



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:22 am GMT

PDB ID : 3W03
Title : XLF-XRCC4 complex
Authors : Wu, Q.; Ochi, T.; Matak-Vinkovic, D.; Robinson, C.V.; Chirgadze, D.Y.;
Blundell, T.L.
Deposited on : 2012-10-17
Resolution : 8.49 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

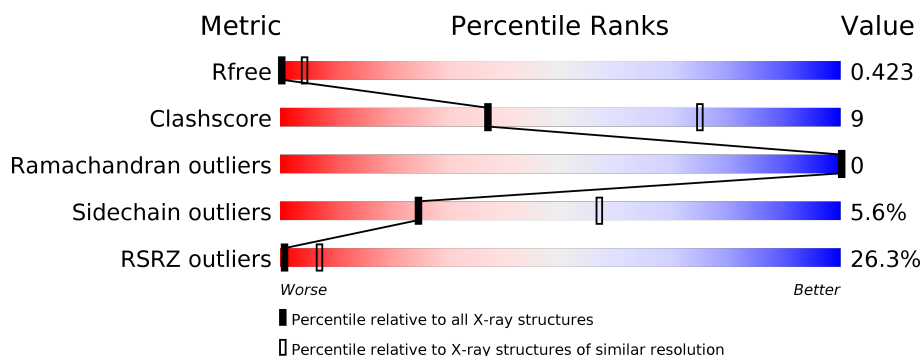
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.49 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}	100719	1100 (10.00-3.70)
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)
RSRZ outliers	101464	1004 (11.50-3.72)

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	235	<div> <div>31%</div> <div>75% 21% . .</div> </div>
1	B	235	<div> <div>26%</div> <div>76% 18% . .</div> </div>
2	C	184	<div> <div>15%</div> <div>57% 30% . 11%</div> </div>
2	D	184	<div> <div>24%</div> <div>58% 29% . 11%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6229 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 Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1818	1159	306	338	15			
1	B	225	Total	C	N	O	S	0	0	0
			1757	1126	292	324	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
A	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
B	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
B	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4

- Molecule 2 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	164	Total	C	N	O	S	0	0	0
			1327	838	224	259	6			
2	D	164	Total	C	N	O	S	0	0	0
			1327	838	224	259	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	EXPRESSION TAG	UNP Q13426
C	-18	GLY	-	EXPRESSION TAG	UNP Q13426
C	-17	SER	-	EXPRESSION TAG	UNP Q13426
C	-16	SER	-	EXPRESSION TAG	UNP Q13426
C	-15	HIS	-	EXPRESSION TAG	UNP Q13426
C	-14	HIS	-	EXPRESSION TAG	UNP Q13426
C	-13	HIS	-	EXPRESSION TAG	UNP Q13426
C	-12	HIS	-	EXPRESSION TAG	UNP Q13426

Continued on next page...

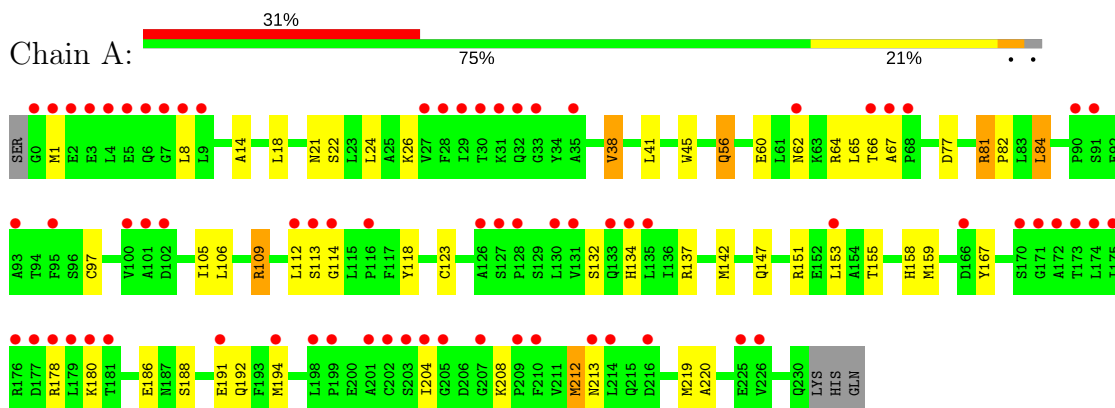
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	EXPRESSION TAG	UNP Q13426
C	-10	HIS	-	EXPRESSION TAG	UNP Q13426
C	-9	SER	-	EXPRESSION TAG	UNP Q13426
C	-8	SER	-	EXPRESSION TAG	UNP Q13426
C	-7	GLY	-	EXPRESSION TAG	UNP Q13426
C	-6	LEU	-	EXPRESSION TAG	UNP Q13426
C	-5	VAL	-	EXPRESSION TAG	UNP Q13426
C	-4	PRO	-	EXPRESSION TAG	UNP Q13426
C	-3	ARG	-	EXPRESSION TAG	UNP Q13426
C	-2	GLY	-	EXPRESSION TAG	UNP Q13426
C	-1	SER	-	EXPRESSION TAG	UNP Q13426
C	0	HIS	-	EXPRESSION TAG	UNP Q13426
D	-19	MET	-	EXPRESSION TAG	UNP Q13426
D	-18	GLY	-	EXPRESSION TAG	UNP Q13426
D	-17	SER	-	EXPRESSION TAG	UNP Q13426
D	-16	SER	-	EXPRESSION TAG	UNP Q13426
D	-15	HIS	-	EXPRESSION TAG	UNP Q13426
D	-14	HIS	-	EXPRESSION TAG	UNP Q13426
D	-13	HIS	-	EXPRESSION TAG	UNP Q13426
D	-12	HIS	-	EXPRESSION TAG	UNP Q13426
D	-11	HIS	-	EXPRESSION TAG	UNP Q13426
D	-10	HIS	-	EXPRESSION TAG	UNP Q13426
D	-9	SER	-	EXPRESSION TAG	UNP Q13426
D	-8	SER	-	EXPRESSION TAG	UNP Q13426
D	-7	GLY	-	EXPRESSION TAG	UNP Q13426
D	-6	LEU	-	EXPRESSION TAG	UNP Q13426
D	-5	VAL	-	EXPRESSION TAG	UNP Q13426
D	-4	PRO	-	EXPRESSION TAG	UNP Q13426
D	-3	ARG	-	EXPRESSION TAG	UNP Q13426
D	-2	GLY	-	EXPRESSION TAG	UNP Q13426
D	-1	SER	-	EXPRESSION TAG	UNP Q13426
D	0	HIS	-	EXPRESSION TAG	UNP Q13426

