Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:43 AM GMT

PDB ID	:	2O0O
Title	:	Crystal structure of TL1A
Authors	:	Jin, T.C.; Kim, S.; Guo, F.; Howard, A.J.; Zhang, Y.Z.
Deposited on	:	2006-11-27
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

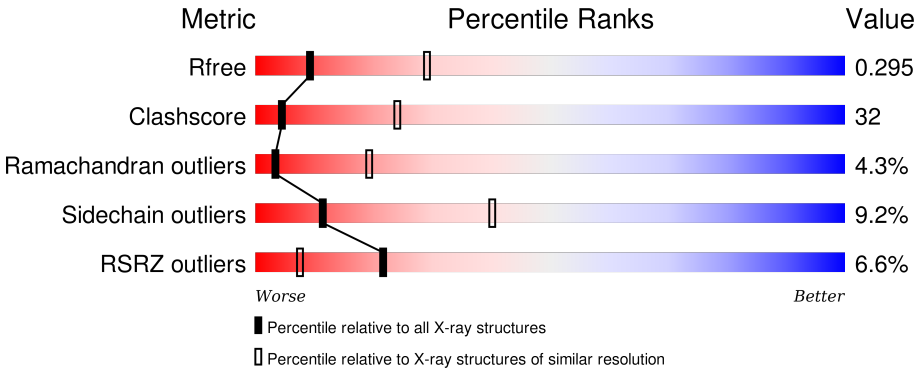
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	180	4% 41% 38% 6% • 15%
1	B	180	7% 42% 37% 6% 15%
1	C	180	6% 34% 44% 6% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	271	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3591 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 TNF superfamily ligand TL1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1200	777	194	222	7			
1	B	153	Total	C	N	O	S	0	0	0
			1183	764	190	223	6			
1	C	152	Total	C	N	O	S	0	0	0
			1170	757	188	219	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

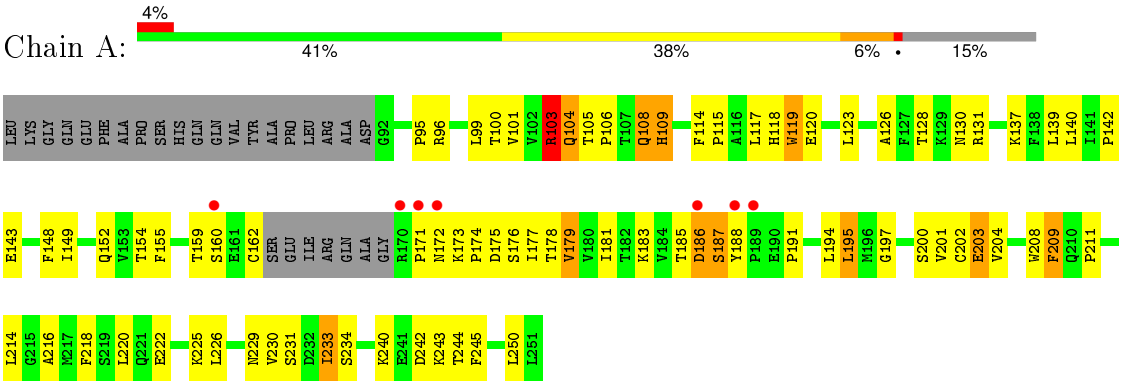
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	12	Total	O	0	0
			12	12		
3	C	9	Total	O	0	0
			9	9		

3 Residue-property plots (i)

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 (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.

