



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:33 PM UTC

PDB ID : 4GYV / pdb_00004gyv
Title : Crystal structure of the DH domain of FARP2
Authors : He, X.; Zhang, X.
Deposited on : 2012-09-05
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

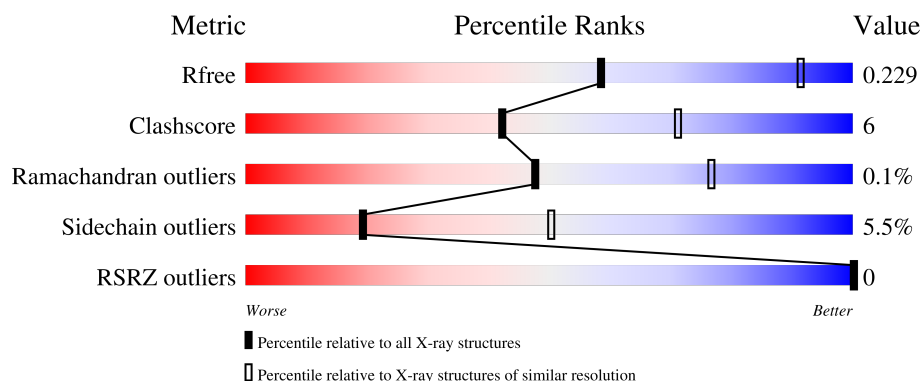
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	218	
1	C	218	
1	D	218	
1	E	218	

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Mol	Chain	Length	Quality of chain
1	F	218	 83% 14% ..
1	G	218	 75% 22% ..
1	H	218	 83% 15% ..
1	I	218	 78% 18% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15733 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 FERM, RhoGEF and pleckstrin domain-containing protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1766	1134	301	323	4	4			
1	B	216	Total	C	N	O	S	Se	0	0	0
			1764	1131	302	323	4	4			
1	C	216	Total	C	N	O	S	Se	0	0	0
			1764	1131	302	323	4	4			
1	D	216	Total	C	N	O	S	Se	0	0	0
			1755	1123	303	321	4	4			
1	E	215	Total	C	N	O	S	Se	0	0	0
			1706	1096	289	313	4	4			
1	F	216	Total	C	N	O	S	Se	0	0	0
			1752	1122	299	323	4	4			
1	G	215	Total	C	N	O	S	Se	0	0	0
			1727	1108	297	314	4	4			
1	H	216	Total	C	N	O	S	Se	0	0	0
			1756	1125	300	323	4	4			
1	I	215	Total	C	N	O	S	Se	0	0	0
			1726	1107	295	316	4	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	GLY	-	expression tag	UNP Q91VS8
A	533	PRO	-	expression tag	UNP Q91VS8
A	534	HIS	-	expression tag	UNP Q91VS8
A	535	MSE	-	expression tag	UNP Q91VS8
B	532	GLY	-	expression tag	UNP Q91VS8
B	533	PRO	-	expression tag	UNP Q91VS8
B	534	HIS	-	expression tag	UNP Q91VS8
B	535	MSE	-	expression tag	UNP Q91VS8
C	532	GLY	-	expression tag	UNP Q91VS8
C	533	PRO	-	expression tag	UNP Q91VS8
C	534	HIS	-	expression tag	UNP Q91VS8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	535	MSE	-	expression tag	UNP Q91VS8
D	532	GLY	-	expression tag	UNP Q91VS8
D	533	PRO	-	expression tag	UNP Q91VS8
D	534	HIS	-	expression tag	UNP Q91VS8
D	535	MSE	-	expression tag	UNP Q91VS8
E	532	GLY	-	expression tag	UNP Q91VS8
E	533	PRO	-	expression tag	UNP Q91VS8
E	534	HIS	-	expression tag	UNP Q91VS8
E	535	MSE	-	expression tag	UNP Q91VS8
F	532	GLY	-	expression tag	UNP Q91VS8
F	533	PRO	-	expression tag	UNP Q91VS8
F	534	HIS	-	expression tag	UNP Q91VS8
F	535	MSE	-	expression tag	UNP Q91VS8
G	532	GLY	-	expression tag	UNP Q91VS8
G	533	PRO	-	expression tag	UNP Q91VS8
G	534	HIS	-	expression tag	UNP Q91VS8
G	535	MSE	-	expression tag	UNP Q91VS8
H	532	GLY	-	expression tag	UNP Q91VS8
H	533	PRO	-	expression tag	UNP Q91VS8
H	534	HIS	-	expression tag	UNP Q91VS8
H	535	MSE	-	expression tag	UNP Q91VS8
I	532	GLY	-	expression tag	UNP Q91VS8
I	533	PRO	-	expression tag	UNP Q91VS8
I	534	HIS	-	expression tag	UNP Q91VS8
I	535	MSE	-	expression tag	UNP Q91VS8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	3	Total O 3 3	0	0
2	C	3	Total O 3 3	0	0
2	D	1	Total O 1 1	0	0
2	F	3	Total O 3 3	0	0
2	G	1	Total O 1 1	0	0
2	H	1	Total O 1 1	0	0