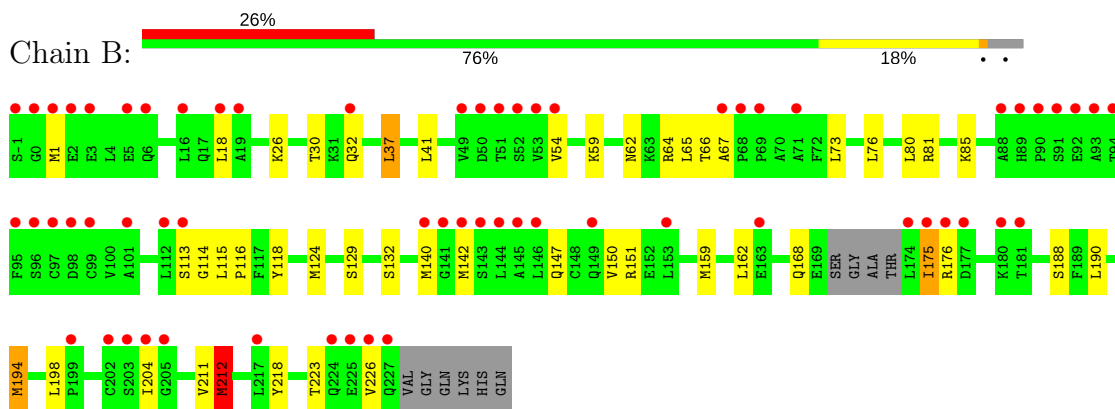
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

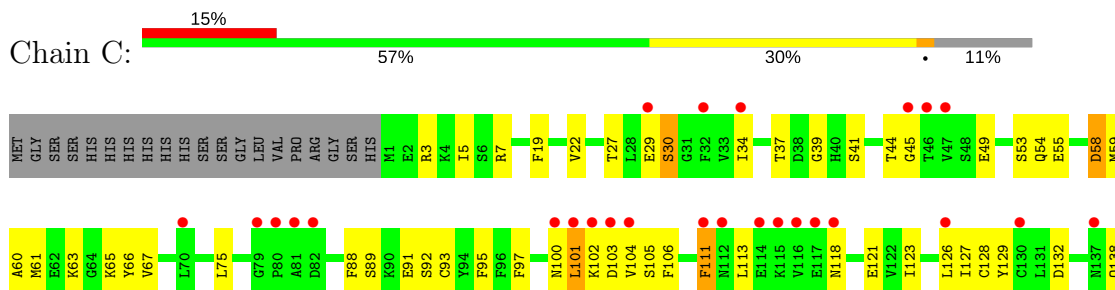
• Molecule 1: Non-homologous end-joining factor 1



• Molecule 1: Non-homologous end-joining factor 1

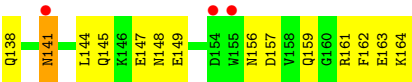
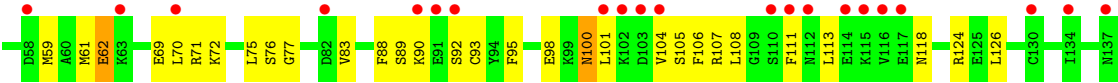
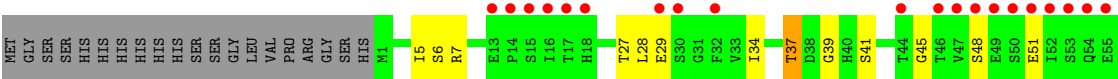