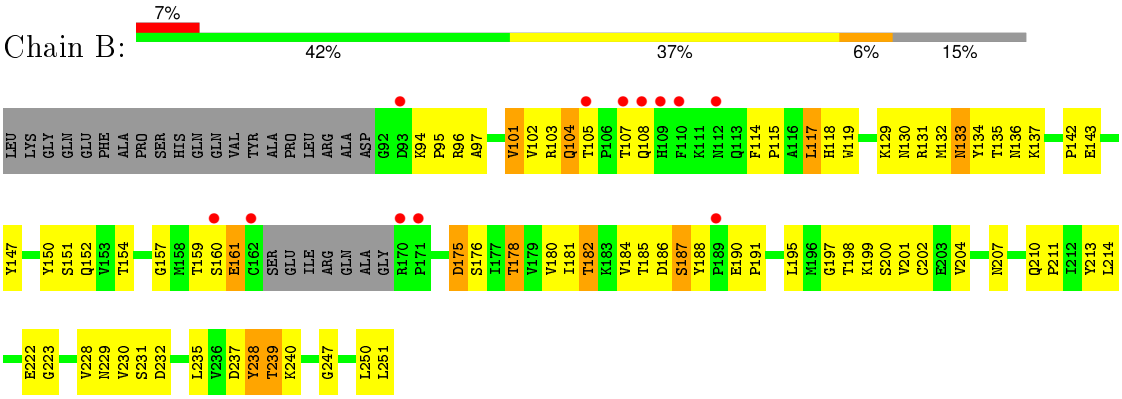
- Molecule 1: TNF superfamily ligand TL1A

Chain A:



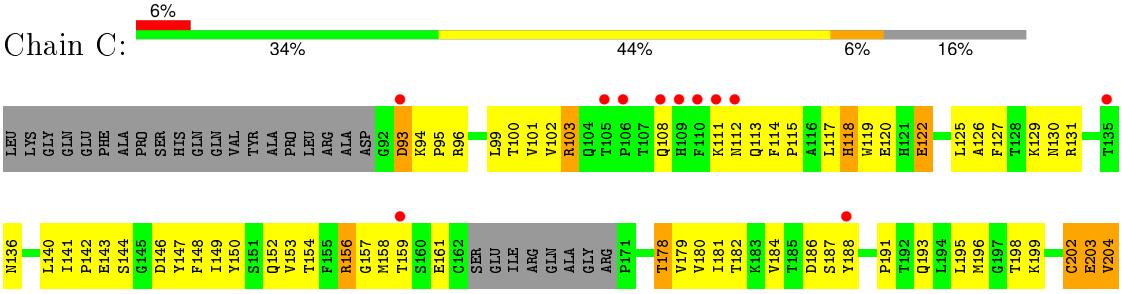
- Molecule 1: TNF superfamily ligand TL1A

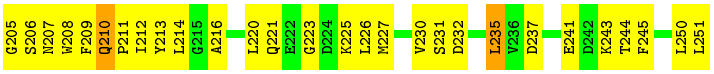
Chain B:



- Molecule 1: TNF superfamily ligand TL1A

Chain C:




G205
S206
N207
W208
F209
Q210
P211
I212
Y213
L214
G215
A216
L220
Q221
E222
G223
D224
K225
L226
M227
V230
S231
D232
I235
V236
D237
E241
D242
K243
T244
F245
L250
L251

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.75Å 116.75Å 118.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 36.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.2 (40.00-3.00) 89.1 (36.99-3.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.295 0.244 , 0.295	Depositor DCC
R_{free} test set	724 reflections (4.77%)	DCC
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 81.0	EDS
Estimated twinning fraction	0.033 for -h,l,k 0.023 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	6 of 17078 reflections (0.035%)	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	3591	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.42	0/1232	0.67	0/1675
1	B	0.43	0/1212	0.68	0/1648
1	C	0.40	0/1201	0.61	0/1637
All	All	0.42	0/3645	0.66	0/4960

There are no bond length outliers.

There are no bond angle outliers.

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	1200	0	1149	72	0
1	B	1183	0	1127	73	0
1	C	1170	0	1100	93	0
2	A	1	0	0	0	0
3	A	16	0	0	0	0
3	B	12	0	0	1	0
3	C	9	0	0	2	0
All	All	3591	0	3376	225	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 32.

