Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:37 PM GMT

PDB ID	:	3RIU
Title	:	Crystal structure of Drosophila hexameric C3PO formed by truncated Translin and Trax
Authors	:	Tian, Y.; Simanshu, D.K.; Patel, D.J.
Deposited on	:	2011-04-14
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 (i)) were used in the production of this report:

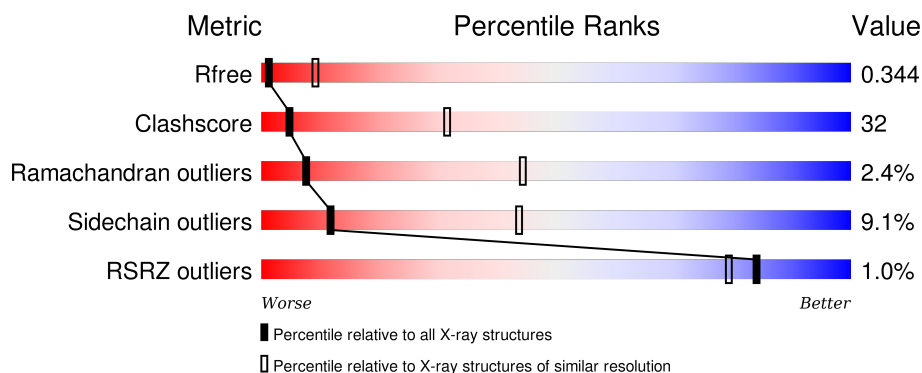|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	Percentile Ranks	Value
Rfree		0.344
Clashscore		32
Ramachandran outliers		2.4%
Sidechain outliers		9.1%
RSRZ outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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	A	218	58% 34% • 6%
1	B	218	46% 42% 6% 7%
2	C	269	2% 25% 38% 9% 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4722 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 Translin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	Se	0	0	0
			1610	1030	270	306	2	2			
1	B	203	Total	C	N	O	S	Se	0	0	0
			1611	1032	268	307	2	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	0	SER	-	EXPRESSION TAG	UNP Q7JVK6

- Molecule 2 is a protein called Translin associated factor X, isoform B.

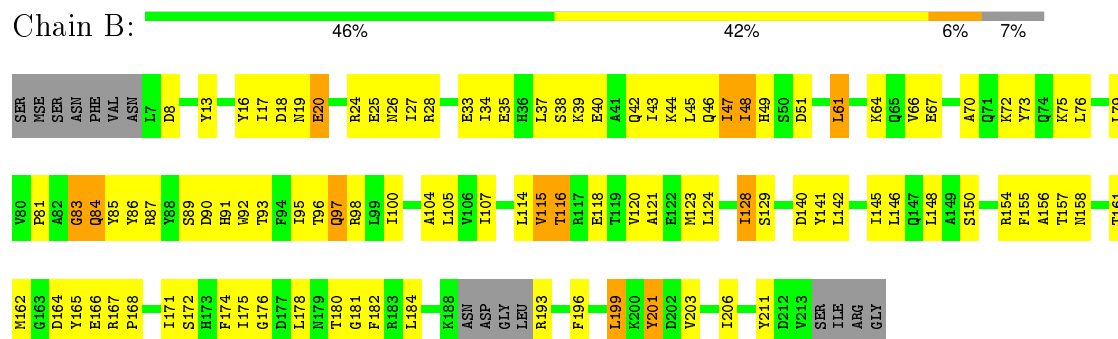| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	190	Total	C	N	O	S	Se	0	0	0
			1501	955	265	270	6	5			

3 Residue-property plots ⓘ

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: Translin

Chain A:

- Molecule 1: Translin

Chain B:
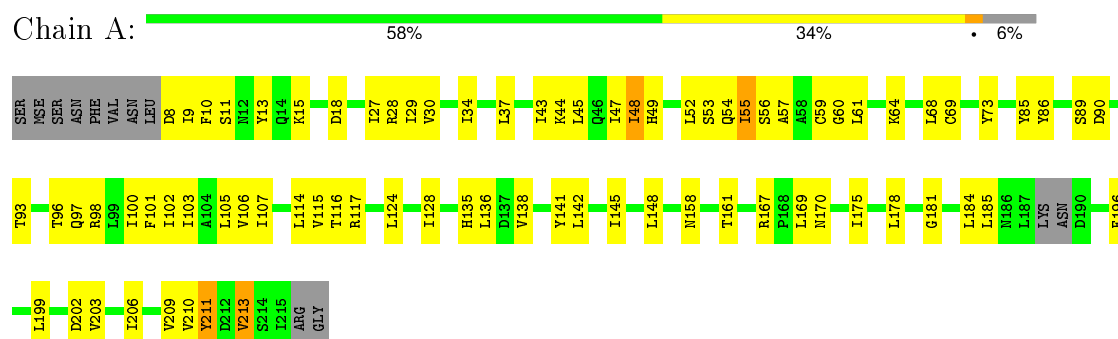
- Molecule 2: Translin associated factor X, isoform B

Chain C:

GLY ASP THR D223 T224 C225 T228 C229 L232 Y236 S237 G238 Y239 I240 S241 L242 N243 C244 GLN ARG ALA ARG E249 L250 W251 R252 K253 I254 T255 T256 M257 K258 Q259 S260 V261 L262 K263 A264 V267 C268 Y269 N270 V271 K272 V273 ARG GLY GLU ALA ALA LYS TRP GLY ALA THR
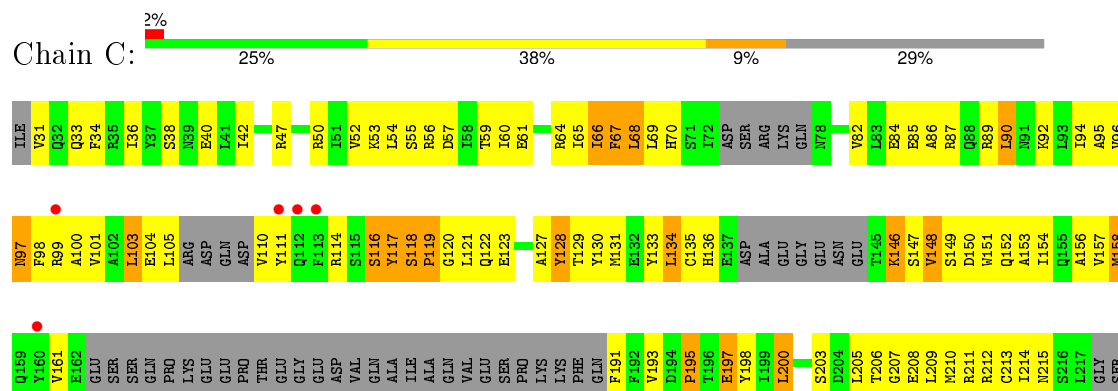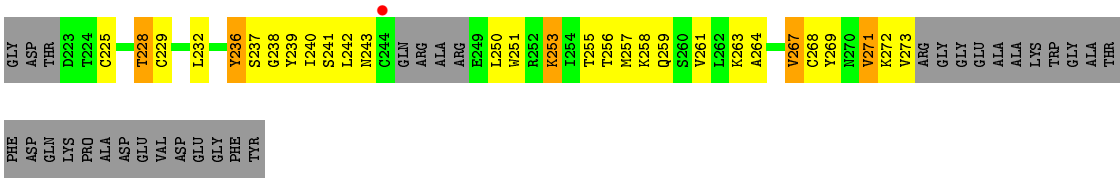
PHE ASP GLN LYS PRO ALA ASP GLU VAL ASP GLU GLY PHE TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	196.03Å 196.03Å 155.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.40 40.94 – 3.21	Depositor EDS