• Molecule 2: DNA repair protein XRCC4





● Molecule 2: DNA repair protein XRCC4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	236.76Å 236.76Å 103.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.81 – 8.49 49.81 – 8.49	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.81-8.49) 99.9 (49.81-8.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.54 (at 8.33Å)	Xtriage
Refinement program	PHENIX (1.7.2_869)	Depositor
R, R_{free}	0.363 , 0.360 0.367 , 0.423	Depositor DCC
R_{free} test set	149 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	931.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 194.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	6229	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.34% 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	0.75	6/1854 (0.3%)	0.69	0/2513
1	B	0.76	7/1793 (0.4%)	0.66	1/2434 (0.0%)
2	C	0.39	0/1353	0.55	0/1821
2	D	0.38	0/1353	0.57	0/1821
All	All	0.63	13/6353 (0.2%)	0.63	1/8589 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CG-SD	6.90	1.99	1.81
1	B	194	MET	CG-SD	6.81	1.98	1.81
1	A	1	MET	CG-SD	6.76	1.98	1.81
1	B	159	MET	CG-SD	6.75	1.98	1.81
1	A	194	MET	CG-SD	6.40	1.97	1.81
1	A	159	MET	CG-SD	6.04	1.96	1.81
1	B	142	MET	CG-SD	5.84	1.96	1.81
1	B	212	MET	CG-SD	5.68	1.96	1.81
1	A	142	MET	CG-SD	5.54	1.95	1.81
1	A	212	MET	CG-SD	5.32	1.95	1.81
1	A	219	MET	CG-SD	5.25	1.94	1.81
1	B	140	MET	CG-SD	5.19	1.94	1.81
1	B	124	MET	CG-SD	5.11	1.94	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LEU	CA-CB-CG	5.54	128.03	115.30

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	1818	0	1818	29	69
1	B	1757	0	1741	20	25
2	C	1327	0	1290	39	36
2	D	1327	0	1290	33	58
All	All	6229	0	6139	110	94

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 9.

