



Full wwPDB X-ray Structure Validation Report

Oct 30, 2014 – 04:50 PM EDT

PDB ID : 4V2C
Title : mouse FLRT2 LRR domain in complex with rat Unc5D Ig1 domain
Authors : Seiradake, E.; del Toro, D.; Nagel, D.; Cop, F.; Haertl, R.; Ruff, T.; Seyit-Bremer, G.; Harlos, K.; Border, E.C.; Acker-Palmer, A.; Jones, E.Y.; Klein, R.
Deposited on : 2014-10-08
Resolution : 4.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

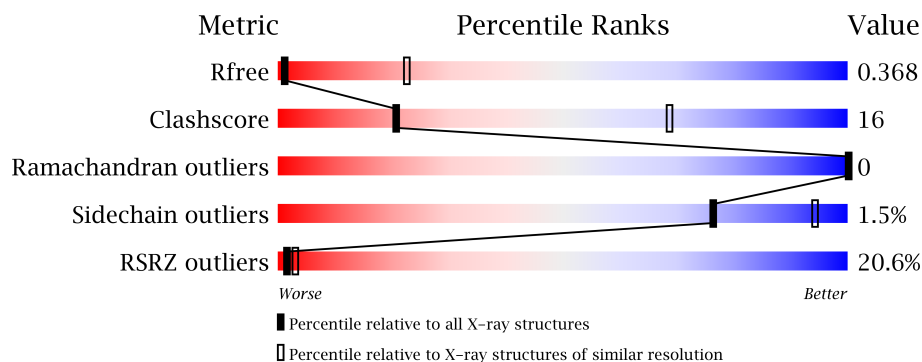
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance





The reported resolution of this entry is 4.00 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}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	328	
1	C	328	
2	B	161	
2	D	161	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6854 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FIBRONECTIN LEUCINE RICH TRANSMEMBRANE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2563	1618	457	474	14			
1	C	323	Total	C	N	O	S	0	0	0
			2563	1618	457	474	14			

- Molecule 2 is a protein called PROTEIN UNC5D.

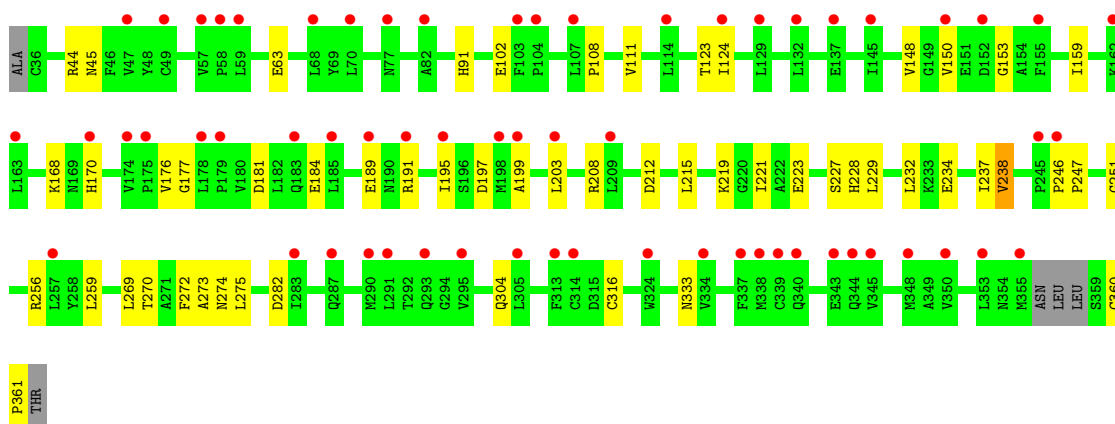
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			864	547	152	160	5			
2	D	106	Total	C	N	O	S	0	0	0
			864	547	152	160	5			

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.

