASP:OD2	2.52	0.42
1:B:87:PRO:HB2	1:B:88:THR:H	1.73	0.41
2:C:46:GLY:HA3	2:C:100:ASN:HB2	2.02	0.41
1:B:90:ILE:CG2	1:B:106:GLN:HE21	2.33	0.41
1:B:50:THR:HB	1:B:98:THR:HG21	2.01	0.41
2:D:31:LEU:CD2	2:D:63:ILE:C	2.89	0.41
2:D:11:ARG:HD3	2:D:99:TYR:OH	2.19	0.41
2:D:76:LYS:HD2	2:D:76:LYS:H	1.86	0.41
1:A:58:THR:CG2	1:A:59:LEU:N	2.83	0.41
1:B:46:ILE:HG12	1:B:73:GLN:HB3	2.02	0.41
2:D:4:MET:CE	2:D:82:THR:CG2	2.80	0.41
1:B:133:ARG:HG3	1:B:142:VAL:CG2	2.51	0.41
1:B:158:HIS:O	1:B:162:VAL:HG23	2.20	0.41
2:D:89:GLU:CG	2:D:94:PHE:H	2.34	0.41
1:A:89:ASN:HB3	1:A:107:TRP:CE3	2.56	0.40
1:A:51:ILE:HD12	1:A:96:ASP:H	1.85	0.40
2:D:14:ALA:N	2:D:27:PHE:HE1	2.20	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	123/270 (46%)	109 (89%)	12 (10%)	2 (2%)	12	48
1	B	122/270 (45%)	103 (84%)	16 (13%)	3 (2%)	7	34
2	C	115/142 (81%)	109 (95%)	5 (4%)	1 (1%)	21	64
2	D	115/142 (81%)	105 (91%)	7 (6%)	3 (3%)	7	33
All	All	475/824 (58%)	426 (90%)	40 (8%)	9 (2%)	10	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	B	87	PRO
2	C	3	ASP
1	A	123	GLU
1	A	152	MET
1	B	72	SER
2	D	3	ASP
2	D	32	GLU
2	D	36	PRO

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	114/228 (50%)	107 (94%)	7 (6%)	23	61
1	B	113/228 (50%)	109 (96%)	4 (4%)	43	80
2	C	102/124 (82%)	100 (98%)	2 (2%)	63	89
2	D	102/124 (82%)	96 (94%)	6 (6%)	24	63
All	All	431/704 (61%)	412 (96%)	19 (4%)	35	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	81	ARG
1	A	90	ILE
1	A	97	MET
1	A	117	ASN
1	A	150	GLU
1	A	155	PHE
1	B	75	THR
1	B	97	MET
1	B	157	THR
1	B	168	VAL

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Mol	Chain	Res	Type
2	C	40	MET
2	C	61	GLU
2	D	44	SER
2	D	59	LEU
2	D	61	GLU
2	D	76	LYS
2	D	84	TYR
2	D	90	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	131	HIS
1	A	153	ASN
1	A	164	ASN
1	A	173	ASN
1	B	106	GLN
1	B	153	ASN
1	B	158	HIS
1	B	173	ASN
2	C	35	HIS
2	D	86	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 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 [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	127/270 (47%)	-0.21	3 (2%) 62 32	60, 79, 99, 110	1 (0%)
1	B	126/270 (46%)	0.28	11 (8%) 13 4	75, 108, 131, 138	1 (0%)
2	C	117/142 (82%)	-0.54	0 100 100	65, 75, 94, 101	0
2	D	117/142 (82%)	-0.21	0 100 100	72, 90, 119, 123	0
All	All	487/824 (59%)	-0.16	14 (2%) 55 26	60, 84, 122, 138	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ASN	4.8
1	B	42	ARG	4.6
1	B	87	PRO	3.7
1	B	85	LYS	3.7
1	B	88	THR	3.4
1	B	119	VAL	3.1
1	B	118	THR	2.8
1	A	42	ARG	2.7
1	B	108	VAL	2.6
1	A	109	ASP	2.3
1	B	59	LEU	2.2
1	B	84	GLU	2.1
1	B	61	ASP	2.1
1	B	90	ILE	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.