All (110) 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:109:ARG:HG3	1:A:109:ARG:HH11	1.24	1.02
1:A:62:ASN:HD21	1:A:118:TYR:H	1.20	0.87
2:D:27:THR:HG22	2:D:29:GLU:H	1.39	0.87
2:C:37:THR:HG22	2:C:39:GLY:H	1.39	0.86
2:C:89:SER:HB3	2:C:92:SER:HB3	1.56	0.85
2:C:141:ASN:HD21	2:D:141:ASN:HB2	1.43	0.82
2:D:71:ARG:HG3	2:D:75:LEU:HD12	1.62	0.81
1:A:26:LYS:HZ3	1:A:134:HIS:HD2	1.29	0.81
1:A:188:SER:O	1:A:192:GLN:HG2	1.81	0.80
1:A:109:ARG:HH11	1:A:109:ARG:CG	1.98	0.75
2:D:159:GLN:O	2:D:163:GLU:HG3	1.87	0.74
2:D:98:GLU:HB3	2:D:107:ARG:HA	1.72	0.72
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.01	0.71
1:B:30:THR:OG1	1:B:32:GLN:HG2	1.91	0.70
2:D:37:THR:HG22	2:D:39:GLY:H	1.57	0.69
2:C:138:GLN:O	2:C:142:GLU:HG3	1.92	0.69
2:D:145:GLN:O	2:D:149:GLU:HG2	1.93	0.68
2:C:118:ASN:ND2	2:C:121:GLU:HB2	2.09	0.67
2:D:48:SER:OG	2:D:51:GLU:HG3	1.94	0.67
2:C:34:ILE:HD13	2:C:111:PHE:CZ	2.30	0.66
2:C:89:SER:CB	2:C:92:SER:HB3	2.26	0.66
2:C:19:PHE:HE2	2:D:124:ARG:HG2	1.60	0.66
1:A:81:ARG:HB3	1:A:82:PRO:HD3	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:ARG:O	2:C:154:ASP:HB2	1.97	0.65
2:C:145:GLN:HG3	2:D:144:LEU:HD11	1.79	0.64
1:B:211:VAL:HG12	1:B:212:MET:HE3	1.79	0.62
1:B:223:THR:O	1:B:226:VAL:HG22	2.00	0.62
1:B:62:ASN:HD21	1:B:118:TYR:H	1.48	0.61
2:D:5:ILE:CD1	2:D:126:LEU:HG	2.31	0.61
2:C:34:ILE:HD13	2:C:111:PHE:HZ	1.67	0.59
2:D:145:GLN:O	2:D:148:ASN:HB3	2.04	0.58
2:C:55:GLU:HG2	2:C:66:TYR:OH	2.03	0.57
1:B:175:ILE:HG23	1:B:176:ARG:H	1.70	0.57
1:A:26:LYS:NZ	1:A:134:HIS:HD2	2.01	0.57
1:B:175:ILE:HG23	1:B:176:ARG:N	2.20	0.57
1:A:21:ASN:CG	1:A:22:SER:H	2.08	0.56
2:C:102:LYS:O	2:C:102:LYS:HG2	2.05	0.56
2:C:29:GLU:O	2:C:49:GLU:HB2	2.06	0.56
1:A:153:LEU:HD11	1:B:150:VAL:HG13	1.87	0.55
1:B:54:VAL:HG21	1:B:73:LEU:HD21	1.88	0.55
2:C:27:THR:HB	2:C:30:SER:OG	2.06	0.55
2:C:53:SER:HB3	2:C:63:LYS:HE3	1.89	0.55
2:C:45:GLY:HA3	2:C:113:LEU:HD23	1.89	0.55
2:D:37:THR:HG23	2:D:41:SER:O	2.07	0.54
1:B:26:LYS:NZ	1:B:218:TYR:OH	2.41	0.54
2:C:100:ASN:OD1	2:C:105:SER:HB3	2.07	0.54
1:A:14:ALA:HB2	1:A:84:LEU:HD12	1.89	0.53
1:B:212:MET:HA	1:B:212:MET:CE	2.39	0.53
1:A:8:LEU:HD11	1:A:26:LYS:HG3	1.92	0.52
2:D:6:SER:HB3	2:D:76:SER:OG	2.11	0.51
1:A:26:LYS:HZ3	1:A:134:HIS:CD2	2.19	0.51
2:D:34:ILE:HD13	2:D:111:PHE:CZ	2.46	0.50
2:C:44:THR:HG22	2:C:45:GLY:N	2.27	0.49
2:C:5:ILE:HD13	2:C:126:LEU:HG	1.95	0.48