% Data completeness (in resolution range)	79.7 (19.88-3.40) 68.1 (40.94-3.21)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.271 , 0.338 0.272 , 0.344	Depositor DCC
R_{free} test set	1009 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.35, < L^2 > = 0.18$	Xtriage
Outliers	1 of 20056 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	4722	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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 (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 RMSZ	Bond lengths #$|Z|$>5	Bond angles RMSZ	Bond angles #$|Z|$>5
1	A	0.25	0/1634	0.41	0/2212
1	B	0.35	0/1636	0.53	0/2213
2	C	0.29	0/1512	0.46	0/2022
All	All	0.30	0/4782	0.47	0/6447

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 (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	1610	0	1551	68	0
1	B	1611	0	1555	94	0
2	C	1501	0	1497	147	0
All	All	4722	0	4603	296	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 (296) 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:C:114:ARG:HG2	2:C:117:TYR:CE2	1.60	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:SER:CB	2:C:119:PRO:CD	2.30	1.10
2:C:147:SER:HA	2:C:148:VAL:HG23	1.37	1.04
2:C:118:SER:CB	2:C:119:PRO:HD2	1.91	1.00
2:C:114:ARG:CG	2:C:117:TYR:CE2	2.45	0.99
1:B:51:ASP:HA	1:B:162:MSE:HE1	1.48	0.92
2:C:114:ARG:HG2	2:C:117:TYR:HE2	1.08	0.90
2:C:98:PHE:HD1	2:C:161:VAL:HG13	1.36	0.89
1:B:92:TRP:O	1:B:96:THR:HG23	1.72	0.88
1:A:45:LEU:HD13	1:A:105:LEU:HD23	1.55	0.87
1:B:27:ILE:HG23	1:B:76:LEU:HD11	1.56	0.86
2:C:195:PRO:HD2	2:C:197:GLU:HG2	1.59	0.83
1:B:73:TYR:OH	1:B:96:THR:HG22	1.76	0.83
1:B:49:HIS:CE1	1:B:154:ARG:HG2	2.13	0.82
1:A:100:ILE:HD13	1:A:141:TYR:HA	1.61	0.81
2:C:131:MSE:O	2:C:135:CYS:HB2	1.79	0.80
2:C:50:ARG:HD2	2:C:103:LEU:HD13	1.64	0.80
1:B:44:LYS:O	1:B:47:ILE:HG22	1.82	0.79
1:B:45:LEU:HA	1:B:48:ILE:HG23	1.65	0.78
2:C:146:LYS:HB2	2:C:148:VAL:HA	1.66	0.76
2:C:118:SER:CB	2:C:119:PRO:HD3	2.14	0.76
1:B:100:ILE:HD13	1:B:141:TYR:HA	1.68	0.75
2:C:98:PHE:CD1	2:C:161:VAL:HG13	2.23	0.74
1:A:117:ARG:HD2	1:A:128:ILE:HG23	1.68	0.73
2:C:52:VAL:O	2:C:56:ARG:HG3	1.89	0.73
1:B:193:ARG:HA	1:B:196:PHE:CE2	2.23	0.73
1:A:141:TYR:HD2	1:A:142:LEU:HD23	1.53	0.73
1:B:114:LEU:HD23	1:B:114:LEU:H	1.54	0.73
1:A:107:ILE:HD13	1:A:114:LEU:HA	1.71	0.71