All (225) 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:C:178:THR:HB	1:C:198:THR:HG22	1.24	1.08
1:A:185:THR:HG22	1:A:187:SER:H	1.29	0.95
1:C:178:THR:HG23	1:C:231:SER:HB3	1.47	0.93
1:A:183:LYS:HB2	1:A:194:LEU:HD11	1.51	0.92
1:C:232:ASP:HB3	1:C:235:LEU:HD22	1.52	0.89
1:C:181:ILE:HD12	1:C:195:LEU:HD12	1.58	0.85
1:B:117:LEU:HD11	1:B:230:VAL:HG13	1.59	0.84
1:A:105:THR:H	1:A:118:HIS:HE1	1.26	0.84
1:C:178:THR:CB	1:C:198:THR:HG22	2.08	0.83
1:B:118:HIS:HB3	1:B:137:LYS:HE3	1.62	0.82
1:B:105:THR:H	1:B:118:HIS:HE1	1.24	0.81
1:C:117:LEU:HD11	1:C:230:VAL:HG13	1.60	0.81
1:B:178:THR:HG23	1:B:231:SER:HB3	1.63	0.79
1:B:94:LYS:HB3	1:B:250:LEU:HB3	1.64	0.78
1:A:178:THR:HG22	1:A:231:SER:HB3	1.67	0.77
1:B:190:GLU:OE1	1:B:191:PRO:HD2	1.86	0.76
1:A:143:GLU:HA	1:A:222:GLU:HG2	1.67	0.76
1:C:94:LYS:HB2	1:C:95:PRO:HD2	1.67	0.76
1:A:200:SER:HB3	1:C:209:PHE:CE2	2.22	0.75
1:C:178:THR:HB	1:C:198:THR:CG2	2.13	0.75
1:B:204:VAL:HG23	1:C:202:CYS:SG	2.27	0.74
1:C:195:LEU:HD21	1:C:216:ALA:HB3	1.70	0.72
1:A:105:THR:H	1:A:118:HIS:CE1	2.12	0.67
1:A:114:PHE:HB3	1:A:229:ASN:HB3	1.74	0.67
1:A:149:ILE:HG21	1:A:181:ILE:HG21	1.76	0.67
1:B:105:THR:H	1:B:118:HIS:CE1	2.10	0.67
1:C:195:LEU:HB3	1:C:214:LEU:HD13	1.76	0.67
1:B:181:ILE:HD12	1:B:195:LEU:HD12	1.77	0.66
1:A:104:GLN:HE22	1:A:118:HIS:H	1.43	0.66
1:B:103:ARG:HA	1:B:238:TYR:CD1	2.31	0.65
1:C:147:TYR:CE1	1:C:250:LEU:HD13	2.32	0.64
1:B:143:GLU:HA	1:B:222:GLU:HB2	1.79	0.64
1:C:159:THR:H	1:C:207:ASN:HA	1.62	0.64
1:A:143:GLU:HA	1:A:222:GLU:CG	2.28	0.64
1:A:159:THR:HG23	1:A:203:GLU:O	1.98	0.63
1:B:115:PRO:HD2	1:B:230:VAL:O	1.98	0.63
1:B:103:ARG:HA	1:B:238:TYR:HD1	1.63	0.63
1:B:103:ARG:O	1:B:104:GLN:HB2	1.99	0.61
1:C:203:GLU:HG3	1:C:208:TRP:CD1	2.35	0.61
1:C:195:LEU:HD21	1:C:216:ALA:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:HD22	1:B:133:ASN:C	2.03	0.61
1:C:120:GLU:OE2	1:C:122:GLU:HG2	2.01	0.60
1:B:117:LEU:N	1:B:117:LEU:HD12	2.16	0.59
1:A:155:PHE:CG	1:A:177:ILE:HD12	2.38	0.59
1:B:129:LYS:HG3	1:B:130:ASN:ND2	2.17	0.59
1:A:108:GLN:HE21	1:A:109:HIS:N	2.01	0.59
