wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 11:22 AM EDT

PDB ID	:	3K77
Title	:	X-ray crystal structure of XRCC1
Authors	:	Cuneo, M.J.; London, R.E.
Deposited on	:	2009-10-12
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

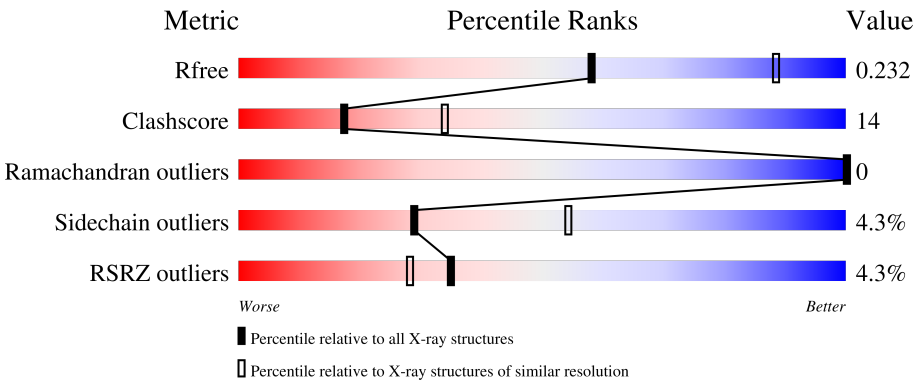
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	161	4% 67% 26% • 6%
1	B	161	4% 66% 27% • 6%
1	C	161	2% 65% 28% • 6%
1	D	161	4% 67% 27% • 6%
1	E	161	5% 71% 22% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	161	4% 66% 27% 6%
1	G	161	4% 68% 24% 6%
1	H	161	5% 70% 24% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9492 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 DNA repair protein XRCC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1172	729	213	225	5	0	0	0
1	B	152	1172	729	213	225	5	0	0	0
1	C	152	1183	735	214	229	5	0	1	0
1	D	152	1184	736	214	228	6	0	1	0
1	E	152	1160	723	207	225	5	0	0	0
1	F	152	1172	729	213	225	5	0	0	0
1	G	152	1165	725	212	223	5	0	0	0
1	H	152	1162	723	209	225	5	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	HIS	-	expression tag	UNP P18887
A	157	HIS	-	expression tag	UNP P18887
A	158	HIS	-	expression tag	UNP P18887
A	159	HIS	-	expression tag	UNP P18887
A	160	HIS	-	expression tag	UNP P18887
A	161	HIS	-	expression tag	UNP P18887
B	156	HIS	-	expression tag	UNP P18887
B	157	HIS	-	expression tag	UNP P18887
B	158	HIS	-	expression tag	UNP P18887
B	159	HIS	-	expression tag	UNP P18887
B	160	HIS	-	expression tag	UNP P18887
B	161	HIS	-	expression tag	UNP P18887
C	156	HIS	-	expression tag	UNP P18887

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	157	HIS	-	expression tag	UNP P18887
C	158	HIS	-	expression tag	UNP P18887
C	159	HIS	-	expression tag	UNP P18887
C	160	HIS	-	expression tag	UNP P18887
C	161	HIS	-	expression tag	UNP P18887
D	156	HIS	-	expression tag	UNP P18887
D	157	HIS	-	expression tag	UNP P18887
D	158	HIS	-	expression tag	UNP P18887
D	159	HIS	-	expression tag	UNP P18887
D	160	HIS	-	expression tag	UNP P18887
D	161	HIS	-	expression tag	UNP P18887
E	156	HIS	-	expression tag	UNP P18887
E	157	HIS	-	expression tag	UNP P18887
E	158	HIS	-	expression tag	UNP P18887
E	159	HIS	-	expression tag	UNP P18887
E	160	HIS	-	expression tag	UNP P18887
E	161	HIS	-	expression tag	UNP P18887
F	156	HIS	-	expression tag	UNP P18887
F	157	HIS	-	expression tag	UNP P18887
F	158	HIS	-	expression tag	UNP P18887
F	159	HIS	-	expression tag	UNP P18887
F	160	HIS	-	expression tag	UNP P18887
F	161	HIS	-	expression tag	UNP P18887
G	156	HIS	-	expression tag	UNP P18887
G	157	HIS	-	expression tag	UNP P18887
G	158	HIS	-	expression tag	UNP P18887
G	159	HIS	-	expression tag	UNP P18887
G	160	HIS	-	expression tag	UNP P18887
G	161	HIS	-	expression tag	UNP P18887
H	156	HIS	-	expression tag	UNP P18887
H	157	HIS	-	expression tag	UNP P18887
H	158	HIS	-	expression tag	UNP P18887
H	159	HIS	-	expression tag	UNP P18887
H	160	HIS	-	expression tag	UNP P18887
H	161	HIS	-	expression tag	UNP P18887

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	14	14	14	0	0
			Total	O		
2	B	20	20	20	0	0

Continued on next page...