2:C:111:TYR:HA	2:C:114:ARG:HG3	1.73	0.70
2:C:116:SER:C	2:C:118:SER:H	1.95	0.70
2:C:33:GLN:O	2:C:36:ILE:HG22	1.90	0.70
2:C:114:ARG:CG	2:C:117:TYR:HE2	1.94	0.69
1:B:49:HIS:CE1	1:B:155:PHE:HA	2.28	0.68
2:C:97:ASN:O	2:C:101:VAL:HG12	1.94	0.68
2:C:84:GLU:O	2:C:87:ARG:HG2	1.94	0.68
2:C:239:TYR:CD1	2:C:257:MSE:HE1	2.28	0.68
2:C:203:SER:HA	2:C:206:THR:HG23	1.77	0.67
1:B:193:ARG:HA	1:B:196:PHE:HE2	1.60	0.67
1:B:45:LEU:O	1:B:48:ILE:HG12	1.93	0.67
1:B:45:LEU:HD23	1:B:105:LEU:HD12	1.75	0.66
1:A:37:LEU:HD21	1:A:68:LEU:HD23	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TYR:CD2	1:A:142:LEU:HD23	2.30	0.66
1:B:35:GLU:HG2	1:B:39:LYS:HE3	1.77	0.65
1:B:42:GLN:NE2	2:C:240:ILE:HD11	2.10	0.65
2:C:147:SER:CA	2:C:148:VAL:HG23	2.20	0.65
2:C:116:SER:O	2:C:118:SER:N	2.30	0.65
1:B:13:TYR:O	1:B:17:ILE:HG23	1.96	0.65
2:C:89:ARG:O	2:C:92:LYS:HG2	1.97	0.64
2:C:66:ILE:HG22	2:C:127:ALA:HB2	1.79	0.64
2:C:114:ARG:HB3	2:C:117:TYR:CD2	2.32	0.64
2:C:129:THR:CG2	2:C:205:LEU:HG	2.27	0.64
1:B:34:ILE:HD11	1:B:72:LYS:HB3	1.79	0.64
2:C:118:SER:O	2:C:120:GLY:N	2.30	0.64
1:A:116:THR:HA	1:A:141:TYR:OH	1.98	0.64
1:A:98:ARG:O	1:A:102:ILE:HG12	1.98	0.64
1:B:174:PHE:CD2	1:B:175:ILE:HD12	2.33	0.63
1:B:199:LEU:HD12	1:B:199:LEU:C	2.20	0.63
1:B:49:HIS:HE1	1:B:155:PHE:HA	1.63	0.63
2:C:67:PHE:HA	2:C:70:HIS:HD2	1.64	0.62
1:A:10:PHE:HA	1:A:13:TYR:CD2	2.34	0.62
2:C:114:ARG:CB	2:C:117:TYR:CD2	2.82	0.62
2:C:65:ILE:CD1	2:C:90:LEU:HD12	2.30	0.62
2:C:158:MSE:HA	2:C:158:MSE:HE2	1.80	0.62
1:A:184:LEU:HD21	2:C:34:PHE:HB2	1.81	0.62
2:C:60:ILE:O	2:C:64:ARG:HG3	2.00	0.62
2:C:129:THR:HG22	2:C:205:LEU:HG	1.82	0.61
1:B:199:LEU:O	1:B:203:VAL:HG23	1.99	0.61
1:B:96:THR:O	1:B:100:ILE:HG13	2.00	0.61
2:C:94:ILE:HG23	2:C:158:MSE:CE	2.30	0.61
2:C:57:ASP:O	2:C:61:GLU:HB2	1.99	0.61
2:C:130:TYR:CZ	2:C:134:LEU:HD23	2.34	0.61
1:B:174:PHE:HD2	1:B:175:ILE:HD12	1.64	0.60
1:A:184:LEU:HD11	2:C:34:PHE:HB3	1.83	0.60
1:A:44:LYS:O	1:A:47:ILE:HB	2.01	0.60
2:C:111:TYR:HA	2:C:114:ARG:CG	2.31	0.60
2:C:65:ILE:HD12	2:C:90:LEU:HD12	1.83	0.60
1:B:17:ILE:HG13	1:B:18:ASP:N	2.16	0.60
1:A:8:ASP:OD1	2:C:146:LYS:HA	2.01	0.60
1:B:49:HIS:CD2	1:B:154:ARG:HE	2.18	0.60
2:C:90:LEU:HD21	2:C:128:TYR:HA	1.84	0.60
1:B:66:VAL:HG11	1:B:123:MSE:HE2	1.83	0.60