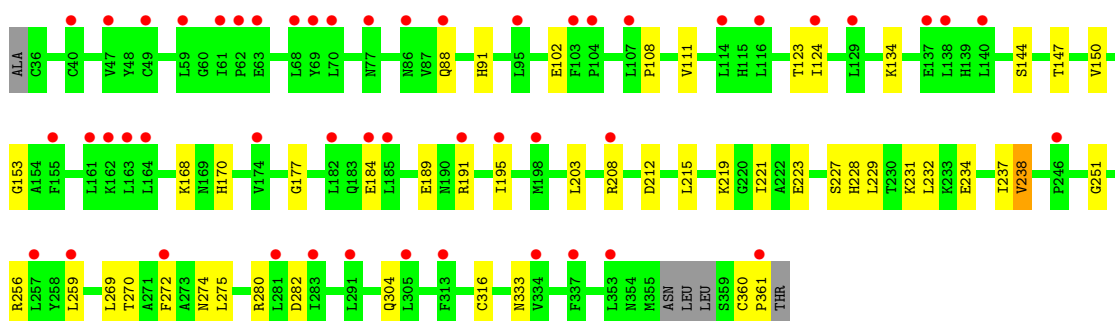
• Molecule 1: FIBRONECTIN LEUCINE RICH TRANSMEMBRANE PROTEIN 2

Chain A: 



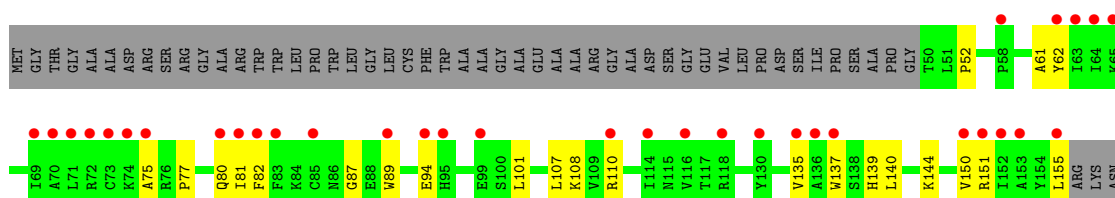
• Molecule 1: FIBRONECTIN LEUCINE RICH TRANSMEMBRANE PROTEIN 2

Chain C: 



• Molecule 2: PROTEIN UNC5D

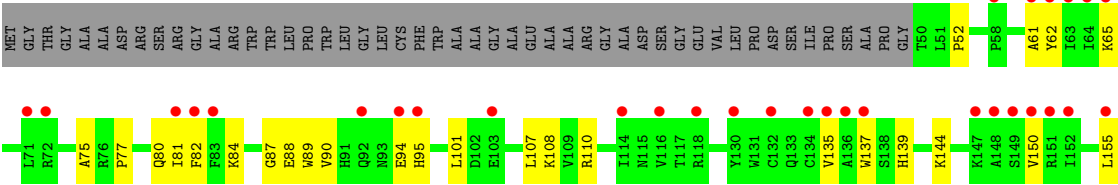
Chain B: 



PHE
GLU
GLN

● Molecule 2: PROTEIN UNC5D

Chain D:



ARG
LYS
ASN
PHE
GLU
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.14Å 150.91Å 67.22Å 90.00° 102.79° 90.00°	Depositor
Resolution (Å)	87.84 – 4.00 87.84 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (87.84-4.00) 99.0 (87.84-4.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 4.01Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.318 , 0.335 0.343 , 0.368	Depositor DCC
R_{free} test set	746 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	157.3	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 14730 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.41	0/2613	0.58	0/3550
1	C	0.41	0/2613	0.58	0/3550
2	B	0.33	0/887	0.55	0/1201
2	D	0.39	0/887	0.57	0/1201
All	All	0.40	0/7000	0.57	0/9502

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2563	0	2565	105	9
1	C	2563	0	2566	87	6
2	B	864	0	826	68	3
2	D	864	0	826	97	3
All	All	6854	0	6783	212	12