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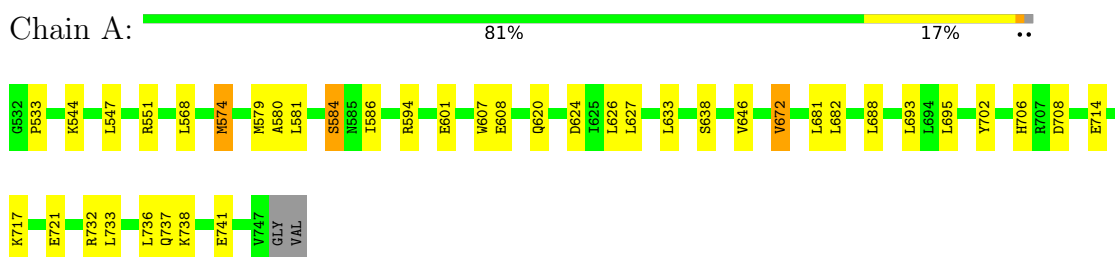
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total	O	0	0
			1	1		

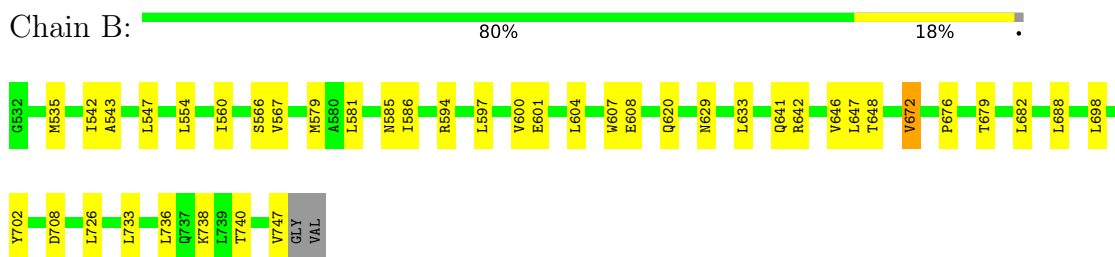
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

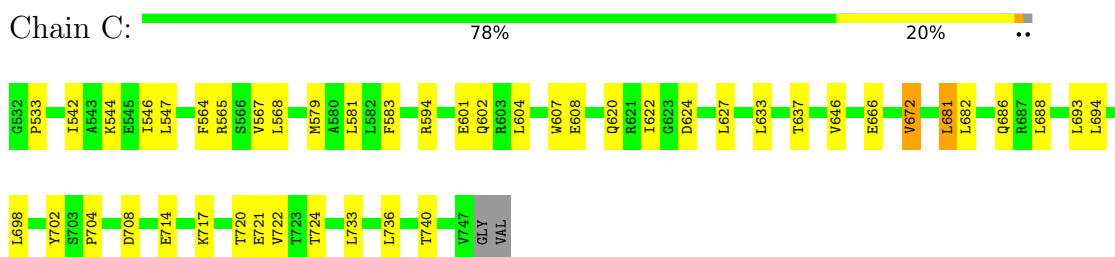
- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2



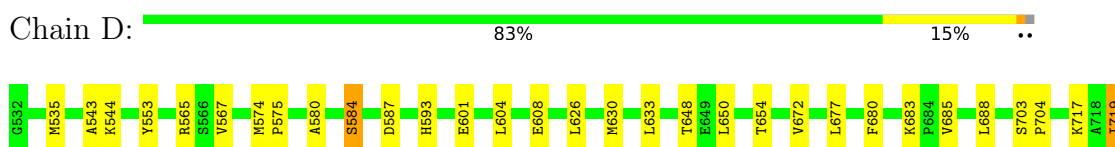
- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2



- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2



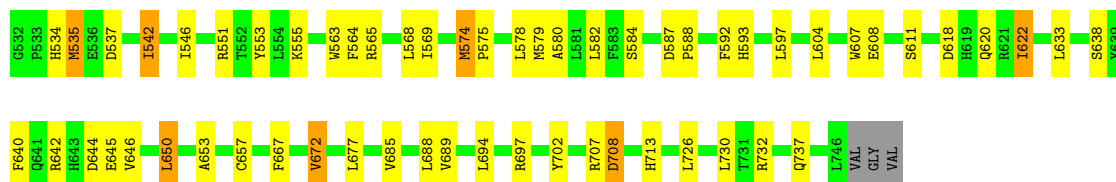
- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2





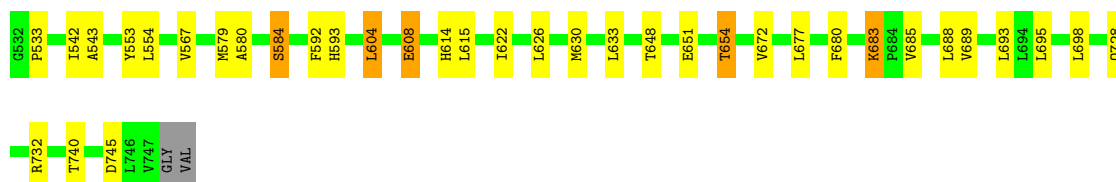
- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2

Chain E: 72% 23% ..



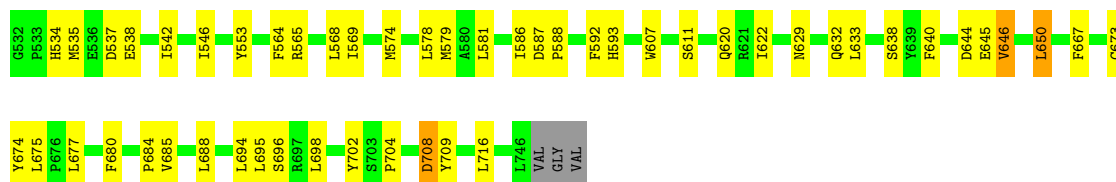
- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2

Chain F: 83% 14% ..



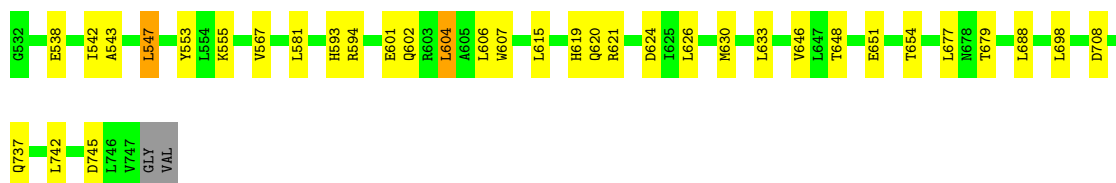
- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2

Chain G: 75% 22% ..



- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2

Chain H: 83% 15% ..



- Molecule 1: FERM, RhoGEF and pleckstrin domain-containing protein 2

Chain I: 78% 18% ..



Q686	R557	L688	L694	L695	S696	Y702	D708	L716	K717	E721	L746	VAL	GLY	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	121.19Å 209.99Å 325.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.90 48.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.58-2.90) 96.6 (48.58-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.178 , 0.221 0.182 , 0.229	Depositor DCC
R_{free} test set	1989 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.487 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15733	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	0/1801	0.91	4/2433 (0.2%)
1	B	0.65	0/1799	0.91	3/2432 (0.1%)
1	C	0.67	0/1799	0.91	1/2432 (0.0%)
1	D	0.57	0/1790	0.86	2/2422 (0.1%)
1	E	0.47	0/1740	0.84	0/2361
1	F	0.57	0/1787	0.86	0/2420
1	G	0.45	0/1762	0.81	0/2387
1	H	0.56	0/1791	0.86	0/2424
1	I	0.47	0/1761	0.85	2/2385 (0.1%)
All	All	0.57	0/16030	0.87	12/21696 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	672	VAL	CB-CA-C	-6.30	103.64	112.14
1	B	672	VAL	CB-CA-C	-6.20	103.67	112.22
1	I	532	GLY	CA-C-N	5.61	125.79	119.90
1	I	532	GLY	C-N-CA	5.61	125.79	119.90
1	D	703	SER	CA-C-N	5.50	126.71	119.84
1	D	703	SER	C-N-CA	5.50	126.71	119.84
1	A	672	VAL	CB-CA-C	-5.45	104.78	112.14
1	A	574	MSE	CA-C-N	5.44	125.36	119.76
1	A	574	MSE	C-N-CA	5.44	125.36	119.76
1	B	560	ILE	CB-CA-C	-5.29	104.99	111.92
1	A	706	HIS	N-CA-C	5.10	117.82	110.28
1	B	629	ASN	N-CA-C	5.08	116.89	111.36

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	1766	0	1748	23	0
1	B	1764	0	1737	20	0
1	C	1764	0	1737	23	0
1	D	1755	0	1713	22	0
1	E	1706	0	1636	33	0
1	F	1752	0	1704	20	0
1	G	1727	0	1672	25	0
1	H	1756	0	1715	16	0
1	I	1726	0	1667	22	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	F	3	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
All	All	15733	0	15329	196	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 6.

