Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 04:06 PM EDT

PDB ID	:	4NKO
Title	:	Crystal structure of engineered anti-EE scFv antibody fragment
Authors	:	Kalyoncu, S.; Hyun, J.; Pai, J.C.; Johnson, J.L.; Etzminger, K.; Jain, A.; Heaner Jr., D.; Molares, I.A.; Truskett, T.M.; Maynard, J.A.; Lieberman, R.L.
Deposited on	:	2013-11-12
Resolution	:	3.50 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 ⓘ 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 ⓘ) were used in the production of this report:

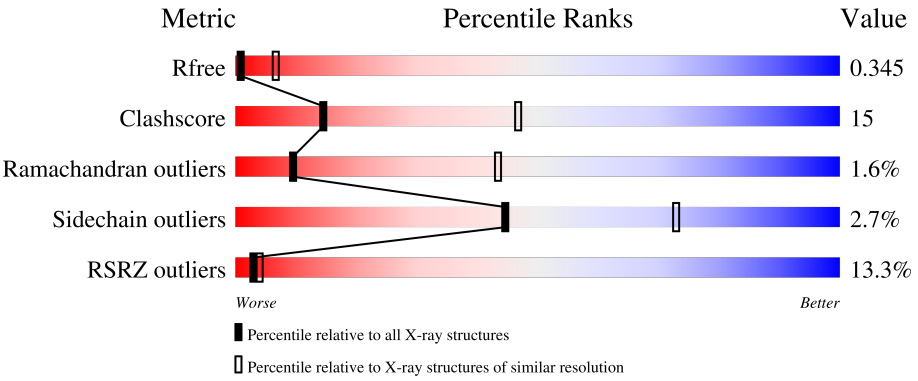
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	269	9% 60% 25% • 12%
1	B	269	13% 62% 25% • 12%
1	C	269	13% 66% 20% • 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5394 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 Engineered scFv.

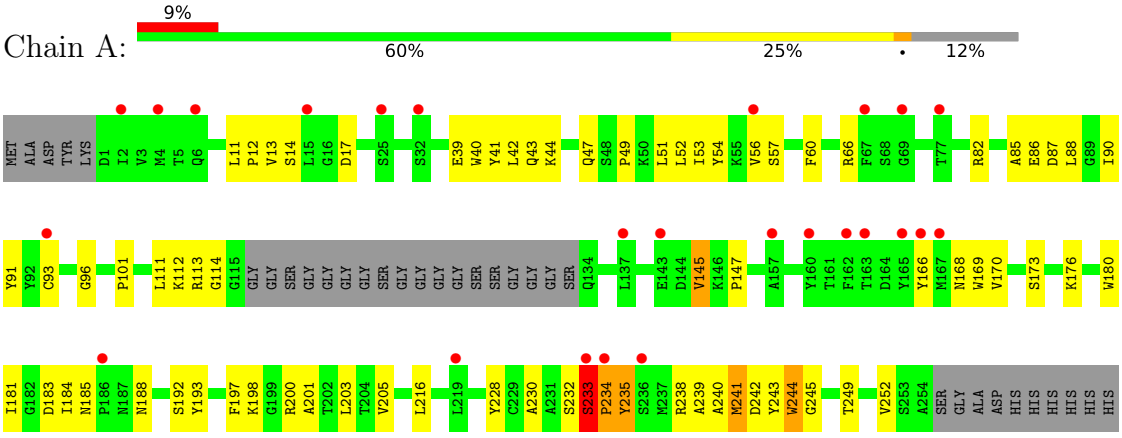
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1798	1128	301	360	9			
1	B	236	Total	C	N	O	S	0	0	0
			1798	1128	301	360	9			
1	C	236	Total	C	N	O	S	0	0	0
			1798	1128	301	360	9			

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.