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (212) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:ALA:CB	2:D:101:LEU:HD11	1.17	1.56
1:A:270:THR:HB	2:D:108:LYS:NZ	1.19	1.51
1:A:273:ALA:CB	2:D:101:LEU:CD1	1.88	1.48
1:C:191:ARG:NH2	2:D:80:GLN:CG	1.75	1.47
1:A:274:ASN:ND2	2:D:101:LEU:CD2	1.78	1.45
1:A:227:SER:HB2	2:D:139:HIS:ND1	1.25	1.43
1:A:227:SER:HB2	2:D:139:HIS:CE1	1.59	1.38
1:A:191:ARG:HD2	2:B:137:TRP:CH2	1.64	1.31
1:A:227:SER:CB	2:D:139:HIS:ND1	1.97	1.28
1:A:273:ALA:HB1	2:D:101:LEU:CD1	1.51	1.26
1:A:227:SER:CB	2:D:139:HIS:CE1	2.19	1.25
1:C:144:SER:OG	2:D:144:LYS:HE2	1.11	1.25
1:C:191:ARG:NH2	2:D:80:GLN:HG3	1.39	1.24
1:C:191:ARG:NH2	2:D:80:GLN:CB	1.98	1.24
1:A:191:ARG:HD2	2:B:137:TRP:CZ2	1.70	1.24
1:C:144:SER:OG	2:D:144:LYS:CE	1.86	1.22
1:C:191:ARG:HH21	2:D:80:GLN:CG	1.45	1.19
2:B:101:LEU:CD2	1:C:274:ASN:HD21	1.55	1.18
1:A:191:ARG:NH2	2:B:80:GLN:CG	2.07	1.18
1:A:227:SER:CB	2:D:139:HIS:HD1	1.52	1.17
1:A:191:ARG:CD	2:B:137:TRP:CZ2	2.30	1.14
1:A:274:ASN:HD21	2:D:101:LEU:CD2	1.48	1.12
1:A:273:ALA:HB3	2:D:101:LEU:HD11	1.23	1.11
1:A:191:ARG:HH22	2:B:80:GLN:HG3	1.14	1.10
1:A:273:ALA:HB2	2:D:101:LEU:HD11	1.23	1.10
1:A:191:ARG:NH2	2:B:80:GLN:CB	2.14	1.10
2:D:89:TRP:CH2	2:D:137:TRP:HH2	1.69	1.10
1:A:270:THR:CB	2:D:108:LYS:NZ	2.14	1.10
2:D:89:TRP:HH2	2:D:137:TRP:CH2	1.69	1.09
1:A:274:ASN:HD21	2:D:101:LEU:HD23	0.99	1.09
1:A:274:ASN:HD22	2:D:101:LEU:HD21	1.13	1.08
1:A:273:ALA:HB1	2:D:101:LEU:HD13	1.36	1.05
1:A:223:GLU:OE2	2:D:80:GLN:HG3	1.56	1.04
2:B:101:LEU:HD22	1:C:274:ASN:HD21	1.21	1.04
2:D:84:LYS:HE2	2:D:89:TRP:HE1	1.22	1.04
1:C:191:ARG:HH21	2:D:80:GLN:CB	1.68	1.03
1:A:191:ARG:HH22	2:B:80:GLN:CG	1.69	1.02
1:A:273:ALA:HB2	2:D:101:LEU:CD1	1.77	1.02
1:A:170:HIS:CE1	2:B:144:LYS:HD3	1.95	1.01
1:A:223:GLU:OE2	2:D:80:GLN:CG	2.08	1.01
1:A:274:ASN:ND2	2:D:101:LEU:HD21	1.65	1.00
1:A:170:HIS:HE1	2:B:144:LYS:HD3	1.27	0.99
1:A:191:ARG:NH2	2:B:80:GLN:HB3	1.76	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:191:ARG:HH22	2:D:80:GLN:HG3	0.82	0.99
2:D:89:TRP:CH2	2:D:137:TRP:CH2	2.48	0.98
1:C:191:ARG:HH21	2:D:80:GLN:CD	1.66	0.97
1:A:191:ARG:CD	2:B:137:TRP:CH2	2.47	0.97
1:A:170:HIS:HD2	2:B:89:TRP:CZ2	1.84	0.96
1:A:270:THR:HB	2:D:108:LYS:HZ1	1.15	0.96
2:B:139:HIS:CE1	1:C:227:SER:HB2	2.00	0.96
1:A:228:HIS:NE2	2:D:139:HIS:O	1.99	0.95