2:D:138:GLN:O	2:D:141:ASN:HB3	2.13	0.48
2:D:157:ASP:O	2:D:161:ARG:HG3	2.14	0.48
1:A:147:GLN:O	1:A:151:ARG:HG2	2.14	0.48
2:D:83:VAL:HB	2:D:100:ASN:HB3	1.94	0.48
1:A:41:LEU:HD13	1:A:204:ILE:CG2	2.44	0.47
2:C:118:ASN:HD21	2:C:121:GLU:HB2	1.80	0.47
2:C:29:GLU:HB3	2:C:67:VAL:HG21	1.96	0.46
1:B:190:LEU:O	1:B:194:MET:HG2	2.16	0.46
1:A:167:TYR:OH	1:B:168:GLN:HG2	2.16	0.46
2:C:88:PHE:HD1	2:C:95:PHE:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:SER:HB3	2:D:92:SER:HB3	1.97	0.46
2:C:37:THR:HG23	2:C:41:SER:O	2.16	0.45
2:C:5:ILE:CD1	2:C:126:LEU:HG	2.47	0.45
1:B:212:MET:HA	1:B:212:MET:HE3	1.99	0.45
2:D:93:CYS:HB3	2:D:113:LEU:O	2.16	0.45
2:D:72:LYS:HG2	2:D:77:GLY:O	2.16	0.45
2:D:5:ILE:HD13	2:D:126:LEU:HG	1.97	0.44
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.68	0.44
1:B:41:LEU:HD13	1:B:204:ILE:HD12	1.99	0.44
2:C:22:VAL:HG11	2:C:75:LEU:HD21	1.98	0.44
1:A:208:LYS:NZ	1:A:212:MET:CE	2.81	0.44
2:D:27:THR:HG22	2:D:28:LEU:N	2.32	0.43
1:A:213:ASN:HB3	1:B:147:GLN:OE1	2.18	0.43
1:A:77:ASP:O	1:A:81:ARG:HB2	2.17	0.43
2:C:102:LYS:O	2:C:103:ASP:CB	2.66	0.43
2:D:89:SER:CB	2:D:92:SER:HB3	2.48	0.43
2:C:3:ARG:HD2	2:C:129:TYR:CD2	2.54	0.43
2:C:44:THR:CG2	2:C:45:GLY:N	2.82	0.43
1:A:38:VAL:HG12	1:A:45:TRP:HB2	2.01	0.43
1:B:175:ILE:CG2	1:B:176:ARG:N	2.82	0.43
2:C:118:ASN:ND2	2:C:121:GLU:CB	2.79	0.43
2:C:27:THR:HG21	2:C:29:GLU:OE1	2.19	0.43
2:D:69:GLU:HB3	2:D:108:LEU:HD21	2.00	0.43
1:A:56:GLN:NE2	1:A:60:GLU:OE2	2.52	0.42
1:A:18:LEU:HD21	1:A:106:LEU:CD1	2.49	0.42
2:C:88:PHE:CD1	2:C:95:PHE:HB2	2.54	0.42
2:D:45:GLY:HA3	2:D:113:LEU:HD23	2.01	0.42
2:C:54:GLN:O	2:C:58:ASP:OD1	2.38	0.42
2:D:62:GLU:HG3	2:D:62:GLU:O	2.18	0.42
1:A:178:ARG:HD2	1:A:180:LYS:HE3	2.01	0.42
1:A:45:TRP:HB3	1:A:123:CYS:HB3	2.01	0.42
2:C:7:ARG:HG3	2:C:7:ARG:O	2.19	0.42
2:C:97:PHE:CD1	2:C:97:PHE:N	2.88	0.42
2:D:5:ILE:HD13	2:D:126:LEU:CD1	2.50	0.41
2:C:132:ASP:OD1	2:D:7:ARG:NH2	2.50	0.41
2:C:128:CYS:SG	2:D:7:ARG:NH1	2.93	0.41
1:A:153:LEU:CD1	1:B:150:VAL:HG13	2.50	0.41
2:C:123:ILE:O	2:C:127:ILE:HG13	2.20	0.41
1:A:220:ALA:HB1	1:B:198:LEU:CD2	2.51	0.41
1:A:137:ARG:CZ	1:B:204:ILE:HD11	2.50	0.41
2:C:3:ARG:HD2	2:C:129:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ASN:C	2:D:100:ASN:HD22	2.24	0.41
1:B:76:LEU:O	1:B:80:LEU:HB2	2.22	0.40
2:D:95:PHE:CD1	2:D:111:PHE:CE1	3.09	0.40
2:D:88:PHE:CE2	2:D:90:LYS:HG2	2.57	0.40
1:A:97:CYS:HA	1:A:105:ILE:O	2.21	0.40

