Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:37 PM GMT

PDB ID	:	4M7L
Title	:	Crystal structure of the complex between human tissue factor extracellular domain and antibody 10H10 FAB fragment
Authors	:	Teplyakov, A.; Obmolova, G.; Malia, T.; Gilliland, G.L.
Deposited on	:	2013-08-12
Resolution	:	3.40 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:

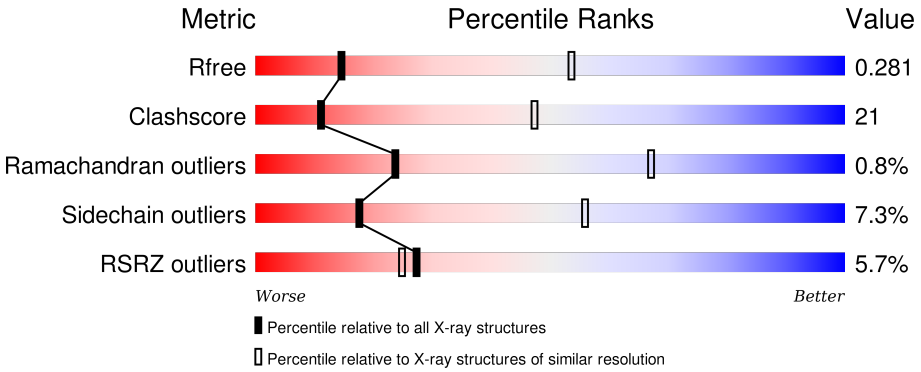
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	T	215	12% 69% 20% 10%
2	L	220	2% 53% 42% 5%
3	H	229	3% 51% 42%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4919 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 Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	194	Total	C	N	O	S	0	0	0
			1571	1000	254	312	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	214	HIS	-	EXPRESSION TAG	UNP P13726
T	215	HIS	-	EXPRESSION TAG	UNP P13726
T	216	HIS	-	EXPRESSION TAG	UNP P13726
T	217	HIS	-	EXPRESSION TAG	UNP P13726
T	218	HIS	-	EXPRESSION TAG	UNP P13726
T	219	HIS	-	EXPRESSION TAG	UNP P13726

- Molecule 2 is a protein called 10H10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	220	Total	C	N	O	S	0	0	0
			1692	1060	279	346	7			

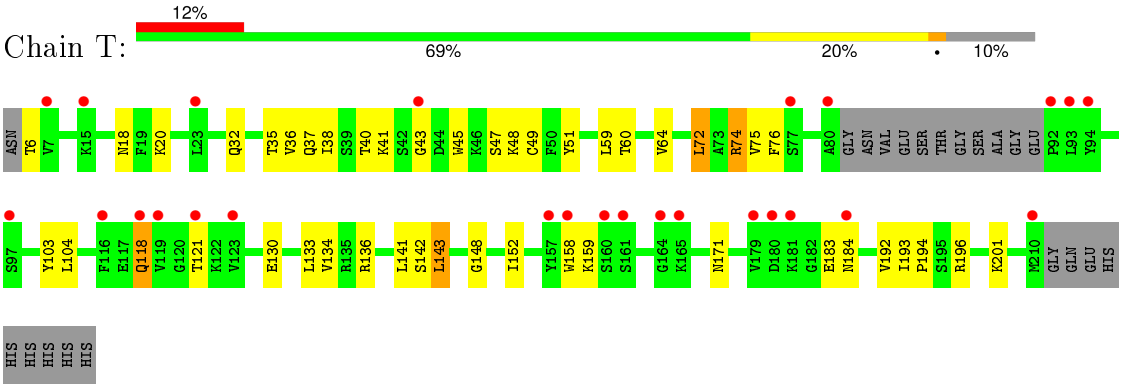
- Molecule 3 is a protein called 10H10 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	223	Total	C	N	O	S	0	0	0
			1656	1048	271	330	7			