1:B:199:LYS:HD3	3:B:252:HOH:O	2.01	0.58
1:B:95:PRO:HA	1:B:130:ASN:HB2	1.84	0.58
1:A:175:ASP:HB2	1:A:201:VAL:HG13	1.85	0.58
1:A:143:GLU:CA	1:A:222:GLU:HG2	2.32	0.58
1:C:157:GLY:O	1:C:207:ASN:HB2	2.04	0.57
1:B:96:ARG:HH21	1:C:146:ASP:HB2	1.69	0.57
1:A:131:ARG:O	1:A:142:PRO:HB3	2.04	0.57
1:B:133:ASN:HD22	1:B:134:TYR:N	2.02	0.57
1:C:100:THR:CG2	1:C:241:GLU:HB2	2.35	0.57
1:B:157:GLY:O	1:B:207:ASN:HB2	2.04	0.57
1:B:114:PHE:CE2	1:B:231:SER:HA	2.40	0.57
1:C:156:ARG:HD2	1:C:237:ASP:HB2	1.86	0.56
1:C:193:GLN:HE22	1:C:196:MET:CE	2.18	0.56
1:C:144:SER:OG	1:C:221:GLN:HA	2.05	0.56
1:A:149:ILE:N	1:A:149:ILE:HD13	2.20	0.56
1:B:239:THR:HG22	1:B:240:LYS:N	2.19	0.56
1:C:220:LEU:HD13	1:C:226:LEU:HD11	1.88	0.56
1:B:180:VAL:HG12	1:B:182:THR:HG22	1.88	0.56
1:A:183:LYS:HB2	1:A:194:LEU:CD1	2.32	0.56
1:B:117:LEU:HD12	1:B:117:LEU:H	1.70	0.55
1:C:203:GLU:HG3	1:C:208:TRP:HB3	1.88	0.55
1:A:104:GLN:HA	1:A:118:HIS:CE1	2.42	0.55
1:A:240:LYS:HB2	1:A:243:LYS:HG3	1.89	0.55
1:B:103:ARG:HG3	1:B:238:TYR:CE1	2.41	0.55
1:A:95:PRO:HD2	1:A:250:LEU:HD22	1.89	0.55
1:C:96:ARG:HD2	1:C:129:LYS:HD2	1.89	0.55
1:C:99:LEU:HB3	1:C:119:TRP:HB3	1.88	0.55
1:C:147:TYR:CZ	1:C:250:LEU:HD13	2.42	0.55
1:A:176:SER:HB3	1:C:209:PHE:HZ	1.72	0.55
1:B:151:SER:HB3	1:B:181:ILE:HD11	1.89	0.54
1:C:141:ILE:CD1	1:C:226:LEU:HD13	2.37	0.54
1:A:115:PRO:HD2	1:A:230:VAL:O	2.07	0.54
1:C:180:VAL:HG22	1:C:196:MET:HG3	1.88	0.54
1:B:238:TYR:N	1:B:238:TYR:CD2	2.74	0.54
1:B:199:LYS:HD2	1:B:210:GLN:OE1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ASP:CB	1:C:235:LEU:HD22	2.32	0.54
1:A:108:GLN:HE21	1:A:108:GLN:C	2.11	0.54
1:B:101:VAL:HG22	1:B:102:VAL:H	1.73	0.54
1:B:96:ARG:HD2	1:C:146:ASP:OD1	2.08	0.54
1:A:197:GLY:N	1:A:214:LEU:HD11	2.23	0.53
1:B:237:ASP:OD1	1:B:239:THR:HB	2.08	0.53
1:C:199:LYS:HD2	1:C:210:GLN:OE1	2.08	0.53
1:C:136:ASN:HB3	3:C:259:HOH:O	2.07	0.53
1:A:185:THR:HG22	1:A:187:SER:N	2.12	0.53
1:B:118:HIS:HB3	1:B:137:LYS:CE	2.37	0.53
1:A:101:VAL:HB	1:A:244:THR:HB	1.90	0.53
1:C:118:HIS:HB3	3:C:254:HOH:O	2.09	0.52