All (94) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:CG2	2:D:105:SER:O[1_556]	0.71	1.49
1:A:64:ARG:NH1	2:C:59:MET:C[6_554]	0.71	1.49
1:B:65:LEU:CD1	2:D:106:PHE:CE2[1_556]	0.79	1.41
1:A:64:ARG:NE	2:C:59:MET:CB[6_554]	0.88	1.32
1:A:186:GLU:CG	2:D:164:LYS:CD[4_655]	0.93	1.27
1:B:64:ARG:NH1	2:D:59:MET:CG[1_556]	0.95	1.25
1:A:151:ARG:NH1	2:D:163:GLU:C[4_655]	0.98	1.22
1:B:113:SER:CB	2:D:101:LEU:CD1[1_556]	1.01	1.19
1:A:67:ALA:CB	2:C:104:VAL:CG1[6_554]	1.02	1.18
1:A:158:HIS:CD2	2:D:161:ARG:CB[4_655]	1.03	1.17
1:A:65:LEU:CB	2:C:106:PHE:CD2[6_554]	1.05	1.15
1:B:113:SER:OG	2:D:101:LEU:CD1[1_556]	1.07	1.13
1:A:64:ARG:CZ	2:C:59:MET:CB[6_554]	1.07	1.13
1:A:186:GLU:CG	2:D:164:LYS:CG[4_655]	1.13	1.07
1:A:151:ARG:CZ	2:D:163:GLU:CA[4_655]	1.17	1.03
1:A:64:ARG:NH1	2:C:59:MET:O[6_554]	1.21	0.99
1:A:65:LEU:CG	2:C:106:PHE:CE2[6_554]	1.22	0.98
1:A:151:ARG:NH2	2:D:163:GLU:CA[4_655]	1.23	0.97
1:A:65:LEU:CB	2:C:106:PHE:CG[6_554]	1.26	0.94
1:A:151:ARG:NH1	2:D:163:GLU:CA[4_655]	1.30	0.90
1:A:65:LEU:CG	2:C:106:PHE:CD2[6_554]	1.30	0.90
1:B:116:PRO:CG	2:D:59:MET:O[1_556]	1.37	0.83
1:B:65:LEU:CD1	2:D:106:PHE:CD2[1_556]	1.42	0.78
1:B:65:LEU:CG	2:D:106:PHE:CE2[1_556]	1.43	0.77
1:A:151:ARG:NH2	2:D:163:GLU:CB[4_655]	1.48	0.72
1:A:186:GLU:CD	2:D:164:LYS:CD[4_655]	1.51	0.69
1:B:115:LEU:CD2	2:D:59:MET:CE[1_556]	1.53	0.67
1:A:158:HIS:CG	2:D:161:ARG:CD[4_655]	1.54	0.66
1:A:64:ARG:NH1	2:C:59:MET:CA[6_554]	1.56	0.64
1:B:116:PRO:CD	2:D:59:MET:O[1_556]	1.58	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:HIS:CB	2:D:161:ARG:CD[4_655]	1.60	0.60
1:A:64:ARG:NE	2:C:59:MET:CG[6_554]	1.63	0.57
1:A:151:ARG:CZ	2:D:163:GLU:C[4_655]	1.68	0.52
1:A:65:LEU:CA	2:C:106:PHE:CD2[6_554]	1.70	0.50
1:A:67:ALA:CA	2:C:104:VAL:CG1[6_554]	1.70	0.50
1:A:158:HIS:NE2	2:D:161:ARG:CB[4_655]	1.71	0.49
1:A:151:ARG:NH1	2:D:164:LYS:N[4_655]	1.72	0.48
1:B:67:ALA:CB	2:D:104:VAL:CG2[1_556]	1.73	0.47
1:A:186:GLU:CG	2:D:164:LYS:CB[4_655]	1.74	0.46
1:A:113:SER:OG	2:C:101:LEU:CD1[6_554]	1.75	0.45
1:A:64:ARG:CZ	2:C:59:MET:CA[6_554]	1.77	0.43
1:A:65:LEU:CD1	2:C:106:PHE:CZ[6_554]	1.78	0.42
1:A:113:SER:CB	2:C:101:LEU:CD1[6_554]	1.78	0.42
1:B:66:THR:CG2	2:D:105:SER:C[1_556]	1.79	0.41
1:A:64:ARG:NH1	2:C:60:ALA:N[6_554]	1.81	0.39
1:A:158:HIS:CD2	2:D:161:ARG:CG[4_655]	1.81	0.39
1:A:65:LEU:CA	2:C:106:PHE:CB[6_554]	1.82	0.38
1:A:66:THR:CG2	2:C:105:SER:O[6_554]	1.82	0.38
1:B:64:ARG:NH2	2:D:59:MET:SD[1_556]	1.83	0.37
1:A:64:ARG:NE	2:C:59:MET:CA[6_554]	1.85	0.35
1:A:65:LEU:CD1	2:C:106:PHE:CE2[6_554]	1.85	0.35
1:A:64:ARG:CD	2:C:59:MET:CA[6_554]	1.87	0.33
1:A:151:ARG:NH1	2:D:163:GLU:O[4_655]	1.87	0.33
1:A:65:LEU:C	2:C:106:PHE:CD2[6_554]	1.88	0.32
1:A:151:ARG:NH1	2:D:163:GLU:N[4_655]	1.89	0.31
1:A:158:HIS:CG	2:D:161:ARG:CG[4_655]	1.90	0.30
1:B:67:ALA:CB	2:D:104:VAL:CG1[1_556]	1.90	0.30
1:B:65:LEU:CD1	2:D:106:PHE:CZ[1_556]	1.90	0.30
1:B:66:THR:CB	2:D:105:SER:O[1_556]	1.91	0.29
1:A:186:GLU:OE2	2:D:164:LYS:CD[4_655]	1.91	0.29
1:A:64:ARG:CB	2:C:59:MET:CE[6_554]	1.92	0.28
1:A:151:ARG:NH1	2:D:162:PHE:O[4_655]	1.93	0.27
1:A:155:THR:OG1	2:D:162:PHE:CD1[4_655]	1.94	0.26
1:A:65:LEU:CA	2:C:106:PHE:CG[6_554]	1.94	0.26
1:B:67:ALA:N	2:D:104:VAL:CG1[1_556]	1.94	0.26
1:A:64:ARG:NH2	2:C:59:MET:CB[6_554]	1.95	0.25
1:B:113:SER:CB	2:D:101:LEU:CG[1_556]	1.95	0.25
1:A:64:ARG:CZ	2:C:59:MET:C[6_554]	1.95	0.25
1:A:151:ARG:NH2	2:D:163:GLU:CG[4_655]	1.96	0.24
1:A:151:ARG:CZ	2:D:163:GLU:O[4_655]	1.98	0.22
1:A:65:LEU:CB	2:C:106:PHE:CB[6_554]	1.98	0.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:CD	2:C:59:MET:CB[6_554]	2.00	0.20
1:A:186:GLU:CB	2:D:164:LYS:CB[4_655]	2.01	0.19
1:A:64:ARG:CZ	2:C:59:MET:O[6_554]	2.01	0.19
1:A:186:GLU:OE1	2:D:164:LYS:CB[4_655]	2.03	0.17
1:A:186:GLU:CD	2:D:164:LYS:CG[4_655]	2.04	0.16
1:A:66:THR:O	2:C:105:SER:O[6_554]	2.05	0.15
1:A:64:ARG:NH1	2:C:59:MET:CB[6_554]	2.05	0.15
1:B:64:ARG:CZ	2:D:59:MET:CG[1_556]	2.08	0.12
1:B:67:ALA:CB	2:D:104:VAL:CB[1_556]	2.08	0.12
1:A:64:ARG:NH2	2:C:61:MET:CE[6_554]	2.10	0.10
1:B:64:ARG:NH1	2:D:59:MET:SD[1_556]	2.10	0.10
1:A:158:HIS:NE2	2:D:161:ARG:CA[4_655]	2.11	0.09
1:B:67:ALA:CA	2:D:104:VAL:CG1[1_556]	2.12	0.08
1:A:158:HIS:CG	2:D:161:ARG:CB[4_655]	2.12	0.08
1:A:151:ARG:NH1	2:D:162:PHE:C[4_655]	2.12	0.08
1:A:114:GLY:O	2:C:65:LYS:NZ[6_554]	2.16	0.04
1:B:114:GLY:O	2:D:61:MET:CE[1_556]	2.16	0.04
1:B:65:LEU:CG	2:D:106:PHE:CD2[1_556]	2.16	0.04
1:B:64:ARG:CZ	2:D:59:MET:SD[1_556]	2.17	0.03
1:A:66:THR:N	2:C:105:SER:O[6_554]	2.18	0.02
1:A:151:ARG:NE	2:D:163:GLU:O[4_655]	2.19	0.01
1:A:186:GLU:CD	2:D:164:LYS:CB[4_655]	2.19	0.01
1:A:158:HIS:NE2	2:D:161:ARG:CG[4_655]	2.19	0.01

