Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 12:30 PM EDT

PDB ID	:	1U8P
Title	:	Crystal structure of the HIV-1 Cross Neutralizing Monoclonal Antibody 2F5 in complex with gp41 Peptide ECDKWCS
Authors	:	Bryson, S.; Julien, J.-P.; Hynes, R.C.; Pai, E.F.
Deposited on	:	2004-08-06
Resolution	:	3.23 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 (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:

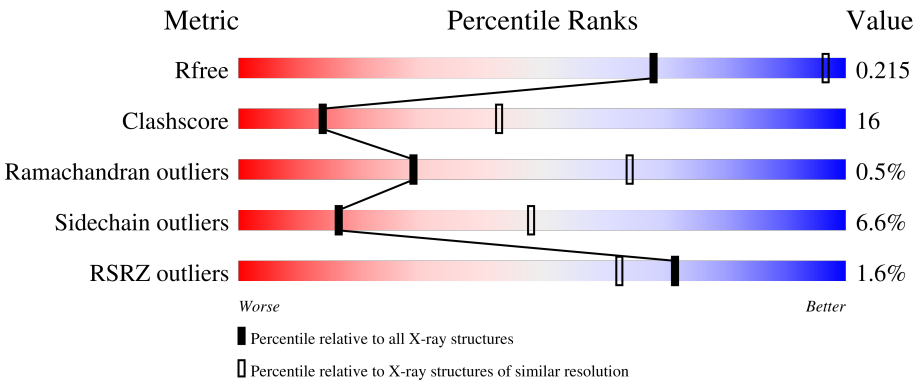
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.23 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	214	71% 26% .
2	B	235	2% 69% 24% . . .
3	C	7	14% 43% 29% 14% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3408 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 ANTIBODY 2F5 (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1644	1025	281	333	5	0	0	0

- Molecule 2 is a protein called ANTIBODY 2F5 (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1705	1084	289	325	7	0	0	0

- Molecule 3 is a protein called GP41 PEPTIDE.

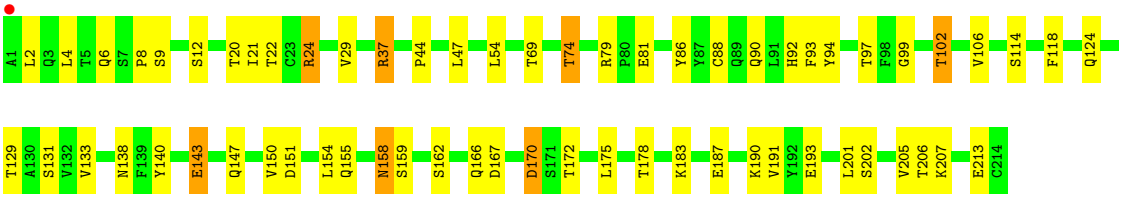
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	7	59	35	9	13	2	0	0	0

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.

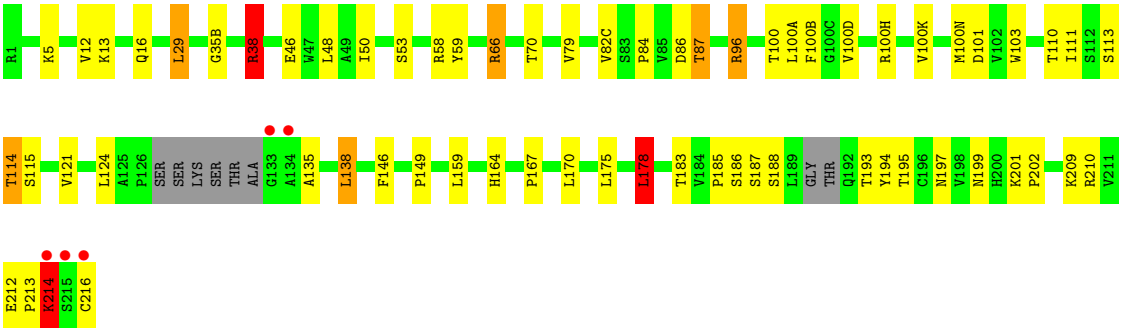
• Molecule 1: ANTIBODY 2F5 (LIGHT CHAIN)

Chain A:



• Molecule 2: ANTIBODY 2F5 (HEAVY CHAIN)

Chain B:



• Molecule 3: GP41 PEPTIDE

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.00Å 65.00Å 176.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.23 14.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-3.23) 91.9 (14.97-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.222 0.211 , 0.215	Depositor DCC
R_{free} test set	1314 reflections (10.31%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3408	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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	0.93	2/1681 (0.1%)	0.94	2/2284 (0.1%)
2	B	0.98	4/1746 (0.2%)	1.08	8/2385 (0.3%)
3	C	1.88	3/60 (5.0%)	1.43	2/78 (2.6%)
All	All	0.98	9/3487 (0.3%)	1.02	12/4747 (0.3%)

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	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	CYS	CB-SG	10.03	1.99	1.82
1	A	193	GLU	CG-CD	8.57	1.64	1.51
1	A	213	GLU	C-N	8.49	1.53	1.34
2	B	114	THR	C-N	-8.41	1.14	1.34
2	B	113	SER	C-N	7.62	1.51	1.34
3	C	7	SER	CA-C	-6.21	1.36	1.52
3	C	5	TRP	CB-CG	-6.16	1.39	1.50
2	B	59	TYR	CD1-CE1	5.30	1.47	1.39
3	C	7	SER	C-OXT	5.01	1.32	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	38	ARG	NE-CZ-NH2	-12.88	113.86	120.30
2	B	38	ARG	NE-CZ-NH1	12.79	126.69	120.30
2	B	66	ARG	NE-CZ-NH1	8.74	124.67	120.30
3	C	7	SER	N-CA-C	-7.41	90.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	66	ARG	NE-CZ-NH2	-6.40	117.10	120.30
3	C	7	SER	N-CA-CB	6.22	119.83	110.50
2	B	216	CYS	CA-CB-SG	6.02	124.83	114.00
2	B	178	LEU	CA-CB-CG	5.81	128.67	115.30
2	B	100(N)	MET	N-CA-C	-5.73	95.54	111.00
1	A	37	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	114	SER	N-CA-C	-5.20	96.97	111.00
2	B	38	ARG	CB-CG-CD	5.13	124.95	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	TYR	Sidechain

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	1644	0	1588	54	0
2	B	1705	0	1720	58	0
3	C	59	0	48	3	0
All	All	3408	0	3356	107	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 16.