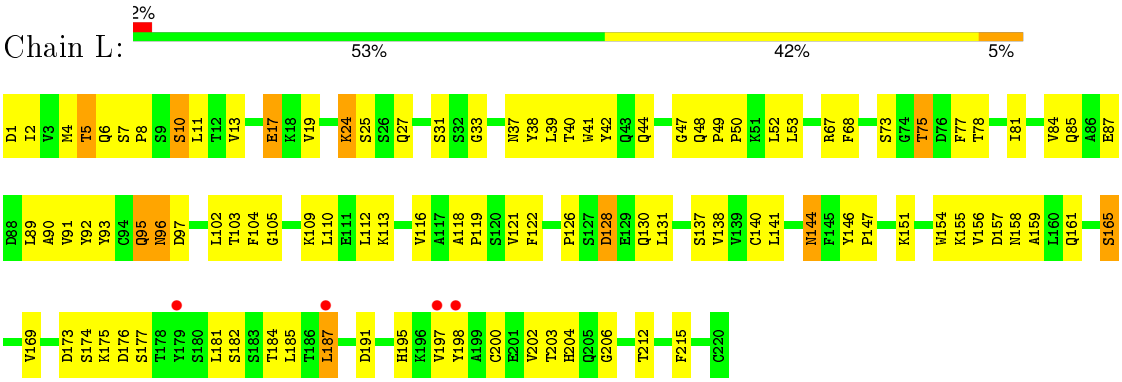
3 Residue-property plots (i)

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.

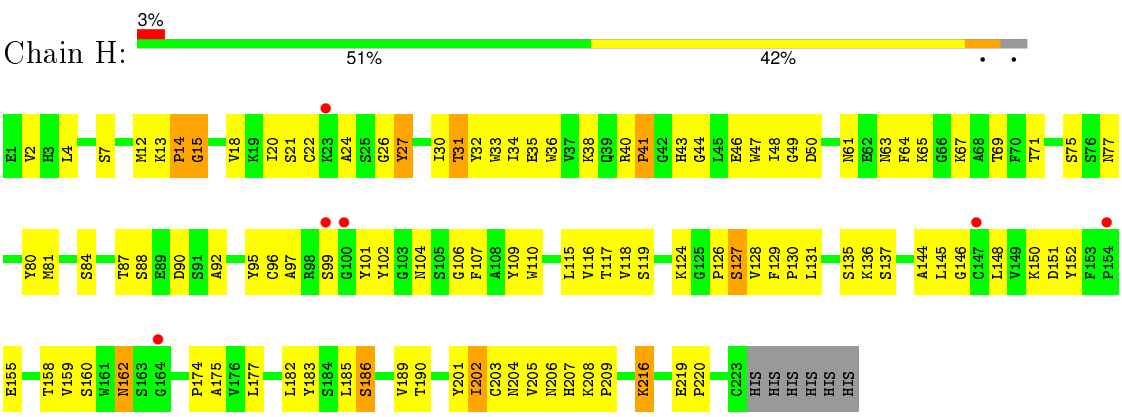
- Molecule 1: Tissue factor



- Molecule 2: 10H10 light chain



- Molecule 3: 10H10 heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	116.86Å 116.86Å 106.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 27.54 – 3.41	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-3.40) 96.9 (27.54-3.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.38Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.242 , 0.289 0.217 , 0.281	Depositor DCC
R_{free} test set	458 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	93.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.9	EDS
Estimated twinning fraction	0.029 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 9573 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4919	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: PCA

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	T	0.58	0/1606	0.68	0/2184
2	L	0.66	1/1728 (0.1%)	0.82	1/2349 (0.0%)
3	H	0.65	0/1693	0.81	0/2310
All	All	0.63	1/5027 (0.0%)	0.77	1/6843 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	154	TRP	CD2-CE2	5.78	1.48	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	187	LEU	CA-CB-CG	5.04	126.89	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	T	1571	0	1534	53	1
2	L	1692	0	1642	88	0
3	H	1656	0	1593	83	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4919	0	4769	201	1

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 21.