2:C:101:VAL:HG21	2:C:191:PHE:O	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:O	1:B:46:GLN:HB2	2.02	0.59
1:A:181:GLY:O	2:C:34:PHE:HD1	1.84	0.59
1:A:211:TYR:O	1:A:211:TYR:HD1	1.84	0.59
1:A:103:ILE:O	1:A:107:ILE:HG13	2.03	0.59
2:C:259:GLN:O	2:C:263:LYS:HG3	2.03	0.58
2:C:68:LEU:HD23	2:C:69:LEU:N	2.19	0.58
2:C:130:TYR:OH	2:C:212:ARG:HB2	2.04	0.58
1:B:83:GLY:O	1:B:85:TYR:N	2.36	0.58
1:B:20:GLU:OE2	1:B:87:ARG:HD2	2.05	0.57
1:B:39:LYS:O	1:B:43:ILE:HG23	2.04	0.57
1:A:49:HIS:HB3	1:A:158:ASN:ND2	2.20	0.57
1:A:60:GLY:O	1:A:64:LYS:HB2	2.05	0.57
2:C:111:TYR:HD1	2:C:114:ARG:HD2	1.70	0.57
1:A:211:TYR:HD1	1:A:211:TYR:C	2.08	0.56
1:B:39:LYS:NZ	2:C:243:ASN:HA	2.20	0.56
1:A:206:ILE:O	1:A:210:VAL:HG23	2.06	0.56
2:C:213:CYS:HB2	2:C:228:THR:HG21	1.87	0.56
2:C:31:VAL:HG23	2:C:33:GLN:H	1.70	0.56
2:C:263:LYS:O	2:C:267:VAL:HG13	2.05	0.56
2:C:114:ARG:CB	2:C:117:TYR:CE2	2.88	0.56
1:B:171:ILE:HG22	1:B:206:ILE:HD13	1.87	0.56
1:A:57:ALA:O	1:A:61:LEU:HD13	2.05	0.56
1:B:25:GLU:HA	1:B:28:ARG:HD2	1.86	0.56
2:C:119:PRO:O	2:C:123:GLU:N	2.33	0.55
1:B:142:LEU:HD22	1:B:182:PHE:CE1	2.41	0.55
1:A:100:ILE:HD11	1:A:136:LEU:HD11	1.87	0.55
1:B:39:LYS:HZ1	2:C:243:ASN:HA	1.70	0.55
2:C:118:SER:O	2:C:119:PRO:C	2.45	0.55
2:C:130:TYR:HA	2:C:205:LEU:HD21	1.87	0.55
1:A:185:LEU:HD23	2:C:38:SER:HB2	1.88	0.55
1:B:45:LEU:CD2	1:B:105:LEU:HD12	2.36	0.55
2:C:38:SER:O	2:C:42:ILE:HG13	2.06	0.55
1:A:181:GLY:O	1:A:184:LEU:HG	2.07	0.55
2:C:232:LEU:HB3	2:C:261:VAL:HG22	1.88	0.55
2:C:104:GLU:C	2:C:105:LEU:HD12	2.28	0.55
2:C:207:GLY:O	2:C:211:ARG:HG3	2.07	0.55
2:C:237:SER:O	2:C:241:SER:HB3	2.07	0.55
1:B:73:TYR:CZ	1:B:96:THR:HG22	2.41	0.54
1:B:81:PRO:HG2	1:B:84:GLN:HG3	1.88	0.54
1:A:27:ILE:HD12	1:A:28:ARG:N	2.23	0.54
2:C:84:GLU:HA	2:C:87:ARG:CD	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HG22	1:A:115:VAL:HG21	1.89	0.54
1:A:34:ILE:HD13	1:A:73:TYR:CE1	2.43	0.54
1:B:114:LEU:H	1:B:114:LEU:CD2	2.19	0.54
1:B:40:GLU:O	1:B:43:ILE:HG12	2.07	0.54
2:C:116:SER:C	2:C:118:SER:N	2.60	0.54
1:B:104:ALA:HA	1:B:115:VAL:HG22	1.90	0.54
1:A:211:TYR:C	1:A:211:TYR:CD1	2.79	0.54
2:C:111:TYR:CD1	2:C:114:ARG:HD2	2.43	0.53
2:C:36:ILE:O	2:C:40:GLU:HB2	2.09	0.53
2:C:119:PRO:O	2:C:123:GLU:HB2	2.09	0.53