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	229/235 (97%)	220 (96%)	9 (4%)	0	100	100
1	B	221/235 (94%)	210 (95%)	11 (5%)	0	100	100
2	C	162/184 (88%)	154 (95%)	8 (5%)	0	100	100
2	D	162/184 (88%)	155 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	774/838 (92%)	739 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	200/207 (97%)	191 (96%)	9 (4%)	32	63
1	B	191/207 (92%)	179 (94%)	12 (6%)	21	53
2	C	146/163 (90%)	137 (94%)	9 (6%)	21	54
2	D	146/163 (90%)	138 (94%)	8 (6%)	25	58
All	All	683/740 (92%)	645 (94%)	38 (6%)	25	57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38	VAL
1	A	56	GLN
1	A	81	ARG
1	A	84	LEU
1	A	109	ARG
1	A	112	LEU
1	A	132	SER
1	A	191	GLU
1	B	18	LEU
1	B	37	LEU
1	B	59	LYS
1	B	81	ARG
1	B	85	LYS
1	B	129	SER
1	B	132	SER
1	B	151	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	162	LEU
1	B	175	ILE
1	B	188	SER
1	B	212	MET
2	C	30	SER
2	C	58	ASP
2	C	91	GLU
2	C	93	CYS
2	C	101	LEU
2	C	111	PHE
2	C	144	LEU
2	C	153	ARG
2	C	156	ASN
2	D	37	THR
2	D	62	GLU
2	D	70	LEU
2	D	100	ASN
2	D	118	ASN
2	D	141	ASN
2	D	147	GLU
2	D	156	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	62	ASN
1	A	134	HIS
1	A	227	GLN
1	B	48	GLN
1	B	62	ASN
2	C	9	HIS
2	C	118	ASN
2	C	137	ASN
2	C	141	ASN
2	C	156	ASN
2	D	100	ASN
2	D	118	ASN
2	D	137	ASN
2	D	141	ASN
2	D	143	HIS