Continued from previous page...

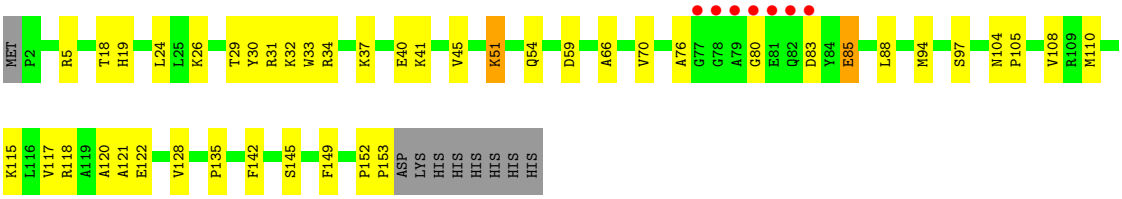
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	C	18	18	18	0	0
			Total	O		
2	D	21	21	21	0	0
			Total	O		
2	E	9	9	9	0	0
			Total	O		
2	F	13	13	13	0	0
			Total	O		
2	G	10	10	10	0	0
			Total	O		
2	H	17	17	17	0	0

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.

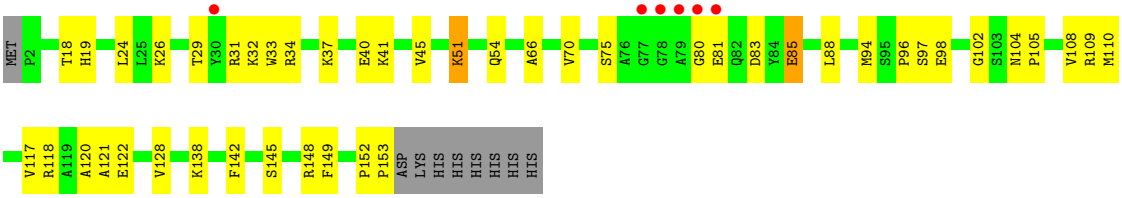
• Molecule 1: DNA repair protein XRCC1

Chain A:



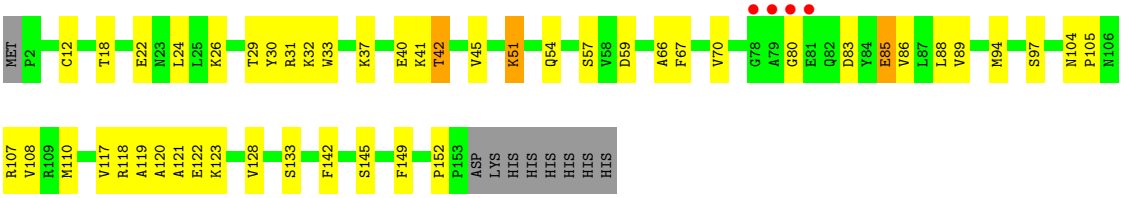
• Molecule 1: DNA repair protein XRCC1

Chain B:



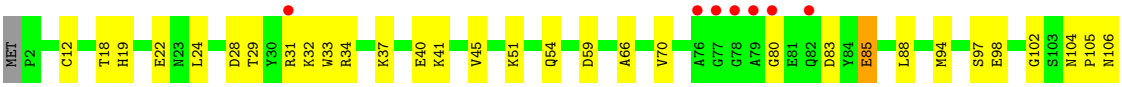
• Molecule 1: DNA repair protein XRCC1

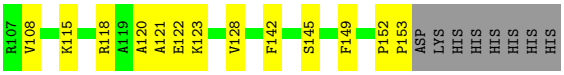
Chain C:



• Molecule 1: DNA repair protein XRCC1

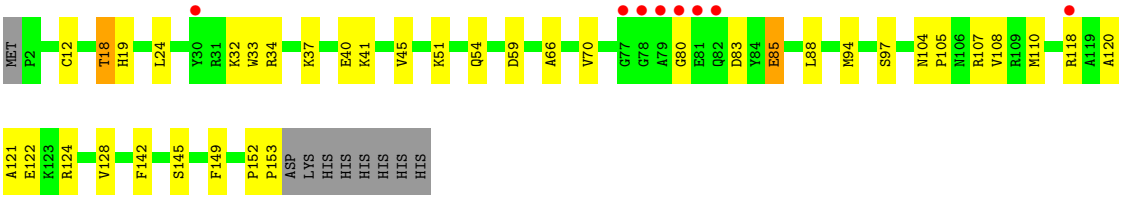
Chain D:





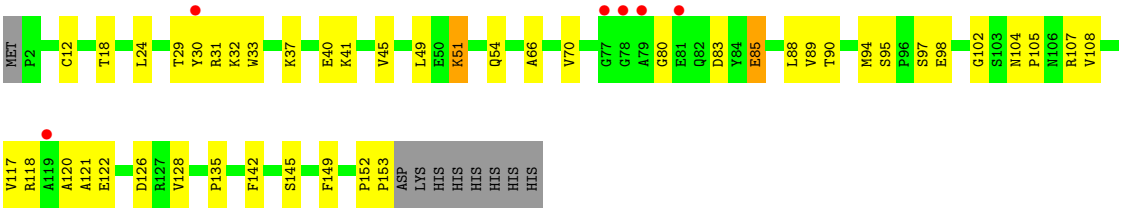
• Molecule 1: DNA repair protein XRCC1

Chain E:



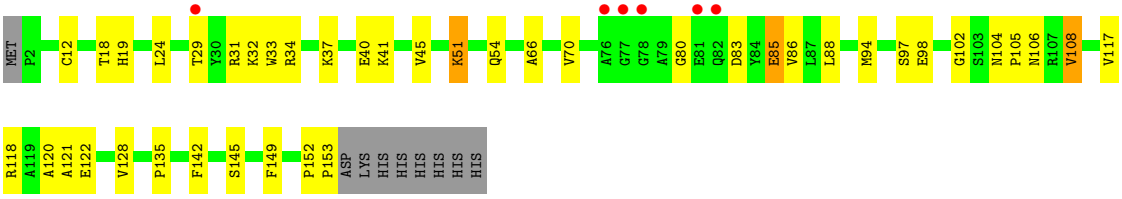
• Molecule 1: DNA repair protein XRCC1

Chain F:



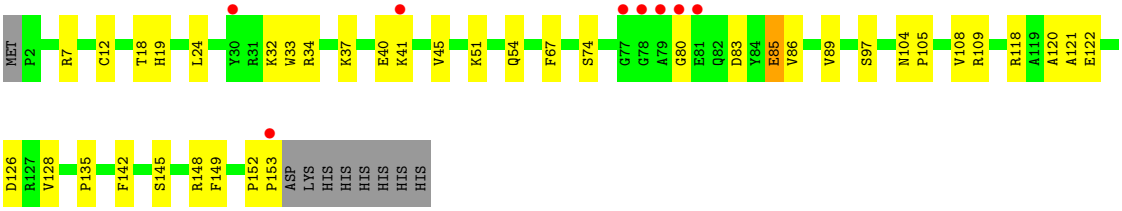
• Molecule 1: DNA repair protein XRCC1

Chain G:



• Molecule 1: DNA repair protein XRCC1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.45Å 89.30Å 93.18Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	29.34 – 2.60 29.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.34-2.60) 98.0 (29.34-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.237 0.203 , 0.232	Depositor DCC
R_{free} test set	1630 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 22.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -h,l,k 0.077 for -h,-l,-k 0.387 for h,-k,-l	Xtriage
Reported twinning fraction	0.394 for h,-k,-l	Depositor
Outliers	1 of 32108 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9492	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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, 0.333 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	0.36	0/1196	0.51	0/1614
1	B	0.40	0/1196	0.54	0/1614
1	C	0.44	1/1207 (0.1%)	0.53	0/1629
1	D	0.47	1/1208 (0.1%)	0.54	0/1629
1	E	0.39	0/1184	0.52	0/1600
1	F	0.37	0/1196	0.53	0/1614
1	G	0.39	0/1189	0.53	0/1606
1	H	0.38	0/1186	0.51	0/1603
All	All	0.40	2/9562 (0.0%)	0.53	0/12909

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	GLU	CD-OE2	8.10	1.34	1.25
1	C	22	GLU	CD-OE2	6.89	1.33	1.25

There are no bond angle outliers.