1:B:145:ILE:O	1:B:148:LEU:HB3	2.09	0.53
1:A:59:CYS:SG	1:A:106:VAL:HG13	2.49	0.53
1:B:34:ILE:HD11	1:B:72:LYS:CB	2.38	0.53
2:C:130:TYR:O	2:C:134:LEU:HG	2.08	0.53
1:B:97:GLN:NE2	1:B:140:ASP:HA	2.23	0.53
1:B:61:LEU:O	1:B:64:LYS:HG2	2.09	0.53
1:B:142:LEU:HD23	1:B:145:ILE:HD11	1.91	0.52
2:C:211:ARG:O	2:C:214:ILE:HG22	2.08	0.52
2:C:212:ARG:O	2:C:215:ASN:HB2	2.10	0.52
2:C:47:ARG:HH22	2:C:105:LEU:HD13	1.74	0.52
1:A:175:ILE:HG23	1:A:203:VAL:HG22	1.92	0.52
2:C:50:ARG:O	2:C:53:LYS:HB2	2.09	0.52
1:A:107:ILE:CD1	1:A:114:LEU:HA	2.37	0.52
1:B:128:ILE:C	1:B:128:ILE:HD13	2.30	0.52
2:C:95:ALA:O	2:C:98:PHE:HB3	2.10	0.52
1:A:184:LEU:HD12	1:A:184:LEU:C	2.30	0.52
1:B:83:GLY:C	1:B:85:TYR:H	2.12	0.52
2:C:114:ARG:O	2:C:117:TYR:HB2	2.10	0.51
1:A:145:ILE:O	1:A:148:LEU:HB3	2.11	0.51
1:B:95:ILE:O	1:B:98:ARG:HB3	2.10	0.51
1:A:10:PHE:CD1	1:A:13:TYR:HD2	2.29	0.51
1:B:34:ILE:HG21	1:B:73:TYR:HE1	1.75	0.51
1:B:35:GLU:HB2	1:B:95:ILE:HD11	1.92	0.51
1:B:100:ILE:HD13	1:B:141:TYR:CA	2.40	0.51
1:B:73:TYR:OH	1:B:96:THR:CG2	2.54	0.51
1:A:114:LEU:HD13	1:A:178:LEU:HD21	1.93	0.51
2:C:103:LEU:H	2:C:103:LEU:HD23	1.76	0.51
1:B:33:GLU:O	1:B:37:LEU:HD13	2.11	0.51
1:B:193:ARG:HA	1:B:196:PHE:CD2	2.46	0.50
2:C:131:MSE:O	2:C:135:CYS:CB	2.56	0.50
2:C:101:VAL:O	2:C:104:GLU:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:HA	1:B:89:SER:HB2	1.93	0.50
2:C:117:TYR:O	2:C:118:SER:O	2.30	0.50
2:C:31:VAL:HG23	2:C:33:GLN:HB2	1.93	0.50
1:B:172:SER:HB2	1:B:206:ILE:HG22	1.94	0.50
2:C:151:TRP:HB3	2:C:198:TYR:CB	2.42	0.50
2:C:271:VAL:O	2:C:273:VAL:N	2.45	0.49
1:B:107:ILE:HG12	1:B:115:VAL:CG1	2.42	0.49
2:C:82:VAL:O	2:C:86:ALA:CB	2.60	0.49
1:A:199:LEU:O	1:A:203:VAL:HG23	2.12	0.49
1:A:48:ILE:HG13	1:A:48:ILE:O	2.12	0.49
1:B:167:ARG:HB2	1:B:168:PRO:HD3	1.94	0.49
1:A:101:PHE:HE1	1:A:148:LEU:HA	1.78	0.49
2:C:55:SER:O	2:C:59:THR:HG22	2.12	0.49
2:C:128:TYR:O	2:C:131:MSE:HB3	2.13	0.49
1:B:8:ASP:N	1:B:8:ASP:OD1	2.45	0.49
2:C:114:ARG:HA	2:C:117:TYR:CD2	2.49	0.48
1:A:107:ILE:HG12	1:A:115:VAL:HG13	1.95	0.48
2:C:94:ILE:HG23	2:C:158:MSE:HE1	1.95	0.48
1:B:89:SER:O	1:B:93:THR:HG23	2.13	0.48
1:A:85:TYR:O	1:A:89:SER:HB3	2.13	0.48
2:C:52:VAL:HG12	2:C:56:ARG:HE	1.77	0.48
2:C:34:PHE:N	2:C:34:PHE:CD2	2.81	0.48