1:A:100:THR:O	1:A:119:TRP:HB3	2.09	0.52
1:B:131:ARG:O	1:B:142:PRO:HB3	2.10	0.52
1:C:117:LEU:N	1:C:117:LEU:HD12	2.25	0.52
1:B:197:GLY:HA3	1:B:214:LEU:HD21	1.92	0.52
1:A:148:PHE:C	1:A:149:ILE:HD13	2.29	0.52
1:C:182:THR:HB	1:C:227:MET:HE2	1.92	0.51
1:C:100:THR:HB	1:C:241:GLU:HB2	1.91	0.51
1:C:112:ASN:CG	1:C:113:GLN:H	2.14	0.51
1:A:173:LYS:HA	1:C:206:SER:HB3	1.91	0.51
1:C:209:PHE:O	1:C:210:GLN:HB3	2.11	0.51
1:C:193:GLN:HE22	1:C:196:MET:HE3	1.76	0.51
1:A:209:PHE:CE2	1:B:200:SER:HB3	2.46	0.51
1:C:203:GLU:HG3	1:C:208:TRP:CG	2.46	0.51
1:C:101:VAL:HG22	1:C:102:VAL:N	2.26	0.51
1:C:140:LEU:HD11	1:C:223:GLY:HA2	1.93	0.51
1:B:117:LEU:HD11	1:B:230:VAL:CG1	2.37	0.50
1:B:186:ASP:O	1:B:187:SER:O	2.30	0.50
1:C:149:ILE:N	1:C:149:ILE:HD12	2.26	0.50
1:C:146:ASP:O	1:C:250:LEU:HD12	2.12	0.50
1:B:107:THR:HG23	1:B:107:THR:O	2.11	0.50
1:B:96:ARG:NH2	1:C:146:ASP:HB2	2.26	0.50
1:C:184:VAL:HG22	1:C:191:PRO:HB3	1.92	0.50
1:A:174:PRO:HB3	1:A:202:CYS:SG	2.52	0.50
1:A:104:GLN:NE2	1:A:117:LEU:HA	2.27	0.50
1:C:148:PHE:HB2	1:C:251:LEU:HD11	1.93	0.50
1:B:152:GLN:HB2	1:B:213:TYR:HD1	1.76	0.50
1:C:149:ILE:CD1	1:C:149:ILE:N	2.75	0.49
1:C:149:ILE:HG21	1:C:181:ILE:HG21	1.94	0.49
1:A:103:ARG:O	1:A:104:GLN:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:HA	1:A:211:PRO:HA	1.95	0.49
1:B:160:SER:O	1:B:161:GLU:C	2.51	0.49
1:B:187:SER:OG	1:B:188:TYR:N	2.46	0.49
1:C:103:ARG:HE	1:C:103:ARG:HA	1.78	0.49
1:C:204:VAL:HG22	1:C:204:VAL:O	2.13	0.48
1:B:105:THR:N	1:B:118:HIS:HE1	2.01	0.48
1:C:95:PRO:HA	1:C:130:ASN:HB2	1.95	0.48
1:C:251:LEU:HD12	1:C:251:LEU:N	2.28	0.48
1:A:105:THR:N	1:A:118:HIS:HE1	2.03	0.48
1:B:133:ASN:C	1:B:133:ASN:ND2	2.67	0.48
1:C:125:LEU:HD12	1:C:241:GLU:HG3	1.96	0.48
1:A:220:LEU:HD13	1:A:226:LEU:HD21	1.96	0.47
1:A:188:TYR:N	1:A:188:TYR:CD1	2.83	0.47
1:A:243:LYS:HE2	1:B:198:THR:HG21	1.96	0.47
1:C:142:PRO:HG2	1:C:143:GLU:H	1.79	0.47
1:C:100:THR:HG21	1:C:241:GLU:HB2	1.96	0.47
1:A:204:VAL:O	1:A:204:VAL:HG23	2.14	0.47
1:A:131:ARG:HH22	1:A:143:GLU:HB3	1.80	0.47
1:C:141:ILE:HD11	1:C:226:LEU:HD13	1.97	0.46