All (201) 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:T:159:LYS:CE	1:T:183:GLU:HB3	1.44	1.47
1:T:159:LYS:HE2	1:T:183:GLU:CB	1.72	1.17
1:T:159:LYS:HE3	1:T:183:GLU:HB3	1.27	1.12
1:T:159:LYS:HE2	1:T:183:GLU:HB3	1.14	1.08
1:T:159:LYS:CE	1:T:183:GLU:CB	2.33	1.03
1:T:159:LYS:HE2	1:T:183:GLU:CD	1.87	0.95
2:L:122:PHE:HD1	3:H:137:SER:HA	1.34	0.90
2:L:102:LEU:HB2	3:H:47:TRP:CD2	2.09	0.87
2:L:96:ASN:HB3	2:L:103:THR:OG1	1.75	0.86
1:T:159:LYS:HE2	1:T:183:GLU:CG	2.07	0.83
1:T:60:THR:HG21	1:T:133:LEU:HD22	1.61	0.82
3:H:126:PRO:HB3	3:H:152:TYR:HB3	1.60	0.82
2:L:130:GLN:HE22	2:L:137:SER:HB2	1.49	0.78
2:L:122:PHE:CD1	3:H:137:SER:HA	2.17	0.78
3:H:33:TRP:HB2	3:H:99:SER:HB3	1.63	0.77
1:T:159:LYS:CE	1:T:183:GLU:CD	2.52	0.77
2:L:67:ARG:HH11	2:L:67:ARG:HG3	1.49	0.76
3:H:175:ALA:HB2	3:H:185:LEU:HB3	1.68	0.76
1:T:64:VAL:HB	1:T:134:VAL:HA	1.69	0.75
2:L:67:ARG:CZ	2:L:85:GLN:HG3	2.18	0.73
2:L:11:LEU:HD21	2:L:110:LEU:HD12	1.70	0.73
1:T:104:LEU:HD12	3:H:30:ILE:HD12	1.71	0.73
1:T:36:VAL:O	1:T:47:SER:HA	1.90	0.72
1:T:104:LEU:CD1	3:H:30:ILE:HD12	2.22	0.70
1:T:159:LYS:HE2	1:T:183:GLU:OE2	1.92	0.69
3:H:64:PHE:O	3:H:65:LYS:C	2.30	0.68
3:H:92:ALA:O	3:H:115:LEU:HD12	1.96	0.66
1:T:45:TRP:CZ3	1:T:74:ARG:HG2	2.32	0.65
3:H:4:LEU:HD22	3:H:22:CYS:SG	2.37	0.65
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.32	0.65
2:L:67:ARG:HG3	2:L:67:ARG:NH1	2.11	0.65
2:L:165:SER:HA	2:L:184:THR:O	1.97	0.65
3:H:32:TYR:OH	3:H:101:TYR:HD1	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:148:GLY:HA3	3:H:104:ASN:OD1	1.96	0.64
2:L:173:ASP:OD1	2:L:175:LYS:N	2.29	0.64
2:L:146:TYR:CD1	2:L:147:PRO:HA	2.33	0.64
3:H:24:ALA:HB1	3:H:27:TYR:HE1	1.63	0.64
3:H:115:LEU:CD2	3:H:155:GLU:HB2	2.28	0.63
2:L:157:ASP:HA	2:L:197:VAL:HB	1.80	0.63
3:H:189:VAL:HG22	3:H:190:THR:O	1.98	0.63
2:L:156:VAL:HG23	2:L:161:GLN:HG3	1.82	0.62
3:H:148:LEU:HD12	3:H:186:SER:HB3	1.80	0.62
2:L:8:PRO:HB2	2:L:10:SER:O	2.00	0.62
2:L:204:HIS:HD2	2:L:206:GLY:H	1.47	0.62
1:T:45:TRP:CD1	1:T:74:ARG:NH1	2.68	0.61
3:H:32:TYR:HH	3:H:101:TYR:HD1	1.47	0.61
3:H:35:GLU:O	3:H:96:CYS:HA	2.01	0.61
2:L:102:LEU:HB2	3:H:47:TRP:CE2	2.35	0.61
3:H:160:SER:OG	3:H:204:ASN:HB2	2.00	0.61
3:H:35:GLU:OE1	3:H:50:ASP:HB3	2.00	0.61
1:T:159:LYS:NZ	1:T:183:GLU:CD	2.55	0.60
3:H:97:ALA:HB1	3:H:109:TYR:O	2.00	0.60
2:L:17:GLU:O	2:L:84:VAL:HG23	2.02	0.59
3:H:61:ASN:OD1	3:H:63:ASN:ND2	2.33	0.59
3:H:115:LEU:HD23	3:H:155:GLU:HB2	1.84	0.59
2:L:144:ASN:N	2:L:144:ASN:HD22	1.98	0.59
1:T:37:GLN:HA	1:T:47:SER:HA	1.83	0.59
2:L:140:CYS:O	2:L:182:SER:HA	2.03	0.59
2:L:39:LEU:HD13	2:L:40:THR:N	2.18	0.58
2:L:93:TYR:CE2	3:H:44:GLY:HA2	2.38	0.58
2:L:19:VAL:HG22	2:L:81:ILE:HB	1.85	0.58
3:H:12:MET:HG3	3:H:18:VAL:HB	1.85	0.57
2:L:137:SER:OG	3:H:150:LYS:HE3	2.05	0.57
2:L:39:LEU:HD22	2:L:40:THR:H	1.69	0.57
2:L:204:HIS:CD2	2:L:206:GLY:H	2.23	0.57
2:L:130:GLN:HE22	2:L:137:SER:CB	2.18	0.57