1:A:227:SER:HB3	2:D:139:HIS:CE1	2.00	0.93
1:A:223:GLU:CD	2:D:80:GLN:HG3	1.86	0.93
2:B:101:LEU:HD21	1:C:274:ASN:ND2	1.83	0.93
2:B:101:LEU:CD2	1:C:274:ASN:ND2	2.31	0.93
1:A:270:THR:HB	2:D:108:LYS:HZ3	1.12	0.93
1:C:191:ARG:HD2	2:D:137:TRP:CH2	2.04	0.92
1:A:170:HIS:HE1	2:B:144:LYS:CD	1.82	0.92
1:C:191:ARG:NH2	2:D:80:GLN:HB3	1.84	0.92
2:B:80:GLN:HG3	1:C:223:GLU:OE1	1.71	0.91
1:A:274:ASN:ND2	2:D:101:LEU:HD22	1.83	0.90
1:A:273:ALA:CB	2:D:101:LEU:HD13	1.93	0.89
2:B:101:LEU:HD21	1:C:274:ASN:HD21	1.37	0.85
1:A:270:THR:CB	2:D:108:LYS:HZ1	1.85	0.85
2:B:139:HIS:CE1	1:C:227:SER:CB	2.60	0.85
1:A:191:ARG:HH21	2:B:80:GLN:CD	1.80	0.84
1:A:191:ARG:HD3	2:B:137:TRP:CZ2	2.11	0.84
1:A:270:THR:HB	2:D:108:LYS:HZ2	1.40	0.83
1:C:168:LYS:HD3	2:D:87:GLY:O	1.77	0.82
2:D:84:LYS:HE2	2:D:89:TRP:NE1	1.95	0.81
1:A:191:ARG:NH2	2:B:80:GLN:CD	2.34	0.81
1:A:191:ARG:HH21	2:B:80:GLN:HB3	1.46	0.80
1:C:191:ARG:HB2	2:D:89:TRP:CH2	2.18	0.79
1:A:227:SER:HB3	2:D:139:HIS:HE1	1.45	0.79
1:C:191:ARG:NH2	2:D:80:GLN:CD	2.31	0.78
1:C:215:LEU:HD21	2:D:82:PHE:CE1	2.18	0.78
1:A:219:LYS:HD2	1:C:219:LYS:HD2	1.66	0.78
1:C:191:ARG:HH22	2:D:80:GLN:CG	1.61	0.77
1:A:170:HIS:HD2	2:B:89:TRP:HZ2	1.32	0.76
1:A:191:ARG:HH21	2:B:80:GLN:CG	1.93	0.76
1:A:191:ARG:HH21	2:B:80:GLN:CB	1.99	0.76
1:A:223:GLU:OE1	2:D:80:GLN:HG3	1.85	0.75
1:A:191:ARG:HD3	2:B:137:TRP:CE2	2.22	0.74
1:C:191:ARG:HH21	2:D:80:GLN:HB3	1.41	0.74
2:B:82:PHE:HB2	2:B:137:TRP:CH2	2.24	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:GLU:OE2	2:D:80:GLN:HG2	1.91	0.71
1:C:191:ARG:HB2	2:D:89:TRP:CZ3	2.26	0.70
1:A:274:ASN:ND2	2:D:101:LEU:HD23	1.67	0.70
1:A:170:HIS:HD2	2:B:89:TRP:CH2	2.09	0.69
1:A:191:ARG:NH2	2:B:80:GLN:HG3	1.85	0.69
1:C:170:HIS:CD2	2:D:135:VAL:HG11	2.27	0.69
1:C:215:LEU:CD2	2:D:82:PHE:CE1	2.76	0.68
1:A:227:SER:HB2	2:D:139:HIS:HD1	1.09	0.67
1:A:228:HIS:HE2	2:D:139:HIS:C	1.94	0.67
1:A:170:HIS:CD2	2:B:89:TRP:CH2	2.83	0.66
1:A:223:GLU:OE1	1:C:191:ARG:NH2	2.29	0.66
2:B:82:PHE:HB2	2:B:137:TRP:HH2	1.59	0.66
1:A:170:HIS:CD2	2:B:89:TRP:CZ2	2.76	0.66
2:B:139:HIS:HE1	1:C:227:SER:CB	2.06	0.66
2:D:90:VAL:O	2:D:95:HIS:HE1	1.77	0.66
1:A:273:ALA:HB1	2:D:101:LEU:CD2	2.24	0.66
1:A:191:ARG:NH2	2:B:80:GLN:NE2	2.43	0.66
1:A:223:GLU:CD	1:C:191:ARG:HH22	2.00	0.64
1:C:191:ARG:HD2	2:D:137:TRP:CZ3	2.33	0.64
1:A:273:ALA:HB1	2:D:101:LEU:CG	2.26	0.64