1:B:156:ALA:HB2	1:B:171:ILE:HD12	1.95	0.48
1:A:209:VAL:O	1:A:213:VAL:HG23	2.14	0.48
2:C:130:TYR:CE1	2:C:134:LEU:HD23	2.48	0.48
1:B:92:TRP:O	1:B:96:THR:CG2	2.54	0.48
1:B:105:LEU:HA	1:B:148:LEU:HD13	1.96	0.48
1:B:16:TYR:O	1:B:19:ASN:HB3	2.14	0.47
1:B:176:GLY:O	1:B:180:THR:HG23	2.14	0.47
1:A:29:ILE:HG13	1:A:30:VAL:N	2.30	0.47
2:C:111:TYR:HA	2:C:114:ARG:CD	2.44	0.47
1:A:10:PHE:CE2	2:C:238:GLY:HA3	2.50	0.47
2:C:34:PHE:HD2	2:C:34:PHE:N	2.12	0.47
1:B:158:ASN:HA	1:B:161:THR:HB	1.97	0.47
1:B:73:TYR:CE2	1:B:96:THR:HG22	2.49	0.47
1:A:138:VAL:O	1:A:141:TYR:HB3	2.15	0.47
2:C:54:LEU:HD13	2:C:100:ALA:CA	2.45	0.47
1:A:86:TYR:O	2:C:111:TYR:HB3	2.15	0.46
2:C:134:LEU:HD12	2:C:135:CYS:N	2.30	0.46
1:B:107:ILE:HG12	1:B:115:VAL:HG13	1.97	0.46
1:A:37:LEU:HD13	1:A:69:CYS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:ALA:O	2:C:156:ALA:HB3	2.14	0.46
2:C:53:LYS:HD2	2:C:56:ARG:CZ	2.45	0.46
1:A:11:SER:O	1:A:15:LYS:HB2	2.16	0.46
1:B:118:GLU:O	1:B:121:ALA:HB3	2.15	0.46
2:C:114:ARG:HA	2:C:117:TYR:CE2	2.49	0.46
2:C:207:GLY:O	2:C:210:MSE:HB3	2.16	0.46
1:B:72:LYS:O	1:B:75:LYS:HB3	2.16	0.46
2:C:200:LEU:HD13	2:C:250:LEU:HD22	1.97	0.46
1:A:103:ILE:HD11	1:A:124:LEU:HD21	1.98	0.46
1:A:93:THR:O	1:A:97:GLN:HG3	2.15	0.46
1:A:52:LEU:C	1:A:54:GLN:H	2.19	0.46
1:B:67:GLU:O	1:B:70:ALA:HB3	2.16	0.46
2:C:92:LYS:O	2:C:95:ALA:HB3	2.16	0.45
2:C:147:SER:N	2:C:148:VAL:HA	2.31	0.45
1:B:178:LEU:HD21	1:B:182:PHE:HE2	1.80	0.45
2:C:82:VAL:O	2:C:86:ALA:HB2	2.15	0.45
1:A:101:PHE:CE1	1:A:148:LEU:HA	2.50	0.45
2:C:158:MSE:HA	2:C:158:MSE:CE	2.47	0.45
1:B:165:TYR:CD2	1:B:165:TYR:N	2.84	0.45
1:B:161:THR:OG1	2:C:269:TYR:HB2	2.17	0.44
1:A:107:ILE:HG12	1:A:115:VAL:HG22	1.98	0.44
2:C:65:ILE:HD11	2:C:89:ARG:HG2	1.99	0.44
1:A:96:THR:O	1:A:100:ILE:HG13	2.16	0.44
2:C:253:LYS:O	2:C:256:THR:HG22	2.16	0.44
1:A:86:TYR:HB2	2:C:110:VAL:HG12	1.99	0.44
1:A:213:VAL:O	1:A:213:VAL:HG12	2.18	0.44
2:C:67:PHE:HD1	2:C:67:PHE:HA	1.66	0.44
1:A:107:ILE:HD12	1:A:107:ILE:C	2.38	0.44
2:C:267:VAL:CG2	2:C:268:CYS:N	2.80	0.44
1:B:201:TYR:C	1:B:201:TYR:CD2	2.91	0.44
1:A:10:PHE:CG	1:A:13:TYR:HD2	2.36	0.44
1:B:178:LEU:O	1:B:181:GLY:N	2.51	0.43
2:C:200:LEU:CD1	2:C:250:LEU:HD22	2.48	0.43
1:A:141:TYR:O	1:A:145:ILE:HG12	2.18	0.43
2:C:68:LEU:HD21	2:C:86:ALA:HB2	1.99	0.43