2:L:6:GLN:OE1	2:L:93:TYR:HA	2.05	0.57
2:L:50:PRO:HB2	3:H:110:TRP:CE2	2.40	0.56
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.87	0.56
3:H:40:ARG:HB3	3:H:43:HIS:CD2	2.41	0.55
1:T:20:LYS:HB2	1:T:133:LEU:HD13	1.87	0.55
3:H:67:LYS:HD2	3:H:84:SER:O	2.07	0.55
1:T:159:LYS:HE3	1:T:183:GLU:CB	2.15	0.54
1:T:45:TRP:CD1	1:T:74:ARG:CZ	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:90:ALA:HB3	2:L:92:TYR:CE1	2.42	0.54
1:T:6:THR:HB	1:T:32:GLN:OE1	2.07	0.54
2:L:169:VAL:HG22	2:L:181:LEU:HD12	1.90	0.54
1:T:159:LYS:CD	1:T:183:GLU:HB3	2.31	0.53
1:T:103:TYR:HB3	3:H:31:THR:CG2	2.38	0.53
3:H:64:PHE:O	3:H:67:LYS:N	2.39	0.53
2:L:38:TYR:CE1	3:H:104:ASN:HB2	2.43	0.53
1:T:45:TRP:NE1	1:T:74:ARG:CZ	2.72	0.53
1:T:37:GLN:HB2	1:T:74:ARG:HG3	1.91	0.53
2:L:37:ASN:HD21	2:L:73:SER:HB2	1.74	0.53
1:T:36:VAL:HG22	1:T:75:VAL:HG22	1.91	0.53
3:H:71:THR:OG1	3:H:80:TYR:HB2	2.08	0.53
2:L:49:PRO:HB3	3:H:95:TYR:CE1	2.44	0.53
3:H:148:LEU:CD1	3:H:186:SER:HB3	2.39	0.52
1:T:104:LEU:HG	3:H:31:THR:HG23	1.90	0.52
3:H:87:THR:O	3:H:118:VAL:HB	2.10	0.52
2:L:47:GLY:O	2:L:48:GLN:HG3	2.10	0.52
2:L:93:TYR:HE2	3:H:44:GLY:HA2	1.73	0.52
3:H:151:ASP:HA	3:H:182:LEU:HB3	1.91	0.52
2:L:144:ASN:N	2:L:144:ASN:ND2	2.57	0.52
2:L:157:ASP:OD1	2:L:195:HIS:HB3	2.10	0.52
2:L:173:ASP:O	2:L:177:SER:HA	2.09	0.51
1:T:38:ILE:HG13	1:T:72:LEU:O	2.09	0.51
2:L:41:TRP:O	2:L:53:LEU:HB2	2.11	0.51
1:T:152:ILE:HG12	1:T:171:ASN:HD22	1.75	0.51
2:L:68:PHE:CD2	2:L:81:ILE:HG12	2.46	0.51
2:L:198:TYR:HB2	2:L:215:PHE:CE1	2.45	0.51
1:T:159:LYS:HZ1	1:T:183:GLU:CD	2.13	0.51
1:T:60:THR:HG21	1:T:133:LEU:CD2	2.37	0.51
1:T:45:TRP:NE1	1:T:74:ARG:NH2	2.59	0.50
2:L:24:LYS:O	2:L:24:LYS:HG2	2.11	0.50
3:H:107:PHE:N	3:H:107:PHE:CD1	2.80	0.50
3:H:41:PRO:O	3:H:43:HIS:CD2	2.64	0.50
2:L:147:PRO:O	2:L:204:HIS:HE1	1.95	0.49
2:L:122:PHE:HD1	3:H:137:SER:CA	2.15	0.49
2:L:10:SER:HB2	2:L:109:LYS:HB3	1.94	0.49
2:L:47:GLY:O	2:L:48:GLN:CG	2.61	0.49
2:L:25:SER:OG	2:L:75:THR:HG22	2.13	0.49
3:H:107:PHE:HD1	3:H:107:PHE:N	2.10	0.49
3:H:7:SER:HB3	3:H:21:SER:OG	2.13	0.49
2:L:7:SER:HA	2:L:8:PRO:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:21:SER:HB3	3:H:80:TYR:CE1	2.48	0.48
3:H:69:THR:O	3:H:81:MET:HA	2.13	0.48
1:T:74:ARG:HD3	1:T:76:PHE:CE2	2.48	0.48
3:H:130:PRO:HD3	3:H:216:LYS:HD3	1.95	0.48
2:L:4:MET:HB2	2:L:105:GLY:HA2	1.95	0.48
2:L:155:LYS:HA	2:L:159:ALA:O	2.14	0.48
2:L:91:VAL:HG22	2:L:109:LYS:HA	1.95	0.48
1:T:192:VAL:HG22	1:T:201:LYS:HG3	1.96	0.48
2:L:42:TYR:O	2:L:92:TYR:HA	2.14	0.48
2:L:102:LEU:HB2	3:H:47:TRP:CE3	2.48	0.48
2:L:156:VAL:HB	2:L:161:GLN:NE2	2.28	0.48
2:L:44:GLN:NE2	2:L:50:PRO:HD3	2.29	0.48
3:H:158:THR:O	3:H:205:VAL:HA	2.14	0.48
2:L:87:GLU:HG2	2:L:87:GLU:H	1.41	0.47
2:L:95:GLN:HB2	2:L:104:PHE:CE1	2.50	0.47
3:H:151:ASP:HB3	3:H:182:LEU:HD13	1.95	0.47
3:H:208:LYS:N	3:H:209:PRO:HD2	2.30	0.47
2:L:128:ASP:HA	2:L:131:LEU:HD12	1.97	0.47