1:C:144:SER:HG	2:D:144:LYS:CE	2.10	0.63
1:A:197:ASP:OD2	1:C:147:THR:HG21	1.98	0.63
1:C:191:ARG:NH2	2:D:80:GLN:NE2	2.47	0.62
2:D:89:TRP:HH2	2:D:137:TRP:CZ2	2.15	0.62
1:A:227:SER:CB	2:D:139:HIS:HE1	1.94	0.61
2:B:101:LEU:HD22	1:C:274:ASN:ND2	2.04	0.61
1:C:191:ARG:HD2	2:D:137:TRP:CZ2	2.36	0.61
1:A:191:ARG:HG3	1:A:215:LEU:CD1	2.32	0.60
1:C:191:ARG:HG3	1:C:215:LEU:CD1	2.32	0.59
1:A:191:ARG:HE	2:B:82:PHE:HD2	1.49	0.59
2:B:139:HIS:ND1	1:C:227:SER:HB2	2.18	0.59
2:B:108:LYS:NZ	1:C:270:THR:HB	2.18	0.58
1:C:170:HIS:CE1	2:D:144:LYS:HD3	2.39	0.58
2:B:80:GLN:HG2	1:C:223:GLU:OE2	2.02	0.58
2:B:80:GLN:HG3	1:C:223:GLU:CD	2.23	0.58
1:A:191:ARG:CD	2:B:137:TRP:CE2	2.80	0.58
1:C:191:ARG:NH2	2:D:80:GLN:HB2	2.11	0.58
1:C:191:ARG:HD3	2:D:137:TRP:CE2	2.40	0.57
2:B:80:GLN:O	2:B:137:TRP:HE3	1.86	0.56
2:B:80:GLN:CG	1:C:223:GLU:OE2	2.54	0.56
1:C:191:ARG:CD	2:D:137:TRP:CZ2	2.88	0.55
1:A:191:ARG:HG3	1:A:215:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:144:SER:OG	2:D:144:LYS:NZ	2.37	0.55
2:D:84:LYS:HG3	2:D:89:TRP:CD1	2.42	0.55
1:C:191:ARG:HG3	1:C:215:LEU:HD11	1.89	0.54
1:C:102:GLU:HG2	1:C:123:THR:HB	1.90	0.54
1:C:144:SER:CB	2:D:144:LYS:HE2	2.29	0.53
1:A:91:HIS:HA	1:A:111:VAL:HA	1.90	0.53
1:A:168:LYS:HD3	2:B:87:GLY:O	2.09	0.53
1:C:170:HIS:HE1	2:D:144:LYS:CD	2.21	0.53
1:C:215:LEU:HD22	2:D:82:PHE:CZ	2.43	0.53
1:A:191:ARG:O	1:A:191:ARG:HG2	2.09	0.53
1:A:102:GLU:HG2	1:A:123:THR:HB	1.90	0.53
1:C:191:ARG:O	1:C:191:ARG:HG2	2.09	0.53
2:D:61:ALA:HB3	2:D:150:VAL:HG22	1.91	0.53
1:C:91:HIS:HA	1:C:111:VAL:HA	1.90	0.52
1:C:215:LEU:CD2	2:D:82:PHE:CZ	2.93	0.52
2:B:108:LYS:HZ1	1:C:270:THR:HB	1.74	0.52
1:A:189:GLU:O	2:B:89:TRP:CD1	2.64	0.52
2:B:61:ALA:HB3	2:B:150:VAL:HG22	1.92	0.51
2:B:139:HIS:HB3	1:C:228:HIS:NE2	2.25	0.51
2:B:139:HIS:HB3	1:C:228:HIS:HE2	1.75	0.51
2:B:139:HIS:ND1	1:C:227:SER:CB	2.73	0.51
1:C:234:GLU:HG3	1:C:256:ARG:HB2	1.93	0.51
1:A:170:HIS:CD2	2:B:89:TRP:HZ2	2.20	0.51
1:A:234:GLU:HG3	1:A:256:ARG:HB2	1.93	0.50
1:A:195:ILE:HB	1:A:221:ILE:HG22	1.94	0.50
1:C:189:GLU:OE2	2:D:88:GLU:OE1	2.22	0.49
1:A:148:VAL:HG11	2:B:140:LEU:O	2.13	0.49
1:C:195:ILE:HB	1:C:221:ILE:HG22	1.94	0.49
1:A:270:THR:CB	2:D:108:LYS:HZ3	1.99	0.49
2:B:139:HIS:HE1	1:C:227:SER:HB3	1.75	0.49
2:D:88:GLU:HG3	2:D:89:TRP:N	2.29	0.48
1:A:170:HIS:NE2	2:B:135:VAL:HG21	2.29	0.48