1:A:202:ASP:O	1:A:206:ILE:HG13	2.17	0.43
1:A:161:THR:HG22	1:A:161:THR:O	2.18	0.43
2:C:251:TRP:O	2:C:255:THR:HG23	2.17	0.43
2:C:128:TYR:CD1	2:C:128:TYR:C	2.92	0.43
1:B:49:HIS:HE1	1:B:155:PHE:CA	2.30	0.43
2:C:209:LEU:HB2	2:C:232:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:LEU:HD13	2:C:100:ALA:HA	2.00	0.43
2:C:133:TYR:CB	2:C:147:SER:HB3	2.49	0.43
2:C:205:LEU:C	2:C:205:LEU:HD13	2.38	0.43
2:C:50:ARG:HD2	2:C:103:LEU:CD1	2.42	0.43
2:C:56:ARG:O	2:C:59:THR:HG22	2.18	0.43
1:B:107:ILE:HD12	1:B:107:ILE:N	2.34	0.43
1:B:158:ASN:O	1:B:162:MSE:HG2	2.19	0.43
2:C:114:ARG:CA	2:C:117:TYR:CD2	3.02	0.43
2:C:205:LEU:O	2:C:205:LEU:HD13	2.19	0.43
2:C:213:CYS:SG	2:C:225:CYS:HB2	2.58	0.43
1:B:45:LEU:CD1	1:B:45:LEU:N	2.82	0.42
1:A:43:ILE:CG2	1:A:44:LYS:N	2.81	0.42
1:B:24:ARG:C	1:B:26:ASN:H	2.21	0.42
2:C:65:ILE:HD13	2:C:90:LEU:HD12	2.01	0.42
1:B:37:LEU:O	1:B:38:SER:C	2.58	0.42
2:C:203:SER:CA	2:C:206:THR:HG23	2.47	0.42
2:C:146:LYS:HG3	2:C:146:LYS:H	1.57	0.42
2:C:96:VAL:O	2:C:99:ARG:HB2	2.19	0.42
1:B:116:THR:O	1:B:120:VAL:HG23	2.19	0.42
2:C:134:LEU:CD1	2:C:134:LEU:C	2.87	0.42
2:C:236:TYR:OH	2:C:258:LYS:HD2	2.19	0.42
1:B:178:LEU:HD21	1:B:182:PHE:CE2	2.55	0.42
1:A:175:ILE:CG2	1:A:203:VAL:HG22	2.48	0.42
2:C:208:GLU:HA	2:C:211:ARG:CD	2.50	0.42
1:B:79:LEU:HA	1:B:79:LEU:HD23	1.94	0.42
2:C:68:LEU:CD2	2:C:86:ALA:HB2	2.50	0.42
2:C:236:TYR:CE1	2:C:258:LYS:HG3	2.54	0.42
2:C:193:VAL:HG12	2:C:195:PRO:HD3	2.02	0.42
1:B:123:MSE:HE2	1:B:123:MSE:HB3	1.95	0.41
2:C:134:LEU:HD12	2:C:134:LEU:C	2.40	0.41
1:A:142:LEU:O	1:A:145:ILE:HB	2.20	0.41
1:B:70:ALA:HB2	1:B:124:LEU:HA	2.03	0.41
1:B:35:GLU:HB2	1:B:95:ILE:CD1	2.50	0.41
1:B:42:GLN:HE21	2:C:240:ILE:HD11	1.85	0.41
2:C:67:PHE:O	2:C:70:HIS:HB2	2.20	0.41
1:B:164:ASP:OD1	1:B:166:GLU:HB3	2.20	0.41
2:C:84:GLU:HA	2:C:87:ARG:HD3	2.03	0.41
2:C:31:VAL:CG2	2:C:33:GLN:HB2	2.51	0.41
1:B:128:ILE:HG23	1:B:129:SER:N	2.36	0.41
1:A:196:PHE:O	1:A:199:LEU:HB3	2.20	0.41
1:A:15:LYS:HA	1:A:18:ASP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:O	1:A:56:SER:C	2.59	0.41
2:C:66:ILE:HG22	2:C:127:ALA:CB	2.49	0.41
2:C:65:ILE:HG21	2:C:90:LEU:HD13	2.02	0.40
1:A:169:LEU:O	1:A:170:ASN:C	2.60	0.40
2:C:149:SER:O	2:C:150:ASP:CB	2.68	0.40
