



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:52 AM UTC

PDB ID : 4C9E / pdb_00004c9e
Title : Mouse ZNRF3 ectodomain in complex with Xenopus RSPO2 Fu1-Fu2 (Seleno Met) crystal form II
Authors : Zebisch, M.; Jones, E.Y.
Deposited on : 2013-10-02
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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

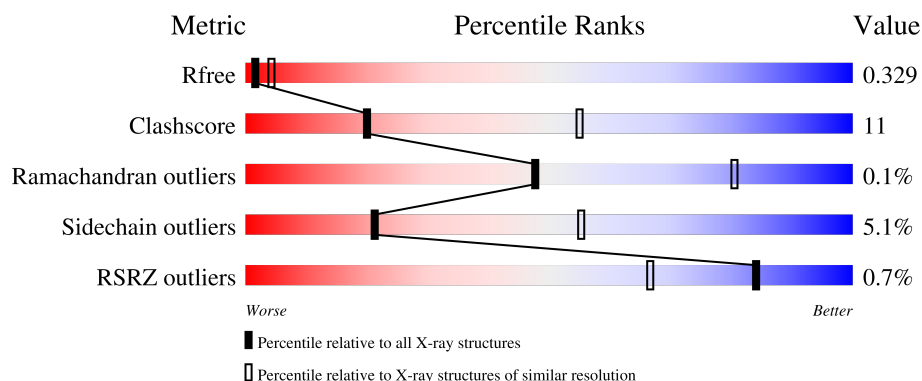
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	165	2% 70% 21% • 7%
1	C	165	% 73% 19% • 8%
1	E	165	% 69% 21% • 7%
1	G	165	68% 24% • 8%
2	B	121	70% 14% • 14%

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Mol	Chain	Length	Quality of chain
2	D	121	70% 14% • 14%
2	F	121	% 69% 15% • 15%
2	H	121	75% 8% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7644 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 E3 UBIQUITIN-PROTEIN LIGASE ZNR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1161	732	202	222	5			
1	C	152	Total	C	N	O	S	0	0	0
			1156	728	199	224	5			
1	E	153	Total	C	N	O	S	0	0	0
			1166	733	204	224	5			
1	G	152	Total	C	N	O	S	0	0	0
			1150	726	197	222	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLU	-	expression tag	UNP Q5SSZ7
A	51	THR	-	expression tag	UNP Q5SSZ7
A	52	GLY	-	expression tag	UNP Q5SSZ7
A	206	GLY	-	expression tag	UNP Q5SSZ7
A	207	THR	-	expression tag	UNP Q5SSZ7
A	208	LYS	-	expression tag	UNP Q5SSZ7
A	209	HIS	-	expression tag	UNP Q5SSZ7
A	210	HIS	-	expression tag	UNP Q5SSZ7
A	211	HIS	-	expression tag	UNP Q5SSZ7
A	212	HIS	-	expression tag	UNP Q5SSZ7
A	213	HIS	-	expression tag	UNP Q5SSZ7
A	214	HIS	-	expression tag	UNP Q5SSZ7
C	50	GLU	-	expression tag	UNP Q5SSZ7
C	51	THR	-	expression tag	UNP Q5SSZ7
C	52	GLY	-	expression tag	UNP Q5SSZ7
C	206	GLY	-	expression tag	UNP Q5SSZ7
C	207	THR	-	expression tag	UNP Q5SSZ7
C	208	LYS	-	expression tag	UNP Q5SSZ7
C	209	HIS	-	expression tag	UNP Q5SSZ7
C	210	HIS	-	expression tag	UNP Q5SSZ7
C	211	HIS	-	expression tag	UNP Q5SSZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	212	HIS	-	expression tag	UNP Q5SSZ7
C	213	HIS	-	expression tag	UNP Q5SSZ7
C	214	HIS	-	expression tag	UNP Q5SSZ7
E	50	GLU	-	expression tag	UNP Q5SSZ7
E	51	THR	-	expression tag	UNP Q5SSZ7
E	52	GLY	-	expression tag	UNP Q5SSZ7
E	206	GLY	-	expression tag	UNP Q5SSZ7
E	207	THR	-	expression tag	UNP Q5SSZ7
E	208	LYS	-	expression tag	UNP Q5SSZ7
E	209	HIS	-	expression tag	UNP Q5SSZ7
E	210	HIS	-	expression tag	UNP Q5SSZ7
E	211	HIS	-	expression tag	UNP Q5SSZ7
E	212	HIS	-	expression tag	UNP Q5SSZ7
E	213	HIS	-	expression tag	UNP Q5SSZ7
E	214	HIS	-	expression tag	UNP Q5SSZ7
G	50	GLU	-	expression tag	UNP Q5SSZ7
G	51	THR	-	expression tag	UNP Q5SSZ7
G	52	GLY	-	expression tag	UNP Q5SSZ7
G	206	GLY	-	expression tag	UNP Q5SSZ7
G	207	THR	-	expression tag	UNP Q5SSZ7
G	208	LYS	-	expression tag	UNP Q5SSZ7
G	209	HIS	-	expression tag	UNP Q5SSZ7
G	210	HIS	-	expression tag	UNP Q5SSZ7
G	211	HIS	-	expression tag	UNP Q5SSZ7
G	212	HIS	-	expression tag	UNP Q5SSZ7
G	213	HIS	-	expression tag	UNP Q5SSZ7
G	214	HIS	-	expression tag	UNP Q5SSZ7