1:C:156:ARG:HH21	1:C:156:ARG:HG3	1.80	0.46
1:A:187:SER:HB2	1:A:188:TYR:CD1	2.51	0.46
1:B:250:LEU:HD13	1:B:251:LEU:N	2.30	0.46
1:C:251:LEU:HD12	1:C:251:LEU:H	1.80	0.46
1:A:152:GLN:O	1:A:244:THR:HA	2.16	0.46
1:C:152:GLN:HB3	1:C:245:PHE:CZ	2.51	0.46
1:A:171:PRO:HG2	1:C:206:SER:HA	1.98	0.45
1:C:100:THR:CB	1:C:241:GLU:HB2	2.46	0.45
1:C:114:PHE:N	1:C:115:PRO:HD3	2.30	0.45
1:A:179:VAL:HA	1:A:229:ASN:O	2.17	0.45
1:A:211:PRO:HD3	1:B:198:THR:O	2.17	0.45
1:A:225:LYS:C	1:A:226:LEU:HD22	2.37	0.45
1:C:204:VAL:HG13	1:C:204:VAL:O	2.17	0.45
1:C:187:SER:OG	1:C:188:TYR:HD1	1.99	0.45
1:B:238:TYR:HD2	1:B:239:THR:N	2.15	0.45
1:C:95:PRO:HG2	1:C:250:LEU:HB2	1.98	0.45
1:A:233:ILE:HG22	1:A:234:SER:N	2.30	0.44
1:B:130:ASN:O	1:B:131:ARG:HB2	2.17	0.44
1:B:159:THR:HG22	1:B:161:GLU:HB3	1.99	0.44
1:A:242:ASP:N	1:A:242:ASP:OD2	2.46	0.44
1:C:153:VAL:HA	1:C:244:THR:HG23	2.00	0.44
1:A:119:TRP:N	1:A:119:TRP:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CD1	1:A:177:ILE:HD12	2.52	0.44
1:A:208:TRP:O	1:A:209:PHE:HB3	2.18	0.44
1:B:180:VAL:HG13	1:B:195:LEU:O	2.17	0.44
1:B:150:TYR:CZ	1:B:247:GLY:HA3	2.52	0.44
1:B:175:ASP:N	1:B:175:ASP:OD2	2.51	0.44
1:C:154:THR:HA	1:C:211:PRO:HA	2.00	0.44
1:A:104:GLN:NE2	1:A:118:HIS:H	2.13	0.43
1:B:104:GLN:HA	1:B:118:HIS:CE1	2.53	0.43
1:C:126:ALA:O	1:C:127:PHE:HB3	2.18	0.43
1:A:104:GLN:HE22	1:A:117:LEU:HA	1.82	0.43
1:A:104:GLN:HE22	1:A:118:HIS:N	2.13	0.43
1:A:105:THR:HG23	1:A:106:PRO:HD2	1.99	0.43
1:B:97:ALA:HB2	1:B:132:MET:HG2	2.00	0.43
1:C:193:GLN:NE2	1:C:196:MET:HE3	2.34	0.43
1:A:195:LEU:HD11	1:A:216:ALA:HB3	2.01	0.43
1:C:150:TYR:HA	1:C:214:LEU:O	2.18	0.43
1:B:101:VAL:HG22	1:B:102:VAL:N	2.33	0.43
1:B:181:ILE:HG12	1:B:228:VAL:HG22	2.00	0.43
1:A:95:PRO:HB3	1:A:142:PRO:HG3	2.00	0.43
1:B:232:ASP:CG	1:B:235:LEU:HD13	2.39	0.43
1:A:162:CYS:HB3	1:A:172:ASN:CB	2.49	0.43
1:C:114:PHE:CE2	1:C:231:SER:HA	2.54	0.43
1:A:103:ARG:HB2	1:A:103:ARG:NH2	2.34	0.43
1:B:119:TRP:CD1	1:B:119:TRP:N	2.87	0.43
1:A:139:LEU:HA	1:A:139:LEU:HD12	1.91	0.43
1:A:195:LEU:HD13	1:A:218:PHE:HZ	1.84	0.42
1:A:152:GLN:HB3	1:A:245:PHE:CE1	2.54	0.42