2:L:25:SER:O	2:L:75:THR:HG22	2.14	0.47
2:L:151:LYS:HB3	2:L:203:THR:HB	1.97	0.47
1:T:159:LYS:HG2	1:T:184:ASN:O	2.14	0.47
3:H:131:LEU:HB2	3:H:146:GLY:H	1.79	0.47
3:H:24:ALA:HB1	3:H:27:TYR:CE1	2.48	0.46
3:H:36:TRP:HB3	3:H:48:ILE:HD12	1.97	0.46
2:L:67:ARG:NH2	2:L:85:GLN:HG3	2.30	0.46
2:L:138:VAL:HB	2:L:185:LEU:HB3	1.98	0.46
3:H:177:LEU:HG	3:H:183:TYR:CE2	2.50	0.46
1:T:38:ILE:HD12	1:T:59:LEU:HD13	1.98	0.46
3:H:206:ASN:OD1	3:H:207:HIS:N	2.49	0.46
3:H:201:TYR:C	3:H:202:ILE:HG13	2.37	0.46
1:T:159:LYS:HD3	1:T:184:ASN:N	2.30	0.45
2:L:89:LEU:HD12	2:L:112:LEU:HD13	1.98	0.45
3:H:159:VAL:HG13	3:H:203:CYS:HB2	1.98	0.45
2:L:68:PHE:HD2	2:L:81:ILE:HG12	1.81	0.45
2:L:77:PHE:O	2:L:78:THR:OG1	2.33	0.45
2:L:121:VAL:HG21	2:L:202:VAL:HG21	1.98	0.45
3:H:127:SER:HB3	3:H:129:PHE:CZ	2.52	0.45
2:L:130:GLN:NE2	2:L:137:SER:HB2	2.27	0.44
3:H:13:LYS:O	3:H:15:GLY:N	2.49	0.44
1:T:35:THR:HG23	1:T:49:CYS:O	2.16	0.44
2:L:122:PHE:CD1	3:H:137:SER:CA	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:103:TYR:O	1:T:196:ARG:NH2	2.50	0.44
1:T:136:ARG:HB3	1:T:141:LEU:HD11	2.00	0.44
1:T:40:THR:O	1:T:41:LYS:HB3	2.18	0.44
1:T:18:ASN:ND2	1:T:130:GLU:OE1	2.51	0.44
2:L:5:THR:OG1	2:L:24:LYS:HE3	2.18	0.43
1:T:104:LEU:HD12	3:H:30:ILE:CD1	2.45	0.43
2:L:44:GLN:HE21	2:L:50:PRO:HD3	1.82	0.43
2:L:52:LEU:HB2	3:H:107:PHE:O	2.19	0.43
1:T:159:LYS:CE	1:T:183:GLU:CG	2.81	0.43
3:H:144:ALA:HB2	3:H:190:THR:HG22	1.99	0.43
2:L:31:SER:O	2:L:33:GLY:N	2.52	0.43
1:T:159:LYS:CE	1:T:183:GLU:OE2	2.64	0.42
3:H:126:PRO:CB	3:H:152:TYR:HB3	2.38	0.42
3:H:38:LYS:HD3	3:H:40:ARG:HD2	2.01	0.42
2:L:87:GLU:HA	2:L:174:SER:O	2.19	0.42
1:T:142:SER:O	1:T:143:LEU:C	2.58	0.42
1:T:48:LYS:HA	1:T:48:LYS:HD2	1.85	0.42
3:H:219:GLU:HA	3:H:220:PRO:HD3	1.66	0.42
3:H:27:TYR:HE2	3:H:32:TYR:HB2	1.84	0.42
2:L:122:PHE:HD2	2:L:141:LEU:HG	1.85	0.42
2:L:87:GLU:C	2:L:89:LEU:H	2.23	0.42
3:H:4:LEU:CD1	3:H:97:ALA:HA	2.49	0.42
2:L:47:GLY:C	2:L:48:GLN:HG3	2.40	0.42
1:T:152:ILE:HD12	1:T:194:PRO:HG2	2.02	0.42
2:L:138:VAL:O	2:L:185:LEU:N	2.53	0.42
2:L:118:ALA:HA	2:L:119:PRO:HD2	1.91	0.41
3:H:128:VAL:O	3:H:216:LYS:HD2	2.20	0.41
3:H:92:ALA:O	3:H:116:VAL:N	2.42	0.41
3:H:87:THR:H	3:H:90:ASP:HB2	1.85	0.41
3:H:162:ASN:OD1	3:H:201:TYR:HA	2.20	0.41
2:L:40:THR:HG22	2:L:41:TRP:N	2.35	0.41
2:L:91:VAL:HG12	2:L:93:TYR:CE1	2.56	0.41
2:L:13:VAL:O	2:L:112:LEU:HA	2.20	0.41
3:H:14:PRO:HD3	3:H:119:SER:C	2.41	0.41
2:L:97:ASP:OD2	3:H:106:GLY:HA2	2.20	0.41
1:T:118:GLN:HB3	1:T:118:GLN:HE21	1.66	0.41
3:H:97:ALA:CB	3:H:109:TYR:O	2.67	0.41
2:L:200:CYS:O	2:L:212:THR:HA	2.20	0.41
2:L:19:VAL:CG2	2:L:81:ILE:HB	2.51	0.41
2:L:176:ASP:C	2:L:176:ASP:OD1	2.59	0.41
3:H:33:TRP:N	3:H:99:SER:OG	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:45:TRP:CE3	1:T:74:ARG:HG2	2.56	0.40
2:L:215:PHE:HA	3:H:136:LYS:NZ	2.37	0.40
1:T:136:ARG:HD2	3:H:102:TYR:CZ	2.56	0.40
2:L:126:PRO:HD3	2:L:137:SER:O	2.22	0.40