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 [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	231/235 (98%)	1.88	72 (31%) 0 6	35, 54, 101, 117	0
1	B	225/235 (95%)	1.52	62 (27%) 1 7	14, 39, 73, 81	0
2	C	164/184 (89%)	0.91	28 (17%) 2 9	47, 88, 114, 127	0
2	D	164/184 (89%)	1.32	44 (26%) 1 7	53, 122, 142, 150	0
All	All	784/838 (93%)	1.46	206 (26%) 1 7	14, 66, 132, 150	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	14.1
1	A	178	ARG	12.3
1	A	3	GLU	12.1
1	A	202	CYS	11.4
1	A	0	GLY	11.0
1	A	177	ASP	10.6
1	A	176	ARG	9.4
1	A	2	GLU	9.0
1	A	30	THR	8.7
1	B	50	ASP	8.5
1	B	91	SER	8.4
1	A	175	ILE	7.1
1	A	5	GLU	7.1
1	B	51	THR	7.1
1	A	4	LEU	7.0
2	D	51	GLU	6.9
1	A	179	LEU	6.5
1	B	95	PHE	6.5
1	B	90	PRO	6.5
1	A	113	SER	6.4
1	A	6	GLN	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	32	GLN	5.9
2	D	47	VAL	5.9
2	C	80	PRO	5.8
1	A	204	ILE	5.8
1	B	97	CYS	5.7
2	D	52	ILE	5.7
1	A	31	LYS	5.5
2	D	48	SER	5.4
1	B	174	LEU	5.3
1	B	96	SER	5.2
1	B	145	ALA	5.2
1	A	7	GLY	5.2
2	C	137	ASN	5.0
2	C	103	ASP	5.0
1	A	134	HIS	5.0
1	B	68	PRO	4.9
1	B	1	MET	4.9
1	B	32	GLN	4.8
2	D	50	SER	4.8
1	B	93	ALA	4.8
2	D	15	SER	4.8
1	A	174	LEU	4.8
2	D	49	GLU	4.7
2	D	29	GLU	4.7
2	C	141	ASN	4.6
1	B	141	GLY	4.6
1	A	1	MET	4.6
1	B	175	ILE	4.4
2	D	46	THR	4.4
2	D	102	LYS	4.4
2	C	32	PHE	4.4
2	D	103	ASP	4.4
1	B	18	LEU	4.4
1	B	144	LEU	4.3
1	A	67	ALA	4.3
1	A	203	SER	4.3
2	C	79	GLY	4.2
2	C	102	LYS	4.2
1	B	2	GLU	4.2
1	A	181	THR	4.2
2	D	82	ASP	4.1
1	B	180	LYS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	53	SER	4.1
2	C	81	ALA	4.1
1	B	-1	SER	4.0
1	A	33	GLY	4.0
1	B	0	GLY	4.0
1	A	29	ILE	3.9
1	B	203	SER	3.9
1	A	173	THR	3.9
1	B	226	VAL	3.9
1	A	101	ALA	3.9
1	A	226	VAL	3.9
1	A	114	GLY	3.8
2	D	13	GLU	3.8
2	D	115	LYS	3.8
2	D	137	ASN	3.7
2	C	47	VAL	3.7
1	B	149	GLN	3.7
2	D	90	LYS	3.6
1	B	202	CYS	3.6
1	B	89	HIS	3.6
1	B	67	ALA	3.6
1	A	91	SER	3.6
1	B	177	ASP	3.6
2	D	16	ILE	3.5
2	D	117	GLU	3.5
1	B	224	GLN	3.5
1	A	205	GLY	3.4
2	C	130	CYS	3.4
1	A	170	SER	3.4
1	A	198	LEU	3.4
1	A	130	LEU	3.4
1	B	3	GLU	3.4
1	A	9	LEU	3.4
2	C	82	ASP	3.4
1	B	94	THR	3.4
1	B	6	GLN	3.4
2	C	46	THR	3.3
2	D	54	GLN	3.3
1	B	227	GLN	3.3
1	A	171	GLY	3.3
1	A	209	PRO	3.3
1	B	49	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	201	ALA	3.3
1	B	143	SER	3.3
2	D	58	ASP	3.3
2	C	117	GLU	3.2
1	A	28	PHE	3.2
1	A	62	ASN	3.2
1	A	90	PRO	3.2
1	A	112	LEU	3.2
1	B	112	LEU	3.2
1	A	8	LEU	3.1
2	D	116	VAL	3.1
2	C	118	ASN	3.1
1	B	205	GLY	3.1
1	B	99	CYS	3.1
1	B	101	ALA	3.1
2	D	14	PRO	3.1
2	D	154	ASP	3.1
2	D	130	CYS	3.1
2	C	104	VAL	3.1
1	B	52	SER	3.0
1	B	176	ARG	3.0
1	B	163	GLU	3.0
1	B	140	MET	3.0
1	A	93	ALA	3.0
1	B	153	LEU	3.0
2	D	30	SER	2.9
1	B	204	ILE	2.9
1	B	92	GLU	2.9
2	D	114	GLU	2.9
1	B	142	MET	2.9
1	A	68	PRO	2.8
2	C	101	LEU	2.8
1	A	225	GLU	2.8
2	D	111	PHE	2.8
1	A	102	ASP	2.8
1	A	214	LEU	2.7
1	A	199	PRO	2.7
1	B	225	GLU	2.7
1	B	217	LEU	2.7
1	B	98	ASP	2.7
1	A	126	ALA	2.6
1	B	16	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	112	ASN	2.6
2	C	115	LYS	2.6
2	C	29	GLU	2.6
1	A	127	SER	2.6
2	C	70	LEU	2.6
2	D	70	LEU	2.6
1	A	27	VAL	2.5
2	C	45	GLY	2.5
2	D	110	SER	2.5
1	B	113	SER	2.5
1	B	88	ALA	2.5
1	A	133	GLN	2.5
1	A	66	THR	2.5
2	D	101	LEU	2.4
1	A	95	PHE	2.4
1	A	194	MET	2.4
2	D	134	ILE	2.4
1	A	166	ASP	2.4
1	A	135	LEU	2.4
1	B	19	ALA	2.4
2	D	104	VAL	2.4
1	A	210	PHE	2.3
2	C	164	LYS	2.3
1	A	35	ALA	2.3
2	D	32	PHE	2.3
1	B	69	PRO	2.3
1	A	128	PRO	2.3
1	A	207	GLY	2.3
1	B	5	GLU	2.3
1	B	53	VAL	2.3
2	D	141	ASN	2.3
1	A	131	VAL	2.2
1	B	71	ALA	2.2
1	A	153	LEU	2.2
2	D	92	SER	2.2
1	B	146	LEU	2.2
2	C	116	VAL	2.2
2	C	111	PHE	2.1
2	D	155	TRP	2.1
2	D	55	GLU	2.1
1	A	191	GLU	2.1
1	A	213	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	63	LYS	2.1
2	C	34	ILE	2.1
1	A	100	VAL	2.1
1	B	199	PRO	2.1
2	D	17	THR	2.1
2	C	126	LEU	2.1
2	D	44	THR	2.1
2	D	91	GLU	2.1
1	A	216	ASP	2.0
1	B	54	VAL	2.0
2	D	18	HIS	2.0
1	A	116	PRO	2.0
2	C	100	ASN	2.0
2	C	112	ASN	2.0
1	B	181	THR	2.0
1	A	172	ALA	2.0
2	C	114	GLU	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.