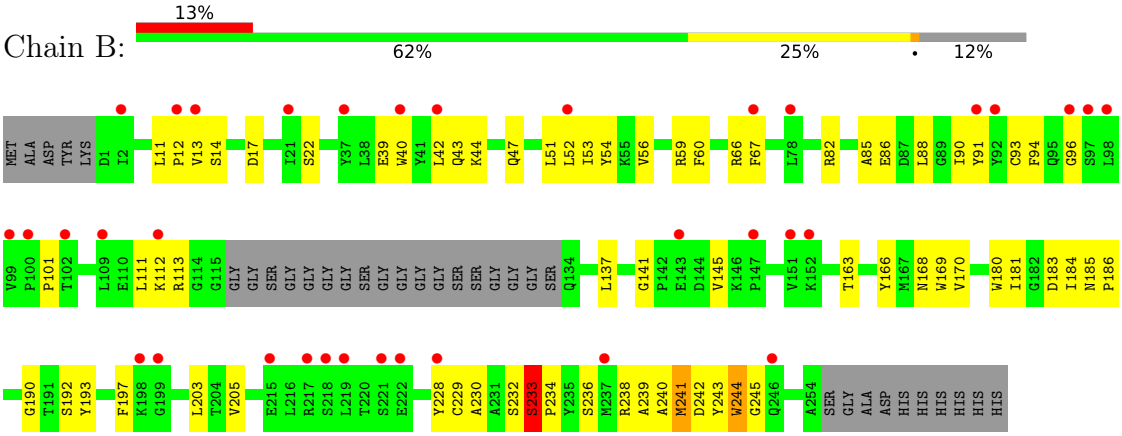
• Molecule 1: Engineered scFv

Chain A:



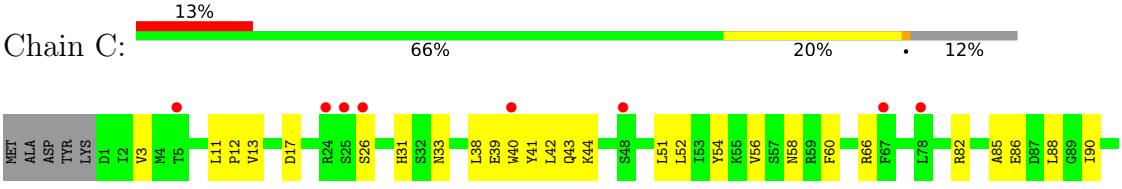
• Molecule 1: Engineered scFv

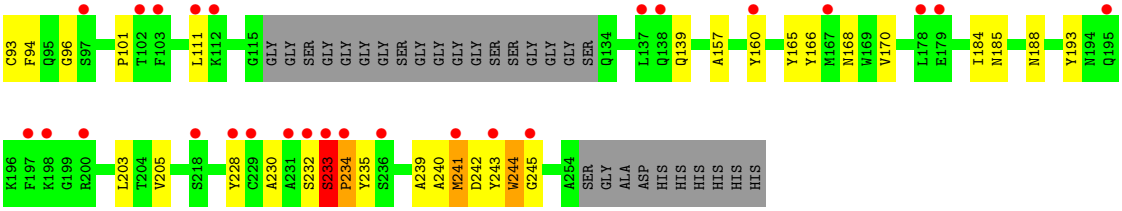
Chain B:



• Molecule 1: Engineered scFv

Chain C:




C93 F94 Q95 G96 S97 P101 T102 F103 L111 K112 G115 GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY GLY SER SER GLY GLY GLY SER Q134 L137 Q138 Q139 A157 Y160 Y165 Y166 M167 N168 W169 V170 L178 E179 I184 N185 N188 Y193 N194 Q195
K196 F197 K198 G199 R200 L203 T204 V205 S218 Y228 C229 A230 A231 S232 S233 P234 Y235 S236 A239 A240 M241 D242 Y243 W244 G245 A254 SER GLY ALA ASP HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	60.59Å 104.92Å 284.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.20 – 3.50 42.22 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.20-3.50) 93.1 (42.22-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.308 , 0.344 0.309 , 0.345	Depositor DCC
R_{free} test set	526 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	104.4	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.388 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.408 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5394	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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