All (196) 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:G:574:MSE:HE2	1:G:578:LEU:HG	1.70	0.73
1:G:646:VAL:O	1:G:650:LEU:HB2	1.92	0.69
1:D:630:MSE:HE3	1:D:630:MSE:HA	1.74	0.69
1:F:580:ALA:O	1:F:584:SER:HB3	1.93	0.69
1:F:689:VAL:HG11	1:G:535:MSE:HG3	1.74	0.69
1:E:568:LEU:HD13	1:E:574:MSE:HG3	1.73	0.68
1:A:633:LEU:HD21	1:A:688:LEU:HD22	1.75	0.68
1:E:535:MSE:HA	1:E:537:ASP:H	1.59	0.67
1:E:633:LEU:HD21	1:E:688:LEU:HD22	1.77	0.66
1:I:546:ILE:HG12	1:I:694:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:604:LEU:O	1:I:608:GLU:HG2	1.96	0.65
1:A:547:LEU:HD11	1:A:601:GLU:HG3	1.79	0.65
1:I:607:TRP:CD1	1:I:620:GLN:HG2	2.31	0.65
1:E:604:LEU:O	1:E:608:GLU:HG2	1.97	0.65
1:H:633:LEU:HD21	1:H:688:LEU:HD22	1.78	0.65
1:I:633:LEU:HD21	1:I:688:LEU:HD22	1.79	0.65
1:D:630:MSE:HE1	1:D:633:LEU:HD23	1.80	0.64
1:A:580:ALA:O	1:A:584:SER:HB3	1.99	0.63
1:B:607:TRP:CD1	1:B:620:GLN:HG2	2.34	0.62
1:C:533:PRO:HD3	1:C:608:GLU:HA	1.81	0.62
1:G:644:ASP:OD1	1:G:645:GLU:N	2.32	0.62
1:C:547:LEU:HD11	1:C:601:GLU:HG3	1.82	0.61
1:E:546:ILE:HG12	1:E:694:LEU:HD13	1.81	0.61
1:A:574:MSE:HB3	1:A:579:MSE:HE3	1.82	0.61
1:D:543:ALA:HB1	1:D:604:LEU:HD21	1.83	0.60
1:A:607:TRP:CD1	1:A:620:GLN:HG2	2.38	0.59
1:C:702:TYR:CE2	1:C:708:ASP:HB3	2.39	0.58
1:C:633:LEU:HD21	1:C:688:LEU:HD22	1.84	0.58
1:E:551:ARG:HG2	1:E:597:LEU:HD11	1.86	0.58
1:A:627:LEU:HD13	1:A:714:GLU:HB3	1.86	0.57
1:G:702:TYR:CE2	1:G:708:ASP:HB3	2.39	0.57
1:B:542:ILE:HG21	1:B:698:LEU:HG	1.86	0.57
1:D:580:ALA:O	1:D:584:SER:HB3	2.04	0.57
1:B:547:LEU:HD11	1:B:601:GLU:HG3	1.86	0.57
1:E:642:ARG:O	1:E:646:VAL:HG23	2.05	0.56
1:C:720:THR:O	1:C:724:THR:HG23	2.07	0.55
1:D:630:MSE:CE	1:D:719:ILE:HD13	2.36	0.55
1:H:543:ALA:HB1	1:H:604:LEU:HD21	1.88	0.55
1:C:717:LYS:O	1:C:721:GLU:HG3	2.08	0.54
1:B:682:LEU:HD23	1:B:733:LEU:HD22	1.89	0.54
1:I:607:TRP:NE1	1:I:620:GLN:HG2	2.22	0.54
1:G:553:TYR:HE2	1:G:593:HIS:CD2	2.25	0.54
1:H:581:LEU:HG	1:H:646:VAL:HG22	1.90	0.54
1:D:650:LEU:O	1:D:654:THR:HG23	2.08	0.54
1:F:533:PRO:HD3	1:F:608:GLU:HA	1.90	0.54
1:E:563:TRP:CD1	1:E:672:VAL:HG11	2.43	0.54
1:A:737:GLN:HG3	1:A:738:LYS:N	2.22	0.54
1:G:538:GLU:HG2	1:G:542:ILE:HD11	1.90	0.53
1:E:534:HIS:O	1:E:537:ASP:HB3	2.07	0.53
1:D:633:LEU:HD21	1:D:688:LEU:HD22	1.89	0.53
1:I:535:MSE:HE3	1:I:541:PHE:HZ	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:MSE:HE1	1:D:719:ILE:HD13	1.90	0.53
1:F:633:LEU:HD21	1:F:688:LEU:HD22	1.90	0.53
1:G:565:ARG:O	1:G:569:ILE:HG12	2.08	0.53
1:C:546:ILE:HG12	1:C:694:LEU:HD13	1.91	0.52
1:E:644:ASP:OD1	1:E:645:GLU:N	2.42	0.52
1:B:585:ASN:OD1	1:B:642:ARG:NH2	2.41	0.52
1:E:702:TYR:CE2	1:E:708:ASP:HB3	2.45	0.52
1:E:564:PHE:O	1:E:568:LEU:HG	2.10	0.52
1:F:543:ALA:HB1	1:F:604:LEU:HD21	1.92	0.52
1:B:633:LEU:HD21	1:B:688:LEU:HD22	1.91	0.52
1:G:673:CYS:SG	1:G:677:LEU:HB3	2.50	0.52
1:H:607:TRP:CD1	1:H:620:GLN:HG2	2.45	0.51
1:A:568:LEU:HB3	1:A:579:MSE:HE2	1.92	0.51