1:C:112:ASN:CG	1:C:113:GLN:N	2.73	0.42
1:A:200:SER:HB3	1:C:209:PHE:CZ	2.55	0.42
1:B:95:PRO:CB	1:B:142:PRO:HG3	2.50	0.42
1:B:147:TYR:CZ	1:B:250:LEU:HD23	2.54	0.42
1:C:152:GLN:HA	1:C:212:ILE:O	2.19	0.42
1:A:123:LEU:O	1:A:126:ALA:HB3	2.19	0.42
1:B:222:GLU:HG3	1:B:223:GLY:N	2.35	0.42
1:C:152:GLN:HB2	1:C:213:TYR:HD1	1.85	0.42
1:B:190:GLU:OE1	1:B:190:GLU:HA	2.19	0.41
1:C:99:LEU:HB3	1:C:119:TRP:CB	2.49	0.41
1:C:154:THR:HG21	1:C:243:LYS:HE2	2.02	0.41
1:C:131:ARG:O	1:C:142:PRO:HB3	2.20	0.41
1:C:225:LYS:HB2	1:C:225:LYS:HE3	1.82	0.41
1:A:181:ILE:N	1:A:181:ILE:HD12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:LEU:HD11	1:C:226:LEU:HD21	2.02	0.41
1:C:156:ARG:HD3	1:C:235:LEU:O	2.20	0.41
1:A:185:THR:HG22	1:A:186:ASP:N	2.35	0.41
1:A:118:HIS:HB3	1:A:137:LYS:HG2	2.01	0.41
1:C:118:HIS:ND1	1:C:118:HIS:N	2.68	0.41
1:B:154:THR:HA	1:B:211:PRO:HA	2.03	0.41
1:B:238:TYR:N	1:B:238:TYR:HD2	2.18	0.41
1:B:182:THR:HG23	1:B:229:ASN:HD22	1.86	0.41
1:B:152:GLN:HE22	1:C:214:LEU:HD21	1.86	0.40
1:A:104:GLN:HA	1:A:118:HIS:HE1	1.84	0.40
1:C:159:THR:HB	1:C:205:GLY:O	2.21	0.40
1:B:114:PHE:HB3	1:B:229:ASN:HB3	2.02	0.40
1:B:190:GLU:HA	1:B:191:PRO:HD2	1.87	0.40
1:C:203:GLU:HG3	1:C:208:TRP:CB	2.50	0.40
1:A:96:ARG:HE	1:A:96:ARG:HB3	1.67	0.40
1:B:103:ARG:O	1:B:104:GLN:CB	2.67	0.40
1:C:94:LYS:CB	1:C:95:PRO:HD2	2.44	0.40
1:C:158:MET:HA	1:C:207:ASN:CB	2.51	0.40
1:C:193:GLN:HE22	1:C:196:MET:HE1	1.85	0.40
1:B:185:THR:OG1	1:B:186:ASP:N	2.54	0.40
1:A:130:ASN:N	1:A:130:ASN:HD22	2.18	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	149/180 (83%)	133 (89%)	10 (7%)	6 (4%)	4 21
1	B	149/180 (83%)	129 (87%)	15 (10%)	5 (3%)	5 25
1	C	148/180 (82%)	120 (81%)	20 (14%)	8 (5%)	2 14
All	All	446/540 (83%)	382 (86%)	45 (10%)	19 (4%)	3 19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	SER
1	A	187	SER
1	A	191	PRO
1	B	161	GLU
1	B	187	SER
1	C	111	LYS
1	C	203	GLU
1	C	204	VAL
1	A	103	ARG
1	A	209	PHE
1	B	108	GLN
1	B	239	THR
1	C	93	ASP
1	C	108	GLN
1	C	202	CYS
1	B	104	GLN
1	C	122	GLU
1	A	104	GLN
1	C	210	GLN