All (1) 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:T:51:TYR:OH	3:H:135:SER:N[2_555]	2.10	0.10

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	T	190/215 (88%)	178 (94%)	11 (6%)	1 (0%)	34 75
2	L	218/220 (99%)	192 (88%)	26 (12%)	0	100 100
3	H	221/229 (96%)	185 (84%)	32 (14%)	4 (2%)	11 50
All	All	629/664 (95%)	555 (88%)	69 (11%)	5 (1%)	24 67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	43	GLY
3	H	14	PRO
3	H	174	PRO
3	H	15	GLY
3	H	41	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	T	182/198 (92%)	175 (96%)	7 (4%)	40	76
2	L	194/195 (100%)	176 (91%)	18 (9%)	11	42
3	H	183/190 (96%)	167 (91%)	16 (9%)	13	47
All	All	559/583 (96%)	518 (93%)	41 (7%)	17	56

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	72	LEU
1	T	74	ARG
1	T	118	GLN
1	T	121	THR
1	T	143	LEU
1	T	158	TRP
1	T	193	ILE
2	L	1	ASP
2	L	2	ILE
2	L	5	THR
2	L	10	SER
2	L	17	GLU
2	L	24	LYS
2	L	27	GLN
2	L	75	THR
2	L	95	GLN
2	L	96	ASN
2	L	113	LYS
2	L	116	VAL
2	L	128	ASP
2	L	144	ASN
2	L	158	ASN
2	L	165	SER
2	L	187	LEU
2	L	191	ASP
3	H	20	ILE