1:C:191:ARG:CZ	2:D:80:GLN:HB3	2.42	0.48
1:A:170:HIS:CE1	2:B:144:LYS:CD	2.68	0.47
1:C:272:PHE:HA	1:C:275:LEU:HD12	1.97	0.47
1:A:219:LYS:HB3	1:C:219:LYS:HB3	1.97	0.47
1:A:272:PHE:HA	1:A:275:LEU:HD12	1.97	0.46
2:B:82:PHE:HB2	2:B:137:TRP:CZ3	2.51	0.46
1:C:229:LEU:HD23	1:C:232:LEU:HD13	1.97	0.46
1:A:170:HIS:CD2	2:B:89:TRP:HH2	2.30	0.46
1:C:251:GLY:HA3	1:C:275:LEU:HA	1.98	0.46
1:C:170:HIS:CE1	2:D:144:LYS:CD	2.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:81:ILE:HD12	2:D:110:ARG:HB3	1.98	0.46
1:A:170:HIS:HE1	2:B:144:LYS:CE	2.29	0.46
1:A:219:LYS:HD3	1:C:219:LYS:HB2	1.98	0.45
1:C:108:PRO:HB2	1:C:111:VAL:HG23	1.99	0.45
1:C:304:GLN:HG3	1:C:333:ASN:HB2	1.99	0.45
1:C:215:LEU:HD22	2:D:82:PHE:CE1	2.51	0.45
1:C:215:LEU:CD1	2:D:82:PHE:CZ	3.00	0.45
1:A:229:LEU:HD23	1:A:232:LEU:HD13	1.97	0.45
1:A:153:GLY:HA2	1:A:177:GLY:HA3	1.99	0.45
1:C:191:ARG:HD3	2:D:137:TRP:CZ2	2.52	0.45
1:A:237:ILE:HD11	1:A:259:LEU:HD23	1.99	0.44
2:B:81:ILE:HD12	2:B:110:ARG:HB3	1.98	0.44
1:C:208:ARG:HG2	1:C:234:GLU:HB3	1.99	0.44
1:A:304:GLN:HG3	1:A:333:ASN:HB2	1.99	0.44
1:A:251:GLY:HA3	1:A:275:LEU:HA	1.98	0.44
1:C:215:LEU:HD13	2:D:82:PHE:CZ	2.52	0.44
1:C:153:GLY:HA2	1:C:177:GLY:HA3	1.99	0.43
1:A:208:ARG:HG2	1:A:234:GLU:HB3	1.99	0.43
1:C:237:ILE:HD11	1:C:259:LEU:HD23	1.99	0.43
1:A:108:PRO:HB2	1:A:111:VAL:HG23	1.99	0.43
1:A:246:PRO:HA	1:A:247:PRO:HD3	1.94	0.43
2:B:75:ALA:HB3	2:B:81:ILE:HD11	2.01	0.43
2:D:84:LYS:HG3	2:D:89:TRP:HD1	1.82	0.43
2:B:82:PHE:N	2:B:137:TRP:HZ3	2.17	0.43
2:B:77:PRO:HB3	2:B:107:LEU:HD23	2.01	0.43
1:C:124:ILE:HB	1:C:150:VAL:HA	2.01	0.42
1:A:360:CYS:HB2	1:A:361:PRO:HD2	2.02	0.42
1:A:212:ASP:HB2	1:A:238:VAL:HG22	2.02	0.42
2:D:52:PRO:HA	2:D:77:PRO:HD2	2.02	0.42
1:A:191:ARG:NE	2:B:137:TRP:CZ3	2.88	0.42
1:C:212:ASP:HB2	1:C:238:VAL:HG22	2.02	0.41
1:A:215:LEU:HD13	2:B:82:PHE:CZ	2.55	0.41
1:C:280:ARG:HG3	1:C:304:GLN:HB3	2.02	0.41
1:C:184:GLU:HG3	1:C:208:ARG:HB2	2.03	0.41
2:D:75:ALA:HB3	2:D:81:ILE:HD11	2.01	0.41
1:A:176:VAL:HA	1:A:199:ALA:HA	2.02	0.41
2:D:77:PRO:HB3	2:D:107:LEU:HD23	2.01	0.41
1:C:360:CYS:HB2	1:C:361:PRO:HD2	2.02	0.41
1:A:124:ILE:HB	1:A:150:VAL:HA	2.01	0.41
1:C:191:ARG:NH2	2:D:80:GLN:HE21	2.19	0.41
2:D:88:GLU:HG3	2:D:89:TRP:H	1.86	0.40
2:B:52:PRO:HA	2:B:77:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:GLU:HG3	1:A:208:ARG:HB2	2.02	0.40