All (107) 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:B:84:PRO:O	2:B:87:THR:HG23	1.65	0.96
1:A:90:GLN:HE22	1:A:93:PHE:H	1.01	0.93
1:A:20:THR:HG22	1:A:74:THR:HB	1.50	0.91
1:A:106:VAL:H	1:A:166:GLN:HE22	1.20	0.86
2:B:100(K):VAL:HG21	3:C:5:TRP:CD1	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASP:HB2	2:B:111:ILE:HD12	1.59	0.84
2:B:38:ARG:HD2	2:B:48:LEU:HD21	1.60	0.80
1:A:90:GLN:NE2	1:A:93:PHE:H	1.81	0.76
1:A:90:GLN:NE2	1:A:92:HIS:H	1.83	0.75
1:A:162:SER:HB2	2:B:167:PRO:HG2	1.70	0.71
2:B:210:ARG:NH1	2:B:212:GLU:OE1	2.25	0.70
2:B:29:LEU:O	2:B:53:SER:HB2	1.93	0.69
1:A:118:PHE:HB2	1:A:133:VAL:HG22	1.77	0.67
1:A:90:GLN:HE21	1:A:92:HIS:H	1.42	0.64
1:A:190:LYS:HG3	1:A:191:VAL:HG23	1.77	0.64
1:A:118:PHE:HD2	1:A:133:VAL:HG23	1.61	0.64
2:B:214:LYS:N	2:B:214:LYS:HE3	2.13	0.64
1:A:12:SER:HB3	1:A:140:TYR:OH	1.98	0.63
2:B:82(C):VAL:HB	2:B:111:ILE:HD13	1.79	0.63
1:A:133:VAL:HG21	2:B:124:LEU:HD22	1.81	0.62
1:A:8:PRO:O	1:A:102:THR:HB	2.01	0.61
1:A:79:ARG:HB3	1:A:81:GLU:OE2	2.01	0.60
1:A:167:ASP:HB3	1:A:170:ASP:HB2	1.83	0.60
2:B:114:THR:HG22	2:B:115:SER:O	2.02	0.60
2:B:213:PRO:C	2:B:214:LYS:HE3	2.23	0.59
2:B:82(C):VAL:CG2	2:B:111:ILE:HD13	2.33	0.59
1:A:29:VAL:HG11	1:A:90:GLN:HG3	1.84	0.59
2:B:114:THR:CG2	2:B:115:SER:O	2.52	0.58
2:B:213:PRO:HA	2:B:214:LYS:HE3	1.84	0.58
1:A:29:VAL:HG11	1:A:90:GLN:CG	2.34	0.57
1:A:90:GLN:NE2	1:A:92:HIS:N	2.51	0.57
2:B:135:ALA:HB1	2:B:183:THR:HG23	1.88	0.56
1:A:183:LYS:O	1:A:187:GLU:HG2	2.05	0.56
2:B:38:ARG:HD3	2:B:46:GLU:OE1	2.06	0.56
2:B:86:ASP:HB2	2:B:111:ILE:CD1	2.34	0.55
2:B:114:THR:HG21	2:B:146:PHE:CB	2.36	0.55
2:B:96:ARG:HD3	2:B:101:ASP:OD2	2.06	0.55
2:B:121:VAL:O	2:B:209:LYS:HE3	2.07	0.55
2:B:38:ARG:HB3	2:B:48:LEU:HD11	1.87	0.54
1:A:4:LEU:HD11	1:A:90:GLN:HB2	1.89	0.54
2:B:185:PRO:O	2:B:187:SER:N	2.40	0.54
1:A:21:ILE:HG23	1:A:102:THR:HG21	1.90	0.54
2:B:100(B):PHE:O	2:B:100(D):VAL:HG23	2.08	0.53
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.74	0.53
2:B:185:PRO:C	2:B:187:SER:H	2.13	0.52
1:A:81:GLU:H	1:A:81:GLU:CD	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.75	0.52
1:A:147:GLN:NE2	1:A:154:LEU:HG	2.25	0.52
1:A:124:GLN:NE2	1:A:131:SER:H	2.07	0.52
2:B:188:SER:HB3	2:B:194:TYR:OH	2.10	0.52
2:B:213:PRO:C	2:B:214:LYS:HZ2	2.13	0.52
2:B:87:THR:HG22	2:B:111:ILE:H	1.75	0.51
1:A:155:GLN:HB3	1:A:158:ASN:HD21	1.76	0.51
1:A:158:ASN:ND2	1:A:158:ASN:H	2.09	0.51
2:B:193:THR:HG22	2:B:210:ARG:HH21	1.76	0.51
1:A:9:SER:O	1:A:102:THR:HA	2.10	0.50
2:B:114:THR:HG21	2:B:175:LEU:HD23	1.92	0.50
3:C:6:CYS:O	3:C:7:SER:OXT	2.29	0.50
2:B:100(K):VAL:CG2	3:C:5:TRP:CD1	2.90	0.50
1:A:118:PHE:HB2	1:A:133:VAL:CG2	2.41	0.50
2:B:84:PRO:O	2:B:87:THR:CG2	2.51	0.50
2:B:12:VAL:O	2:B:111:ILE:HA	2.13	0.49
1:A:133:VAL:CG2	2:B:124:LEU:HD22	2.43	0.48
1:A:170:ASP:HB3	1:A:172:THR:HG23	1.95	0.48
2:B:87:THR:HB	2:B:110:THR:HA	1.95	0.48
1:A:147:GLN:CD	1:A:154:LEU:HD11	2.34	0.48
2:B:82(C):VAL:CB	2:B:111:ILE:HD13	2.43	0.48
2:B:82(C):VAL:HB	2:B:111:ILE:CD1	2.42	0.47
2:B:201:LYS:HB2	2:B:202:PRO:HD3	1.96	0.47
1:A:2:LEU:C	1:A:2:LEU:HD23	2.34	0.47
1:A:158:ASN:H	1:A:158:ASN:HD22	1.62	0.47
1:A:118:PHE:CD2	1:A:133:VAL:HG23	2.47	0.47
1:A:90:GLN:HE22	1:A:93:PHE:N	1.87	0.47
1:A:37:ARG:HB2	1:A:47:LEU:HD11	1.96	0.47
2:B:29:LEU:O	2:B:53:SER:CB	2.62	0.46
1:A:94:TYR:CZ	2:B:58:ARG:HG3	2.51	0.46
2:B:13:LYS:H	2:B:16:GLN:NE2	2.13	0.45
2:B:213:PRO:C	2:B:214:LYS:NZ	2.69	0.45
1:A:143:GLU:CD	1:A:143:GLU:H	2.20	0.45
2:B:35(B):GLY:HA2	2:B:50:ILE:HA	1.97	0.45
1:A:147:GLN:CG	1:A:154:LEU:HD11	2.47	0.45
2:B:213:PRO:C	2:B:214:LYS:CE	2.85	0.45
1:A:124:GLN:HG2	1:A:129:THR:O	2.16	0.44
1:A:201:LEU:HD13	1:A:205:VAL:HG12	1.99	0.44
1:A:44:PRO:HD2	2:B:103:TRP:CE3	2.53	0.44
1:A:206:THR:O	1:A:207:LYS:HD2	2.18	0.44
1:A:201:LEU:CD1	1:A:205:VAL:HG12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:C	1:A:175:LEU:HD23	2.38	0.43
2:B:114:THR:HG21	2:B:146:PHE:HB3	1.99	0.43
2:B:178:LEU:HD12	2:B:178:LEU:C	2.39	0.43
1:A:158:ASN:ND2	1:A:158:ASN:N	2.66	0.43
1:A:138:ASN:OD1	2:B:164:HIS:HE1	2.01	0.42
2:B:100(H):ARG:O	2:B:100(K):VAL:HG22	2.20	0.42
2:B:70:THR:CG2	2:B:79:VAL:HB	2.50	0.41
2:B:100(A):LEU:HG	2:B:100(B):PHE:CD1	2.55	0.41
2:B:138:LEU:CD2	2:B:138:LEU:N	2.83	0.41
1:A:6:GLN:NE2	1:A:88:CYS:H	2.19	0.41
1:A:159:SER:HA	1:A:178:THR:O	2.21	0.41
2:B:100:THR:HA	2:B:100(D):VAL:O	2.21	0.41
2:B:185:PRO:C	2:B:187:SER:N	2.73	0.41
2:B:87:THR:CG2	2:B:111:ILE:H	2.34	0.41
2:B:138:LEU:N	2:B:138:LEU:HD23	2.36	0.41
1:A:29:VAL:HG11	1:A:90:GLN:HG2	2.03	0.41
1:A:150:VAL:O	1:A:151:ASP:C	2.60	0.41
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.53	0.40
1:A:24:ARG:HA	1:A:69:THR:O	2.21	0.40
2:B:213:PRO:CA	2:B:214:LYS:HE3	2.48	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	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
2	B	221/235 (94%)	212 (96%)	7 (3%)	2 (1%)	17	52
3	C	5/7 (71%)	3 (60%)	2 (40%)	0	100	100
All	All	438/456 (96%)	419 (96%)	17 (4%)	2 (0%)	29	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	214	LYS
2	B	186	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	187/187 (100%)	177 (95%)	10 (5%)	22	56
2	B	197/203 (97%)	183 (93%)	14 (7%)	14	45
3	C	7/7 (100%)	5 (71%)	2 (29%)	0	1
All	All	391/397 (98%)	365 (93%)	26 (7%)	16	48