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Mol	Chain	Res	Type
3	H	27	TYR
3	H	31	THR
3	H	34	ILE
3	H	46	GLU
3	H	75	SER
3	H	77	ASN
3	H	88	SER
3	H	117	THR
3	H	124	LYS
3	H	127	SER
3	H	145	LEU
3	H	162	ASN
3	H	186	SER
3	H	202	ILE
3	H	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	37	GLN
1	T	96	ASN
1	T	107	ASN
1	T	118	GLN
1	T	171	ASN
1	T	184	ASN
2	L	27	GLN
2	L	130	GLN
2	L	144	ASN
2	L	204	HIS
3	H	5	GLN
3	H	43	HIS
3	H	77	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PCA	H	1	3	7,8,9	0.87	1 (14%)	9,10,12	1.08	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	PCA	CA-N	-2.02	1.44	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	PCA	CB-CA-C	-2.34	109.56	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates 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	T	194/215 (90%)	0.75	26 (13%) 4 4	75, 120, 196, 255	0
2	L	220/220 (100%)	-0.11	4 (1%) 71 65	54, 82, 126, 165	0
3	H	222/229 (96%)	-0.05	6 (2%) 58 53	56, 92, 119, 146	0
All	All	636/664 (95%)	0.17	36 (5%) 27 25	54, 97, 165, 255	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	93	LEU	8.2
1	T	164	GLY	6.6
1	T	92	PRO	6.2
1	T	179	VAL	6.0
1	T	116	PHE	4.3
1	T	181	LYS	4.2
1	T	121	THR	3.3
2	L	187	LEU	3.3
2	L	198	TYR	3.2
1	T	77	SER	3.1
1	T	180	ASP	2.9
1	T	165	LYS	2.8
1	T	160	SER	2.8
3	H	99	SER	2.7
1	T	157	TYR	2.6
1	T	80	ALA	2.6
1	T	7	VAL	2.6
1	T	158	TRP	2.6
1	T	23	LEU	2.5
1	T	119	VAL	2.4
2	L	197	VAL	2.3
1	T	118	GLN	2.3
3	H	164	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	T	184	ASN	2.3
1	T	94	TYR	2.3
3	H	147	CYS	2.2
3	H	100	GLY	2.2
3	H	154	PRO	2.2
1	T	97	SER	2.2
1	T	15	LYS	2.1
1	T	210	MET	2.1
2	L	179	TYR	2.1
1	T	123	VAL	2.1
3	H	23	LYS	2.1
1	T	43	GLY	2.1
1	T	161	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	PCA	H	1	8/9	0.86	0.23	-	68,87,104,106	0

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.