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	0.29	0/1838	0.57	1/2489 (0.0%)
1	B	0.27	0/1838	0.57	1/2489 (0.0%)
1	C	0.28	0/1838	0.59	1/2489 (0.0%)
All	All	0.28	0/5514	0.57	3/7467 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	SER	C-N-CD	-5.82	107.80	120.60
1	B	233	SER	C-N-CD	-5.75	107.96	120.60
1	A	233	SER	C-N-CD	-5.71	108.03	120.60

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	1798	0	1745	60	0
1	B	1798	0	1743	55	0
1	C	1798	0	1743	53	0
All	All	5394	0	5231	164	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 (164) 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:168:ASN:HB2	1:A:230:ALA:HB3	1.46	0.95
1:B:168:ASN:HB2	1:B:230:ALA:HB3	1.48	0.95
1:C:168:ASN:HB2	1:C:230:ALA:HB3	1.52	0.90
1:C:230:ALA:HA	1:C:243:TYR:HB2	1.66	0.77
1:C:233:SER:HB3	1:C:234:PRO:HA	1.67	0.77
1:B:230:ALA:HA	1:B:243:TYR:HB2	1.68	0.76
1:B:243:TYR:HA	1:B:244:TRP:HB3	1.69	0.74
1:C:243:TYR:HA	1:C:244:TRP:HB3	1.68	0.73
1:A:243:TYR:HA	1:A:244:TRP:HB3	1.72	0.71
1:A:230:ALA:HA	1:A:243:TYR:HB2	1.71	0.71
1:A:66:ARG:HD2	1:A:82:ARG:HB2	1.74	0.70
1:A:181:ILE:HG12	1:A:197:PHE:HE2	1.59	0.67
1:C:193:TYR:HE1	1:C:203:LEU:HD13	1.61	0.66
1:B:193:TYR:HE1	1:B:203:LEU:HD13	1.61	0.66
1:C:44:LYS:NZ	1:C:86:GLU:O	2.28	0.65
1:B:44:LYS:NZ	1:B:86:GLU:O	2.31	0.63
1:C:243:TYR:CZ	1:C:245:GLY:HA3	2.34	0.62
1:C:85:ALA:HA	1:C:88:LEU:HD23	1.82	0.61
1:A:44:LYS:NZ	1:A:86:GLU:O	2.27	0.61
1:B:166:TYR:HB2	1:B:240:ALA:HB3	1.82	0.61
1:C:243:TYR:CA	1:C:244:TRP:HB3	2.31	0.60
1:B:184:ILE:HD13	1:B:205:VAL:HG23	1.82	0.60
1:C:243:TYR:CE1	1:C:245:GLY:HA3	2.35	0.60
1:A:243:TYR:CA	1:A:244:TRP:HB3	2.31	0.60
1:A:47:GLN:N	1:B:113:ARG:HH22	2.00	0.59
1:B:243:TYR:CE1	1:B:245:GLY:HA3	2.37	0.59
1:A:193:TYR:HE1	1:A:203:LEU:HD13	1.67	0.59
1:A:185:ASN:ND2	1:A:188:ASN:OD1	2.36	0.59
1:A:243:TYR:CE1	1:A:245:GLY:HA3	2.38	0.59
1:A:39:GLU:HG3	1:A:54:TYR:HA	1.85	0.59
1:C:166:TYR:HB2	1:C:240:ALA:HB3	1.85	0.58
1:A:114:GLY:HA3	1:B:141:GLY:HA2	1.86	0.58
1:B:243:TYR:CA	1:B:244:TRP:HB3	2.32	0.58