2:C:264:ALA:O	2:C:267:VAL:HG22	2.21	0.40
2:C:154:ILE:O	2:C:157:VAL:HG22	2.22	0.40
1:B:104:ALA:HB1	1:B:148:LEU:HD22	2.02	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	202/218 (93%)	176 (87%)	21 (10%)	5 (2%)	7	43
1	B	199/218 (91%)	176 (88%)	21 (11%)	2 (1%)	19	63
2	C	176/269 (65%)	153 (87%)	16 (9%)	7 (4%)	4	31
All	All	577/705 (82%)	505 (88%)	58 (10%)	14 (2%)	7	44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	117	TYR
2	C	118	SER
2	C	195	PRO
1	A	55	ILE
1	B	83	GLY
2	C	148	VAL
2	C	272	LYS
1	A	53	SER
1	B	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	119	PRO
1	A	213	VAL
1	A	90	ASP
2	C	271	VAL
1	A	9	ILE

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	166/191 (87%)	162 (98%)	4 (2%)	57	85
1	B	168/191 (88%)	151 (90%)	17 (10%)	9	38
2	C	161/235 (68%)	137 (85%)	24 (15%)	4	20
All	All	495/617 (80%)	450 (91%)	45 (9%)	12	44

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	135	HIS
1	A	167	ARG
1	A	211	TYR
1	B	20	GLU
1	B	47	ILE
1	B	48	ILE
1	B	61	LEU
1	B	90	ASP
1	B	91	HIS
1	B	97	GLN
1	B	115	VAL
1	B	116	THR
1	B	128	ILE
1	B	146	LEU
1	B	150	SER
1	B	157	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	LEU
1	B	199	LEU
1	B	201	TYR
1	B	211	TYR
2	C	66	ILE
2	C	67	PHE
2	C	68	LEU
2	C	85	GLU
2	C	90	LEU
2	C	97	ASN
2	C	103	LEU
2	C	116	SER
2	C	121	LEU
2	C	122	GLN
2	C	128	TYR
2	C	134	LEU
2	C	136	HIS
2	C	146	LYS
2	C	152	GLN
2	C	158	MSE
2	C	197	GLU
2	C	200	LEU
2	C	228	THR
2	C	229	CYS
2	C	236	TYR
2	C	242	LEU
2	C	253	LYS
2	C	267	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	91	HIS
1	A	97	GLN
1	A	135	HIS
1	A	158	ASN
1	B	49	HIS
1	B	97	GLN
2	C	70	HIS
2	C	97	ASN
2	C	112	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 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 (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	204/218 (93%)	-0.27	0	100	100	45, 96, 190, 239	0
1	B	201/218 (92%)	-0.45	0	100	100	27, 58, 146, 228	0
2	C	185/269 (68%)	-0.11	6 (3%)	51	47	26, 95, 205, 313	0
All	All	590/705 (83%)	-0.28	6 (1%)	84	79	26, 84, 188, 313	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	112	GLN	3.4
2	C	111	TYR	2.8
2	C	99	ARG	2.3
2	C	160	TYR	2.3
2	C	113	PHE	2.2
2	C	244	CYS	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.