All (12) 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	Distance(Å)	Clash(Å)
1:A:45:ASN:OD1	1:A:63:GLU:OE1[2_857]	0.56	1.64
1:A:181:ASP:OD1	1:C:88:GLN:OE1[2_858]	0.86	1.34
1:A:181:ASP:CG	1:C:88:GLN:OE1[2_858]	1.29	0.91
1:A:44:ARG:NH1	1:C:231:LYS:NZ[1_554]	1.32	0.88
1:A:45:ASN:CG	1:A:63:GLU:OE1[2_857]	1.58	0.62
1:A:181:ASP:OD1	1:C:88:GLN:CD[2_858]	1.60	0.60
1:A:181:ASP:OD2	1:C:88:GLN:OE1[2_858]	1.71	0.49
1:A:45:ASN:OD1	1:A:63:GLU:CD[2_857]	1.71	0.49
2:B:155:LEU:CD1	2:D:62:TYR:CE1[4_748]	1.82	0.38
2:B:62:TYR:CE1	2:D:155:LEU:CD1[4_748]	1.85	0.35
1:A:159:ILE:CD1	1:C:134:LYS:CE[2_858]	2.00	0.20
2:B:151:ARG:NH1	2:D:65:LYS:NZ[4_748]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	319/328 (97%)	293 (92%)	26 (8%)	0	100	100
1	C	319/328 (97%)	293 (92%)	26 (8%)	0	100	100
2	B	104/161 (65%)	100 (96%)	4 (4%)	0	100	100
2	D	104/161 (65%)	100 (96%)	4 (4%)	0	100	100
All	All	846/978 (86%)	786 (93%)	60 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	294/298 (99%)	289 (98%)	5 (2%)	73	94
1	C	294/298 (99%)	289 (98%)	5 (2%)	73	94
2	B	95/132 (72%)	94 (99%)	1 (1%)	84	95
2	D	95/132 (72%)	94 (99%)	1 (1%)	84	95
All	All	778/860 (90%)	766 (98%)	12 (2%)	76	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LEU
1	A	238	VAL
1	A	269	LEU
1	A	282	ASP
1	A	316	CYS
2	B	94	GLU
1	C	203	LEU
1	C	238	VAL
1	C	269	LEU
1	C	282	ASP
1	C	316	CYS
2	D	94	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	218	ASN
1	A	304	GLN
1	C	170	HIS
1	C	218	ASN
1	C	274	ASN
1	C	304	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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, 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	323/328 (98%)	1.11	62 (19%) 2 3	37, 97, 207, 223	0
1	C	323/328 (98%)	0.90	50 (15%) 3 5	42, 97, 214, 235	0
2	B	106/161 (65%)	1.54	34 (32%) 1 2	68, 97, 156, 178	0
2	D	106/161 (65%)	1.37	31 (29%) 1 2	74, 106, 171, 198	0
All	All	858/978 (87%)	1.12	177 (20%) 1 3	37, 99, 207, 235	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	155	LEU	11.7
1	A	353	LEU	8.8
2	D	155	LEU	8.6
1	C	49	CYS	7.6
2	D	62	TYR	5.7
1	A	344	GLN	5.7
2	B	152	ILE	5.4
1	A	337	PHE	5.1
2	D	82	PHE	5.0
2	B	65	LYS	4.9
1	A	191	ARG	4.9
1	C	63	GLU	4.8
2	D	83	PHE	4.8
1	A	49	CYS	4.7
2	B	137	TRP	4.6
1	C	47	VAL	4.6
1	C	88	GLN	4.4
2	B	64	ILE	4.3
1	A	58	PRO	4.2
1	A	334	VAL	4.2
1	A	338	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	340	GLN	4.1
2	B	114	ILE	4.1
2	B	136	ALA	4.0
2	B	81	ILE	4.0
2	D	64	ILE	3.9
1	A	155	PHE	3.9
2	B	71	LEU	3.9
2	D	94	GLU	3.9
1	C	191	ARG	3.9
2	B	151	ARG	3.9