1:E:565:ARG:O	1:E:569:ILE:HG12	2.10	0.51
1:G:546:ILE:HG12	1:G:694:LEU:HD13	1.93	0.51
1:G:607:TRP:CD1	1:G:620:GLN:HG2	2.45	0.51
1:C:607:TRP:CD1	1:C:620:GLN:HG2	2.46	0.51
1:A:533:PRO:HD3	1:A:608:GLU:HA	1.91	0.51
1:C:682:LEU:HD23	1:C:733:LEU:HD22	1.92	0.51
1:E:553:TYR:HE2	1:E:593:HIS:CD2	2.29	0.51
1:I:702:TYR:CE2	1:I:708:ASP:HB3	2.45	0.51
1:C:542:ILE:HG21	1:C:698:LEU:HG	1.93	0.51
1:F:680:PHE:HA	1:F:683:LYS:HG3	1.92	0.50
1:E:607:TRP:CD1	1:E:620:GLN:HG2	2.47	0.50
1:A:594:ARG:NH2	1:F:745:ASP:O	2.45	0.50
1:B:747:VAL:HG21	1:F:554:LEU:HB3	1.94	0.50
1:G:633:LEU:HD21	1:G:688:LEU:HD22	1.94	0.49
1:G:564:PHE:O	1:G:568:LEU:HG	2.13	0.49
1:F:728:GLN:HB3	1:F:732:ARG:NH2	2.28	0.49
1:G:574:MSE:HB3	1:G:579:MSE:HG3	1.94	0.49
1:A:581:LEU:HG	1:A:646:VAL:HG22	1.95	0.48
1:H:651:GLU:HA	1:H:654:THR:HG22	1.95	0.48
1:E:640:PHE:CE2	1:E:688:LEU:HD11	2.48	0.48
1:A:702:TYR:CE2	1:A:708:ASP:HB3	2.48	0.48
1:A:717:LYS:O	1:A:721:GLU:HG3	2.13	0.48
1:E:575:PRO:HD2	1:E:578:LEU:HD12	1.94	0.48
1:F:651:GLU:OE2	1:F:740:THR:HG21	2.14	0.48
1:G:677:LEU:HA	1:G:680:PHE:HD1	1.78	0.48
1:I:614:HIS:CD2	1:I:615:LEU:HG	2.49	0.48
1:D:553:TYR:HE2	1:D:593:HIS:CD2	2.32	0.48
1:F:604:LEU:O	1:F:608:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:626:LEU:O	1:F:630:MSE:HG2	2.13	0.48
1:D:626:LEU:O	1:D:630:MSE:HG2	2.14	0.47
1:I:646:VAL:O	1:I:650:LEU:HB2	2.14	0.47
1:E:575:PRO:HG2	1:E:578:LEU:HD12	1.95	0.47
1:H:542:ILE:HG21	1:H:698:LEU:HG	1.96	0.47
1:G:592:PHE:CE2	1:G:633:LEU:HD13	2.50	0.47
1:C:627:LEU:HD13	1:C:714:GLU:HB3	1.97	0.46
1:D:677:LEU:O	1:D:677:LEU:HG	2.13	0.46
1:I:717:LYS:O	1:I:721:GLU:HG3	2.16	0.46
1:F:651:GLU:HA	1:F:654:THR:HG22	1.98	0.46
1:A:624:ASP:OD1	1:A:624:ASP:N	2.47	0.46
1:E:618:ASP:OD2	1:E:707:ARG:NH2	2.49	0.46
1:B:535:MSE:HE3	1:C:686:GLN:HB2	1.97	0.45
1:B:594:ARG:NH2	1:H:745:ASP:O	2.49	0.45
1:D:544:LYS:HA	1:D:544:LYS:HD2	1.77	0.45
1:D:565:ARG:NH1	1:D:587:ASP:OD2	2.42	0.45
1:D:630:MSE:HE2	1:D:719:ILE:HB	1.98	0.45
1:I:592:PHE:CE2	1:I:633:LEU:HD13	2.52	0.45
1:B:736:LEU:HD23	1:B:736:LEU:HA	1.56	0.45
1:E:646:VAL:HG12	1:E:650:LEU:HD12	1.99	0.45
1:A:626:LEU:HD13	1:A:695:LEU:HD21	1.98	0.45
1:D:535:MSE:HE2	1:E:689:VAL:HG21	1.99	0.45
1:E:580:ALA:O	1:E:584:SER:HB2	2.17	0.45
1:F:553:TYR:HE2	1:F:593:HIS:CD2	2.35	0.45
1:G:704:PRO:HA	1:G:709:TYR:CG	2.52	0.45
1:A:736:LEU:HA	1:A:736:LEU:HD23	1.73	0.45
1:I:618:ASP:HA	1:I:621:ARG:HE	1.82	0.45
1:B:547:LEU:HD13	1:B:600:VAL:HG12	1.99	0.44
1:F:592:PHE:CE2	1:F:633:LEU:HD13	2.51	0.44
1:B:604:LEU:O	1:B:608:GLU:HG2	2.17	0.44
1:D:604:LEU:O	1:D:608:GLU:HG2	2.17	0.44
1:F:677:LEU:O	1:F:677:LEU:HG	2.15	0.44
1:G:534:HIS:O	1:G:537:ASP:HB3	2.16	0.44
1:H:626:LEU:O	1:H:630:MSE:HG2	2.18	0.44
1:B:586:ILE:HD13	1:B:586:ILE:HA	1.86	0.44
1:B:702:TYR:CE2	1:B:708:ASP:HB3	2.52	0.44
1:F:698:LEU:HD23	1:F:698:LEU:HA	1.81	0.44
1:A:681:LEU:HD23	1:A:681:LEU:HA	1.85	0.44