1:C:3:VAL:HG12	1:C:26:SER:HB3	1.85	0.58
1:B:137:LEU:HB2	1:B:243:TYR:HE1	1.68	0.58
1:B:168:ASN:O	1:B:230:ALA:N	2.36	0.58
1:A:184:ILE:HD13	1:A:205:VAL:HG23	1.86	0.57
1:C:41:TYR:HE1	1:C:242:ASP:HB3	1.69	0.57
1:C:43:GLN:HB3	1:C:90:ILE:HG23	1.84	0.57
1:C:96:GLY:HA2	1:C:101:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLY:HA2	1:B:101:PRO:HB3	1.87	0.56
1:C:165:TYR:CE1	1:C:233:SER:HB2	2.39	0.56
1:A:85:ALA:HA	1:A:88:LEU:HD23	1.86	0.56
1:B:243:TYR:CZ	1:B:245:GLY:HA3	2.41	0.56
1:C:228:TYR:HB3	1:C:243:TYR:HD2	1.70	0.56
1:A:96:GLY:HA2	1:A:101:PRO:HB3	1.89	0.55
1:A:113:ARG:HH22	1:B:47:GLN:N	2.04	0.55
1:A:43:GLN:HB3	1:A:90:ILE:HG23	1.87	0.55
1:C:185:ASN:ND2	1:C:188:ASN:OD1	2.40	0.54
1:C:243:TYR:HA	1:C:244:TRP:CB	2.38	0.54
1:C:3:VAL:H	1:C:26:SER:HB3	1.72	0.54
1:B:43:GLN:HB3	1:B:90:ILE:HG23	1.90	0.53
1:C:228:TYR:HB3	1:C:243:TYR:CD2	2.43	0.53
1:A:168:ASN:O	1:A:230:ALA:N	2.40	0.53
1:A:173:SER:HB3	1:A:176:LYS:HG2	1.90	0.53
1:A:243:TYR:CZ	1:A:245:GLY:HA3	2.44	0.53
1:B:168:ASN:HB3	1:B:180:TRP:HE1	1.74	0.53
1:C:233:SER:HB3	1:C:234:PRO:CA	2.39	0.53
1:C:233:SER:OG	1:C:240:ALA:N	2.38	0.53
1:A:243:TYR:HA	1:A:244:TRP:CB	2.40	0.52
1:C:170:VAL:HG13	1:C:228:TYR:HB2	1.90	0.52
1:B:42:LEU:HB2	1:B:52:LEU:HD11	1.92	0.52
1:B:170:VAL:HG13	1:B:228:TYR:HB2	1.90	0.52
1:A:13:VAL:HG13	1:A:17:ASP:HB2	1.92	0.52
1:B:85:ALA:HA	1:B:88:LEU:HD23	1.92	0.51
1:A:42:LEU:HB2	1:A:52:LEU:HD11	1.92	0.51
1:A:145:VAL:HG23	1:A:252:VAL:HA	1.92	0.51
1:A:166:TYR:HB2	1:A:240:ALA:HB3	1.94	0.50
1:A:235:TYR:OH	1:A:239:ALA:O	2.29	0.50
1:A:170:VAL:HG13	1:A:228:TYR:HB2	1.94	0.50
1:A:232:SER:O	1:A:241:MET:HG2	2.12	0.49
1:B:243:TYR:HA	1:B:244:TRP:CB	2.39	0.49
1:A:41:TYR:HE1	1:A:242:ASP:HB3	1.78	0.48
1:B:232:SER:OG	1:B:242:ASP:O	2.31	0.48
1:A:169:TRP:HB3	1:A:181:ILE:HD12	1.96	0.48
1:B:184:ILE:HA	1:B:190:GLY:O	2.13	0.48
1:C:241:MET:HG2	1:C:242:ASP:N	2.28	0.48
1:A:51:LEU:HD21	1:A:54:TYR:HB3	1.96	0.48
1:C:39:GLU:HG3	1:C:54:TYR:HA	1.97	0.47
1:B:51:LEU:HB2	1:B:242:ASP:CB	2.44	0.47