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	130/160 (81%)	117 (90%)	13 (10%)	9 34
1	B	127/160 (79%)	114 (90%)	13 (10%)	9 33
1	C	124/160 (78%)	115 (93%)	9 (7%)	17 52
All	All	381/480 (79%)	346 (91%)	35 (9%)	11 40

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	103	ARG

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Mol	Chain	Res	Type
1	A	108	GLN
1	A	109	HIS
1	A	119	TRP
1	A	120	GLU
1	A	128	THR
1	A	140	LEU
1	A	179	VAL
1	A	186	ASP
1	A	195	LEU
1	A	203	GLU
1	A	233	ILE
1	B	101	VAL
1	B	117	LEU
1	B	133	ASN
1	B	135	THR
1	B	136	ASN
1	B	175	ASP
1	B	176	SER
1	B	178	THR
1	B	182	THR
1	B	184	VAL
1	B	201	VAL
1	B	202	CYS
1	B	238	TYR
1	C	93	ASP
1	C	103	ARG
1	C	118	HIS
1	C	156	ARG
1	C	161	GLU
1	C	178	THR
1	C	179	VAL
1	C	186	ASP
1	C	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	108	GLN
1	A	118	HIS
1	A	130	ASN
1	A	221	GLN

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Mol	Chain	Res	Type
1	B	113	GLN
1	B	118	HIS
1	B	130	ASN
1	B	133	ASN
1	B	136	ASN
1	B	152	GLN
1	B	210	GLN
1	C	112	ASN
1	C	130	ASN
1	C	136	ASN
1	C	193	GLN
1	C	221	GLN
1	C	229	ASN

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	153/180 (85%)	0.04	7 (4%)	36	14	14, 39, 93, 113	0
1	B	153/180 (85%)	0.19	12 (7%)	16	6	16, 37, 100, 124	0
1	C	152/180 (84%)	0.39	11 (7%)	18	7	20, 56, 118, 153	0
All	All	458/540 (84%)	0.21	30 (6%)	22	7	14, 44, 98, 153	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	GLN	6.2
1	C	109	HIS	4.8
1	B	112	ASN	4.6
1	B	109	HIS	3.8
1	C	111	LYS	3.6
1	B	162	CYS	3.6
1	C	93	ASP	3.4
1	B	110	PHE	3.3
1	A	171	PRO	3.2
1	B	107	THR	3.2
1	B	189	PRO	3.1
1	A	188	TYR	3.1
1	C	112	ASN	3.0
1	C	110	PHE	2.9
1	A	170	ARG	2.9
1	B	108	GLN	2.8
1	B	170	ARG	2.8
1	A	186	ASP	2.7
1	A	189	PRO	2.7
1	A	172	ASN	2.6
1	B	160	SER	2.6
1	B	105	THR	2.5
1	B	171	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	160	SER	2.4
1	C	159	THR	2.3
1	C	135	THR	2.3
1	C	105	THR	2.2
1	C	106	PRO	2.2
1	C	188	TYR	2.2
1	B	93	ASP	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	271	1/1	0.97	0.32	10.25	6,6,6,6	0

6.5 Other polymers (i)

There are no such residues in this entry.