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	24	ARG
1	A	54	LEU
1	A	74	THR
1	A	97	THR
1	A	102	THR
1	A	143	GLU
1	A	158	ASN
1	A	170	ASP
1	A	202	SER
2	B	5	LYS
2	B	29	LEU
2	B	38	ARG
2	B	87	THR
2	B	96	ARG
2	B	138	LEU
2	B	149	PRO
2	B	159	LEU
2	B	170	LEU

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Mol	Chain	Res	Type
2	B	178	LEU
2	B	195	THR
2	B	197	ASN
2	B	199	ASN
2	B	214	LYS
3	C	2	CYS
3	C	7	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	38	GLN
1	A	90	GLN
1	A	124	GLN
1	A	137	ASN
1	A	147	GLN
1	A	155	GLN
1	A	158	ASN
1	A	166	GLN
1	A	199	GLN
2	B	16	GLN
2	B	39	GLN
2	B	164	HIS
2	B	192	GLN
2	B	199	ASN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	114:THR	C	115:SER	N	1.14

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	214/214 (100%)	-0.44	1 (0%)	91	87	18, 30, 45, 51	0
2	B	227/235 (96%)	-0.48	5 (2%)	62	52	16, 28, 51, 71	0
3	C	7/7 (100%)	0.03	1 (14%)	2	2	24, 29, 42, 60	0
All	All	448/456 (98%)	-0.45	7 (1%)	72	63	16, 29, 49, 71	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	216	CYS	5.6
2	B	133	GLY	4.7
2	B	134	ALA	3.7
2	B	215	SER	2.5
1	A	1	ALA	2.3
3	C	7	SER	2.2
2	B	214	LYS	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 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.