1:A:228:TYR:HB3	1:A:243:TYR:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HA	1:A:12:PRO:HD3	1.72	0.47
1:A:168:ASN:HB3	1:A:180:TRP:HE1	1.80	0.46
1:C:241:MET:HG2	1:C:242:ASP:H	1.80	0.46
1:A:183:ASP:OD2	1:A:192:SER:HB3	2.15	0.46
1:A:43:GLN:OE1	1:A:49:PRO:HG3	2.15	0.46
1:B:42:LEU:HD13	1:B:91:TYR:CZ	2.51	0.46
1:B:43:GLN:NE2	1:B:47:GLN:O	2.43	0.46
1:B:183:ASP:OD2	1:B:192:SER:HB3	2.16	0.46
1:B:230:ALA:HA	1:B:243:TYR:CB	2.42	0.46
1:C:184:ILE:HD13	1:C:205:VAL:HG23	1.97	0.46
1:C:31:HIS:HD1	1:C:33:ASN:H	1.63	0.46
1:C:168:ASN:HB2	1:C:230:ALA:CB	2.36	0.46
1:A:166:TYR:CE2	1:A:185:ASN:HB2	2.51	0.46
1:C:168:ASN:O	1:C:230:ALA:N	2.43	0.46
1:B:11:LEU:HA	1:B:12:PRO:HD3	1.77	0.46
1:B:54:TYR:HB2	1:B:241:MET:HE1	1.98	0.46
1:B:238:ARG:HA	1:B:238:ARG:HD2	1.67	0.46
1:C:11:LEU:HA	1:C:12:PRO:HD3	1.53	0.46
1:C:42:LEU:HB2	1:C:52:LEU:HD11	1.98	0.46
1:A:14:SER:OG	1:A:112:LYS:HB2	2.16	0.45
1:B:51:LEU:HD23	1:B:60:PHE:CD1	2.51	0.45
1:A:228:TYR:HB3	1:A:243:TYR:CD2	2.51	0.45
1:B:244:TRP:CD1	1:B:244:TRP:O	2.69	0.45
1:B:40:TRP:CZ3	1:B:93:CYS:HB3	2.52	0.45
1:B:228:TYR:HB3	1:B:243:TYR:HD2	1.80	0.45
1:A:66:ARG:HH22	1:A:87:ASP:CG	2.20	0.45
1:A:233:SER:HB3	1:A:234:PRO:HA	1.99	0.45
1:B:14:SER:OG	1:B:112:LYS:HB2	2.16	0.45
1:C:54:TYR:O	1:C:58:ASN:HB2	2.16	0.44
1:A:238:ARG:HA	1:A:238:ARG:HD2	1.59	0.44
1:A:66:ARG:NH1	1:A:82:ARG:O	2.50	0.44
1:B:228:TYR:HB3	1:B:243:TYR:CD2	2.53	0.44
1:A:244:TRP:CD1	1:A:244:TRP:O	2.70	0.44
1:B:181:ILE:HG12	1:B:197:PHE:HE2	1.82	0.44
1:C:51:LEU:HD23	1:C:60:PHE:CD1	2.53	0.44
1:C:244:TRP:O	1:C:244:TRP:CD1	2.71	0.44
1:B:241:MET:HG2	1:B:242:ASP:N	2.33	0.44
1:B:66:ARG:HD2	1:B:82:ARG:HB2	1.98	0.43
1:C:232:SER:OG	1:C:242:ASP:O	2.36	0.43
1:C:235:TYR:OH	1:C:239:ALA:O	2.35	0.43
1:B:233:SER:OG	1:B:239:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASN:HB2	1:B:230:ALA:CB	2.34	0.43
1:A:51:LEU:HB2	1:A:242:ASP:HB3	2.00	0.43
1:A:51:LEU:HB2	1:A:242:ASP:CB	2.49	0.43
1:A:230:ALA:HA	1:A:243:TYR:CB	2.45	0.43
1:B:166:TYR:CE2	1:B:185:ASN:HB2	2.54	0.43