1:I:660:LEU:HD23	1:I:660:LEU:HA	1.69	0.44
1:C:604:LEU:O	1:C:608:GLU:HG2	2.18	0.43
1:D:680:PHE:HA	1:D:683:LYS:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:PHE:CE2	1:E:633:LEU:HD13	2.54	0.43
1:E:644:ASP:OD2	1:E:732:ARG:HD3	2.18	0.43
1:G:629:ASN:HA	1:G:632:GLN:HG2	2.00	0.43
1:C:594:ARG:NH2	1:D:745:ASP:O	2.51	0.43
1:G:587:ASP:N	1:G:588:PRO:HD2	2.32	0.43
1:I:642:ARG:O	1:I:646:VAL:HG23	2.18	0.43
1:A:682:LEU:HD23	1:A:733:LEU:HD22	2.01	0.43
1:A:682:LEU:HD11	1:A:737:GLN:HB3	1.99	0.43
1:G:542:ILE:HG21	1:G:698:LEU:HG	2.00	0.43
1:G:674:TYR:CD1	1:G:675:LEU:HG	2.53	0.43
1:E:542:ILE:HD13	1:E:697:ARG:NH2	2.34	0.43
1:H:547:LEU:HD23	1:H:604:LEU:HG	2.00	0.43
1:H:742:LEU:HD23	1:H:742:LEU:HA	1.90	0.43
1:E:587:ASP:N	1:E:588:PRO:HD2	2.34	0.42
1:I:696:SER:HA	1:I:716:LEU:HD22	2.01	0.42
1:B:554:LEU:HD12	1:B:597:LEU:HD22	2.01	0.42
1:I:676:PRO:HB2	1:I:679:THR:HG23	2.01	0.42
1:E:653:ALA:O	1:E:657:CYS:HB3	2.19	0.42
1:I:586:ILE:HD13	1:I:586:ILE:HA	1.80	0.42
1:H:553:TYR:HE2	1:H:593:HIS:CD2	2.38	0.42
1:B:543:ALA:HB1	1:B:604:LEU:HD21	2.01	0.42
1:C:564:PHE:CE2	1:C:568:LEU:HD11	2.54	0.42
1:C:565:ARG:HG3	1:C:583:PHE:CZ	2.55	0.42
1:C:637:THR:HG22	1:C:722:VAL:HG13	2.02	0.42
1:E:726:LEU:HA	1:E:726:LEU:HD23	1.81	0.42
1:F:614:HIS:CD2	1:F:615:LEU:HG	2.54	0.42
1:H:624:ASP:OD1	1:H:624:ASP:N	2.51	0.42
1:I:582:LEU:C	1:I:584:SER:H	2.27	0.42
1:C:624:ASP:OD1	1:C:624:ASP:N	2.53	0.42
1:C:681:LEU:HA	1:C:681:LEU:HD12	1.82	0.42
1:F:542:ILE:HG21	1:F:698:LEU:HG	2.01	0.42
1:G:564:PHE:HA	1:G:667:PHE:CE2	2.54	0.42
1:H:606:LEU:HD13	1:H:619:HIS:CE1	2.55	0.42
1:B:581:LEU:HG	1:B:646:VAL:HG22	2.01	0.42
1:H:621:ARG:HB2	1:H:708:ASP:CG	2.45	0.42
1:A:586:ILE:HD12	1:A:586:ILE:HG23	1.73	0.42
1:A:586:ILE:HD13	1:A:586:ILE:HA	1.90	0.42
1:D:574:MSE:HA	1:D:575:PRO:HD3	1.94	0.42
1:D:633:LEU:HD12	1:D:633:LEU:HA	1.73	0.42
1:D:717:LYS:O	1:D:721:GLU:HG3	2.20	0.41
1:I:568:LEU:HD23	1:I:568:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:587:ASP:N	1:I:588:PRO:HD2	2.35	0.41
1:B:641:GLN:HG3	1:B:726:LEU:HD23	2.03	0.41
1:C:637:THR:CG2	1:C:722:VAL:HG13	2.50	0.41
1:E:535:MSE:HA	1:E:537:ASP:N	2.29	0.41
1:B:586:ILE:HD12	1:B:586:ILE:HG23	1.85	0.41
1:E:564:PHE:HA	1:E:667:PHE:CE2	2.55	0.41
1:F:626:LEU:HD13	1:F:695:LEU:HD21	2.03	0.41
1:G:640:PHE:HE1	1:G:684:PRO:HB3	1.85	0.41
1:H:615:LEU:HB3	1:H:619:HIS:CD2	2.56	0.41
1:C:581:LEU:HG	1:C:646:VAL:HG22	2.02	0.41
1:B:676:PRO:HG2	1:B:679:THR:CG2	2.51	0.41
1:E:574:MSE:HE3	1:E:579:MSE:HA	2.02	0.41
1:C:594:ARG:NE	1:D:747:VAL:HG12	2.36	0.41
1:H:677:LEU:O	1:H:677:LEU:HG	2.15	0.41
1:A:737:GLN:HG3	1:A:738:LYS:H	1.84	0.40
1:A:737:GLN:O	1:A:741:GLU:HG2	2.21	0.40
1:C:736:LEU:HD23	1:C:736:LEU:HA	1.79	0.40
1:E:582:LEU:C	1:E:584:SER:H	2.30	0.40
1:G:696:SER:HA	1:G:716:LEU:HD22	2.03	0.40
1:E:555:LYS:HA	1:E:555:LYS:HD3	1.93	0.40
1:I:563:TRP:CE3	1:I:672:VAL:HG21	2.57	0.40
1:I:682:LEU:O	1:I:686:GLN:HG3	2.22	0.40