2	D	150	VAL	3.9
2	D	147	LYS	3.9
1	C	291	LEU	3.9
2	B	62	TYR	3.8
1	A	305	LEU	3.8
2	D	95	HIS	3.8
1	C	353	LEU	3.8
1	C	198	MET	3.8
1	A	152	ASP	3.8
1	A	189	GLU	3.7
1	A	57	VAL	3.7
1	A	70	LEU	3.7
2	D	81	ILE	3.7
1	A	283	ILE	3.6
1	C	70	LEU	3.6
2	B	153	ALA	3.6
1	C	184	GLU	3.6
2	B	63	ILE	3.5
1	C	334	VAL	3.5
1	A	162	LYS	3.5
2	D	65	LYS	3.5
2	B	83	PHE	3.5
1	C	259	LEU	3.4
1	A	195	ILE	3.4
1	A	170	HIS	3.3
2	B	82	PHE	3.3
1	A	59	LEU	3.3
1	C	337	PHE	3.3
1	C	361	PRO	3.2
1	A	291	LEU	3.2
1	C	116	LEU	3.2
1	A	124	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	73	CYS	3.2
2	D	148	ALA	3.2
1	A	174	VAL	3.2
1	A	175	PRO	3.2
1	C	164	LEU	3.2
1	A	163	LEU	3.2
1	A	104	PRO	3.2
1	C	59	LEU	3.1
1	C	283	ILE	3.1
1	C	68	LEU	3.1
2	D	71	LEU	3.1
1	A	129	LEU	3.1
1	A	339	CYS	3.1
1	A	287	GLN	3.1
1	C	208	ARG	3.0
1	A	137	GLU	3.0
1	C	162	LYS	3.0
1	A	82	ALA	3.0
2	D	118	ARG	3.0
1	A	246	PRO	2.9
1	A	68	LEU	2.9
2	D	132	CYS	2.8
1	C	174	VAL	2.8
1	A	350	VAL	2.8
1	A	314	CYS	2.8
1	A	114	LEU	2.8
1	A	293	GLN	2.8
1	A	313	PHE	2.8
2	D	134	CYS	2.7
1	C	137	GLU	2.7
2	D	63	ILE	2.7
1	C	124	ILE	2.7
1	C	62	PRO	2.7
1	A	47	VAL	2.7
1	C	114	LEU	2.7
2	B	135	VAL	2.6
2	D	151	ARG	2.6
1	A	355	MET	2.6
1	C	69	TYR	2.6
2	B	95	HIS	2.6
1	A	343	GLU	2.6
1	C	185	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	103	PHE	2.6
1	A	178	LEU	2.6
1	C	103	PHE	2.5
2	B	99	GLU	2.5
1	A	107	LEU	2.5
1	C	182	LEU	2.5
2	B	74	LYS	2.5
1	A	179	PRO	2.5
2	B	70	ALA	2.5
2	D	137	TRP	2.5
2	D	130	TYR	2.5
1	C	195	ILE	2.5
1	A	183	GLN	2.5
2	B	130	TYR	2.5
2	B	118	ARG	2.5
2	B	150	VAL	2.5
2	B	94	GLU	2.5
1	C	104	PRO	2.4
1	A	348	MET	2.4
2	D	92	GLN	2.4
2	B	85	CYS	2.4
1	C	272	PHE	2.4
1	A	245	PRO	2.4
1	C	61	ILE	2.4
1	C	281	LEU	2.4
2	B	80	GLN	2.4
2	D	61	ALA	2.4
1	C	257	LEU	2.4
1	C	40	CYS	2.4
2	B	89	TRP	2.3
2	B	58	PRO	2.3
1	C	129	LEU	2.3
1	A	199	ALA	2.3
1	C	138	LEU	2.3
1	A	345	VAL	2.3
1	C	161	LEU	2.3
2	D	72	ARG	2.3
1	C	155	PHE	2.3
1	A	290	MET	2.3
2	D	149	SER	2.3
2	B	69	ILE	2.3
1	C	107	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	163	LEU	2.2
2	B	72	ARG	2.2
2	B	75	ALA	2.2
2	D	136	ALA	2.2
1	C	95	LEU	2.2
1	A	203	LEU	2.2
1	A	209	LEU	2.2
1	A	132	LEU	2.2
1	C	77	ASN	2.1
2	D	114	ILE	2.1
2	D	58	PRO	2.1
1	A	145	ILE	2.1
1	A	150	VAL	2.1
1	C	246	PRO	2.1
1	C	305	LEU	2.1
1	A	295	VAL	2.1
1	C	140	LEU	2.1
2	D	116	VAL	2.1
1	C	86	ASN	2.1
2	D	152	ILE	2.1
2	D	103	GLU	2.1
1	A	198	MET	2.0
2	B	116	VAL	2.0
2	B	110	ARG	2.0
2	D	135	VAL	2.0
1	C	313	PHE	2.0
1	A	324	TRP	2.0
1	A	77	ASN	2.0
1	A	185	LEU	2.0
1	A	257	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.