1:C:38:LEU:HB3	1:C:56:VAL:HG22	2.00	0.43
1:B:241:MET:HG2	1:B:242:ASP:H	1.83	0.43
1:A:40:TRP:HB2	1:A:53:ILE:HB	1.99	0.42
1:A:198:LYS:HB2	1:A:200:ARG:HG3	2.01	0.42
1:A:201:ALA:HB2	1:A:216:LEU:HD13	2.01	0.42
1:B:13:VAL:HG13	1:B:17:ASP:HB2	2.00	0.42
1:A:181:ILE:HG23	1:A:197:PHE:CD2	2.55	0.42
1:B:59:ARG:HD3	1:B:67:PHE:O	2.19	0.42
1:B:229:CYS:O	1:B:243:TYR:CD1	2.72	0.42
1:A:180:TRP:HZ2	1:A:183:ASP:HB3	1.84	0.42
1:C:94:PHE:CE2	1:C:101:PRO:HB2	2.54	0.42
1:C:41:TYR:HE1	1:C:242:ASP:CB	2.33	0.42
1:C:66:ARG:HD2	1:C:82:ARG:HB2	2.00	0.42
1:C:139:GLN:HE22	1:C:228:TYR:HA	1.84	0.42
1:B:40:TRP:HB2	1:B:53:ILE:HB	2.01	0.42
1:C:232:SER:OG	1:C:242:ASP:OD2	2.37	0.42
1:C:233:SER:OG	1:C:239:ALA:HA	2.20	0.42
1:C:94:PHE:HE2	1:C:101:PRO:HB2	1.85	0.42
1:A:249:THR:OG1	1:B:113:ARG:N	2.51	0.41
1:B:180:TRP:HZ2	1:B:183:ASP:HB3	1.84	0.41
1:B:51:LEU:HB2	1:B:242:ASP:HB3	2.02	0.41
1:C:168:ASN:ND2	1:C:240:ALA:O	2.52	0.41
1:C:230:ALA:HA	1:C:243:TYR:CB	2.44	0.41
1:A:181:ILE:HG12	1:A:197:PHE:CE2	2.48	0.41
1:B:169:TRP:HB3	1:B:181:ILE:HD12	2.02	0.41
1:C:157:ALA:HB1	1:C:160:TYR:CE1	2.55	0.41
1:A:51:LEU:HD23	1:A:60:PHE:CD1	2.56	0.41
1:C:40:TRP:CZ3	1:C:93:CYS:HB3	2.56	0.41
1:C:166:TYR:CE2	1:C:185:ASN:HB2	2.56	0.41
1:A:54:TYR:HE1	1:A:60:PHE:HA	1.86	0.40
1:B:163:THR:HA	1:B:186:PRO:HB2	2.03	0.40
1:A:181:ILE:HG23	1:A:197:PHE:HD2	1.86	0.40
1:B:39:GLU:HB2	1:B:94:PHE:HD1	1.85	0.40
1:A:40:TRP:CZ3	1:A:93:CYS:HB3	2.56	0.40
1:C:13:VAL:HG13	1:C:17:ASP:HB2	2.04	0.40
1:C:170:VAL:CG1	1:C:228:TYR:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD13	1:A:91:TYR:CZ	2.56	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	232/269 (86%)	213 (92%)	14 (6%)	5 (2%)	6 37
1	B	232/269 (86%)	216 (93%)	12 (5%)	4 (2%)	9 42
1	C	232/269 (86%)	214 (92%)	16 (7%)	2 (1%)	17 56
All	All	696/807 (86%)	643 (92%)	42 (6%)	11 (2%)	9 43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	B	56	VAL
1	A	235	TYR
1	B	233	SER
1	C	233	SER
1	A	147	PRO
1	A	233	SER
1	B	236	SER
1	B	234	PRO
1	C	234	PRO
1	A	234	PRO