There are no symmetry-related clashes.

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	214/218 (98%)	209 (98%)	5 (2%)	0	100	100
1	B	214/218 (98%)	208 (97%)	6 (3%)	0	100	100
1	C	214/218 (98%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	214/218 (98%)	204 (95%)	10 (5%)	0	100	100
1	E	213/218 (98%)	196 (92%)	16 (8%)	1 (0%)	24	54
1	F	214/218 (98%)	204 (95%)	10 (5%)	0	100	100
1	G	213/218 (98%)	204 (96%)	9 (4%)	0	100	100
1	H	214/218 (98%)	208 (97%)	6 (3%)	0	100	100
1	I	213/218 (98%)	200 (94%)	12 (6%)	1 (0%)	24	54
All	All	1923/1962 (98%)	1838 (96%)	83 (4%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	583	PHE
1	E	622	ILE

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	190/192 (99%)	183 (96%)	7 (4%)	30	64
1	B	189/192 (98%)	181 (96%)	8 (4%)	26	60
1	C	189/192 (98%)	178 (94%)	11 (6%)	18	49
1	D	186/192 (97%)	177 (95%)	9 (5%)	23	55
1	E	176/192 (92%)	162 (92%)	14 (8%)	11	34
1	F	186/192 (97%)	174 (94%)	12 (6%)	15	44
1	G	180/192 (94%)	170 (94%)	10 (6%)	19	50
1	H	187/192 (97%)	176 (94%)	11 (6%)	18	48
1	I	180/192 (94%)	171 (95%)	9 (5%)	22	53
All	All	1663/1728 (96%)	1572 (94%)	91 (6%)	19	50