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	1172	0	1154	32	0
1	B	1172	0	1154	40	2
1	C	1183	0	1164	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1184	0	1166	30	2
1	E	1160	0	1132	32	0
1	F	1172	0	1154	41	2
1	G	1165	0	1141	28	2
1	H	1162	0	1132	38	0
2	A	14	0	0	3	0
2	B	20	0	0	6	0
2	C	18	0	0	6	0
2	D	21	0	0	3	0
2	E	9	0	0	0	0
2	F	13	0	0	4	0
2	G	10	0	0	0	0
2	H	17	0	0	3	0
All	All	9492	0	9197	257	4

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 14.

The worst 5 of 257 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:E:153:PRO:HB3	1:F:153:PRO:CB	1.83	1.09
1:E:153:PRO:HB3	1:F:153:PRO:HB2	1.29	1.06
1:F:49:LEU:HD12	2:F:164:HOH:O	1.64	0.94
1:F:126:ASP:HA	2:F:164:HOH:O	1.68	0.93
1:B:118:ARG:HB3	1:C:122:GLU:HG2	1.55	0.88

All (4) 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:26:LYS:NZ	1:D:59:ASP:OD2[2_646]	2.06	0.14
1:F:31:ARG:NH1	1:G:106:ASN:O[2_555]	2.13	0.07
1:B:31:ARG:NH1	1:D:106:ASN:O[2_646]	2.16	0.04
1:F:31:ARG:NH1	1:G:108:VAL:N[2_555]	2.18	0.02

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	150/161 (93%)	146 (97%)	4 (3%)	0	100	100
1	B	150/161 (93%)	146 (97%)	4 (3%)	0	100	100
1	C	151/161 (94%)	145 (96%)	6 (4%)	0	100	100
1	D	151/161 (94%)	147 (97%)	4 (3%)	0	100	100
1	E	150/161 (93%)	146 (97%)	4 (3%)	0	100	100
1	F	150/161 (93%)	146 (97%)	4 (3%)	0	100	100
1	G	150/161 (93%)	147 (98%)	3 (2%)	0	100	100
1	H	150/161 (93%)	146 (97%)	4 (3%)	0	100	100
All	All	1202/1288 (93%)	1169 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	130/140 (93%)	124 (95%)	6 (5%)	27	51
1	B	130/140 (93%)	124 (95%)	6 (5%)	27	51
1	C	132/140 (94%)	124 (94%)	8 (6%)	18	38
1	D	132/140 (94%)	127 (96%)	5 (4%)	33	59
1	E	128/140 (91%)	123 (96%)	5 (4%)	32	58
1	F	130/140 (93%)	124 (95%)	6 (5%)	27	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	128/140 (91%)	123 (96%)	5 (4%)	32	58
1	H	128/140 (91%)	123 (96%)	5 (4%)	32	58
All	All	1038/1120 (93%)	992 (96%)	46 (4%)	29	53

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	97	SER
1	F	117	VAL
1	E	108	VAL
1	F	85	GLU
1	G	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	104	ASN
1	G	82	GLN
1	H	82	GLN
1	C	104	ASN
1	D	82	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 monosaccharides 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 (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	152/161 (94%)	-0.15	7 (4%)	32	26	16, 33, 80, 130	0
1	B	152/161 (94%)	-0.07	6 (3%)	39	32	15, 32, 79, 130	0
1	C	152/161 (94%)	-0.13	4 (2%)	56	50	13, 32, 77, 129	0
1	D	152/161 (94%)	0.02	7 (4%)	32	26	17, 32, 78, 130	0
1	E	152/161 (94%)	-0.02	8 (5%)	26	20	19, 34, 77, 131	0
1	F	152/161 (94%)	-0.07	6 (3%)	39	32	13, 34, 79, 129	0
1	G	152/161 (94%)	0.00	6 (3%)	39	32	17, 33, 78, 128	0
1	H	152/161 (94%)	0.05	8 (5%)	26	20	18, 37, 77, 130	0
All	All	1216/1288 (94%)	-0.05	52 (4%)	35	28	13, 34, 80, 131	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	GLY	10.3
1	D	79	ALA	9.8
1	F	79	ALA	7.6
1	D	78	GLY	7.3
1	H	78	GLY	7.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.