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	200/217 (92%)	194 (97%)	6 (3%)	41	71
1	B	200/217 (92%)	194 (97%)	6 (3%)	41	71
1	C	200/217 (92%)	196 (98%)	4 (2%)	55	79
All	All	600/651 (92%)	584 (97%)	16 (3%)	44	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	111	LEU
1	A	145	VAL
1	A	233	SER
1	A	241	MET
1	A	244	TRP
1	B	22	SER
1	B	111	LEU
1	B	145	VAL
1	B	233	SER
1	B	241	MET
1	B	244	TRP
1	C	111	LEU
1	C	233	SER
1	C	241	MET
1	C	244	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	138	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 monosaccharides 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	236/269 (87%)	0.69	25 (10%)	6	7	67, 89, 108, 121	0
1	B	236/269 (87%)	0.75	35 (14%)	2	3	68, 91, 110, 131	0
1	C	236/269 (87%)	0.88	34 (14%)	2	3	71, 90, 108, 119	0
All	All	708/807 (87%)	0.77	94 (13%)	3	4	67, 90, 109, 131	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	SER	10.4
1	C	178	LEU	8.6
1	B	97	SER	7.2
1	C	236	SER	6.5
1	C	234	PRO	6.0
1	B	98	LEU	5.9
1	A	137	LEU	5.4
1	A	157	ALA	5.4
1	C	179	GLU	5.2
1	A	6	GLN	5.1
1	A	233	SER	4.7
1	B	78	LEU	4.7
1	C	243	TYR	4.6
1	B	219	LEU	4.5
1	C	103	PHE	4.4
1	B	143	GLU	4.4
1	C	25	SER	4.2
1	B	92	TYR	4.0
1	C	197	PHE	4.0
1	A	67	PHE	3.8
1	B	198	LYS	3.7
1	A	160	TYR	3.6
1	C	195	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	91	TYR	3.5
1	C	231	ALA	3.5
1	C	245	GLY	3.4
1	B	222	GLU	3.4
1	C	137	LEU	3.3
1	C	232	SER	3.3
1	C	112	LYS	3.3
1	B	2	ILE	3.3
1	A	162	PHE	3.3
1	A	236	SER	3.1
1	C	138	GLN	3.1
1	C	102	THR	3.1
1	C	167	MET	3.1
1	C	229	CYS	2.9
1	B	151	VAL	2.9
1	B	199	GLY	2.9
1	B	21	ILE	2.8
1	B	112	LYS	2.8
1	C	111	LEU	2.8
1	A	4	MET	2.8
1	C	218	SER	2.7
1	B	102	THR	2.7
1	C	40	TRP	2.7
1	B	237	MET	2.7
1	C	67	PHE	2.6
1	C	160	TYR	2.6
1	C	228	TYR	2.6
1	A	56	VAL	2.6
1	B	96	GLY	2.5
1	A	219	LEU	2.5
1	B	217	ARG	2.5
1	C	24	ARG	2.5
1	A	69	GLY	2.5
1	B	99	VAL	2.5
1	A	32	SER	2.5
1	C	5	THR	2.5
1	C	78	LEU	2.4
1	B	12	PRO	2.4
1	B	37	TYR	2.4
1	B	100	PRO	2.4
1	A	93	CYS	2.4
1	A	143	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	MET	2.3
1	A	166	TYR	2.3
1	A	2	ILE	2.3
1	C	241	MET	2.3
1	B	52	LEU	2.3
1	A	234	PRO	2.3
1	B	67	PHE	2.3
1	B	228	TYR	2.3
1	A	163	THR	2.2
1	C	26	SER	2.2
1	A	165	TYR	2.2
1	B	147	PRO	2.2
1	C	200	ARG	2.2
1	B	42	LEU	2.2
1	C	97	SER	2.2
1	A	186	PRO	2.2
1	C	198	LYS	2.2
1	B	152	LYS	2.1
1	B	40	TRP	2.1
1	B	221	SER	2.1
1	B	13	VAL	2.1
1	B	109	LEU	2.1
1	A	15	LEU	2.1
1	B	246	GLN	2.1
1	C	48	SER	2.1
1	A	77	THR	2.1
1	A	25	SER	2.1
1	B	218	SER	2.1
1	B	215	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 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.