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LYS
1	A	551	ARG
1	A	584	SER
1	A	638	SER
1	A	672	VAL
1	A	693	LEU
1	A	732	ARG
1	B	566	SER
1	B	567	VAL
1	B	579	MSE
1	B	647	LEU
1	B	648	THR
1	B	672	VAL
1	B	738	LYS
1	B	740	THR
1	C	544	LYS
1	C	567	VAL
1	C	579	MSE
1	C	602	GLN
1	C	622	ILE
1	C	666	GLU
1	C	672	VAL
1	C	681	LEU
1	C	693	LEU
1	C	704	PRO
1	C	740	THR
1	D	567	VAL
1	D	584	SER
1	D	601	GLU
1	D	648	THR
1	D	672	VAL
1	D	685	VAL
1	D	704	PRO
1	D	719	ILE
1	D	727	GLN
1	E	535	MSE
1	E	542	ILE
1	E	574	MSE
1	E	611	SER
1	E	622	ILE
1	E	638	SER
1	E	650	LEU
1	E	672	VAL

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Mol	Chain	Res	Type
1	E	677	LEU
1	E	685	VAL
1	E	708	ASP
1	E	713	HIS
1	E	730	LEU
1	E	737	GLN
1	F	567	VAL
1	F	579	MSE
1	F	584	SER
1	F	604	LEU
1	F	608	GLU
1	F	622	ILE
1	F	648	THR
1	F	654	THR
1	F	672	VAL
1	F	683	LYS
1	F	685	VAL
1	F	693	LEU
1	G	581	LEU
1	G	586	ILE
1	G	611	SER
1	G	622	ILE
1	G	638	SER
1	G	646	VAL
1	G	650	LEU
1	G	685	VAL
1	G	695	LEU
1	G	708	ASP
1	H	538	GLU
1	H	547	LEU
1	H	555	LYS
1	H	567	VAL
1	H	594	ARG
1	H	601	GLU
1	H	602	GLN
1	H	604	LEU
1	H	648	THR
1	H	679	THR
1	H	737	GLN
1	I	542	ILE
1	I	554	LEU
1	I	569	ILE

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Mol	Chain	Res	Type
1	I	581	LEU
1	I	586	ILE
1	I	612	SER
1	I	650	LEU
1	I	672	VAL
1	I	708	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	629	ASN
1	B	656	HIS
1	B	743	GLN
1	C	632	GLN
1	C	678	ASN
1	C	727	GLN
1	D	678	ASN
1	E	593	HIS
1	E	619	HIS
1	E	686	GLN
1	E	727	GLN
1	F	629	ASN
1	G	619	HIS
1	G	629	ASN
1	H	641	GLN
1	I	614	HIS
1	I	713	HIS

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 oligosaccharides 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	212/218 (97%)	-1.12	0 100 100	42, 66, 97, 126	0
1	B	212/218 (97%)	-1.14	0 100 100	43, 67, 96, 124	0
1	C	212/218 (97%)	-1.09	0 100 100	43, 68, 96, 127	0
1	D	212/218 (97%)	-0.97	0 100 100	56, 79, 133, 184	0
1	E	211/218 (96%)	-0.52	0 100 100	65, 117, 161, 197	0
1	F	212/218 (97%)	-1.01	0 100 100	58, 80, 133, 177	0
1	G	211/218 (96%)	-0.55	0 100 100	64, 117, 165, 191	0
1	H	212/218 (97%)	-0.95	0 100 100	59, 80, 130, 173	0
1	I	211/218 (96%)	-0.55	0 100 100	66, 119, 166, 196	0
All	All	1905/1962 (97%)	-0.88	0 100 100	42, 84, 152, 197	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.