- Molecule 2 is a protein called R-SPONDIN-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	Se	0	0	0
			732	447	136	131	17	1			
2	D	104	Total	C	N	O	S	Se	0	0	0
			774	475	143	138	17	1			
2	F	103	Total	C	N	O	S	Se	0	0	0
			736	450	135	133	17	1			
2	H	103	Total	C	N	O	S	Se	0	0	0
			769	472	142	137	17	1			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	GLU	-	expression tag	UNP Q5M7L6
B	33	THR	-	expression tag	UNP Q5M7L6
B	34	GLY	-	expression tag	UNP Q5M7L6
B	145	THR	-	expression tag	UNP Q5M7L6
B	146	LYS	-	expression tag	UNP Q5M7L6
B	147	HIS	-	expression tag	UNP Q5M7L6
B	148	HIS	-	expression tag	UNP Q5M7L6
B	149	HIS	-	expression tag	UNP Q5M7L6
B	150	HIS	-	expression tag	UNP Q5M7L6
B	151	HIS	-	expression tag	UNP Q5M7L6
B	152	HIS	-	expression tag	UNP Q5M7L6
D	32	GLU	-	expression tag	UNP Q5M7L6
D	33	THR	-	expression tag	UNP Q5M7L6
D	34	GLY	-	expression tag	UNP Q5M7L6
D	145	THR	-	expression tag	UNP Q5M7L6
D	146	LYS	-	expression tag	UNP Q5M7L6
D	147	HIS	-	expression tag	UNP Q5M7L6
D	148	HIS	-	expression tag	UNP Q5M7L6
D	149	HIS	-	expression tag	UNP Q5M7L6
D	150	HIS	-	expression tag	UNP Q5M7L6
D	151	HIS	-	expression tag	UNP Q5M7L6
D	152	HIS	-	expression tag	UNP Q5M7L6
F	32	GLU	-	expression tag	UNP Q5M7L6
F	33	THR	-	expression tag	UNP Q5M7L6
F	34	GLY	-	expression tag	UNP Q5M7L6
F	145	THR	-	expression tag	UNP Q5M7L6
F	146	LYS	-	expression tag	UNP Q5M7L6
F	147	HIS	-	expression tag	UNP Q5M7L6
F	148	HIS	-	expression tag	UNP Q5M7L6
F	149	HIS	-	expression tag	UNP Q5M7L6
F	150	HIS	-	expression tag	UNP Q5M7L6
F	151	HIS	-	expression tag	UNP Q5M7L6
F	152	HIS	-	expression tag	UNP Q5M7L6
H	32	GLU	-	expression tag	UNP Q5M7L6
H	33	THR	-	expression tag	UNP Q5M7L6
H	34	GLY	-	expression tag	UNP Q5M7L6
H	145	THR	-	expression tag	UNP Q5M7L6
H	146	LYS	-	expression tag	UNP Q5M7L6
H	147	HIS	-	expression tag	UNP Q5M7L6
H	148	HIS	-	expression tag	UNP Q5M7L6
H	149	HIS	-	expression tag	UNP Q5M7L6
H	150	HIS	-	expression tag	UNP Q5M7L6
H	151	HIS	-	expression tag	UNP Q5M7L6

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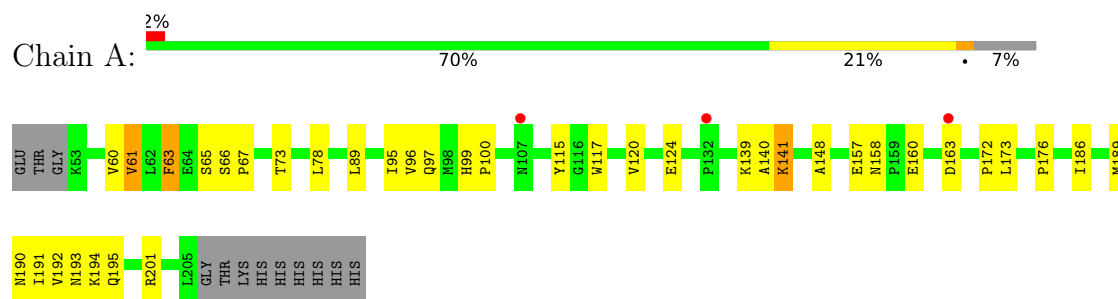
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Chain	Residue	Modelled	Actual	Comment	Reference
H	152	HIS	-	expression tag	UNP Q5M7L6

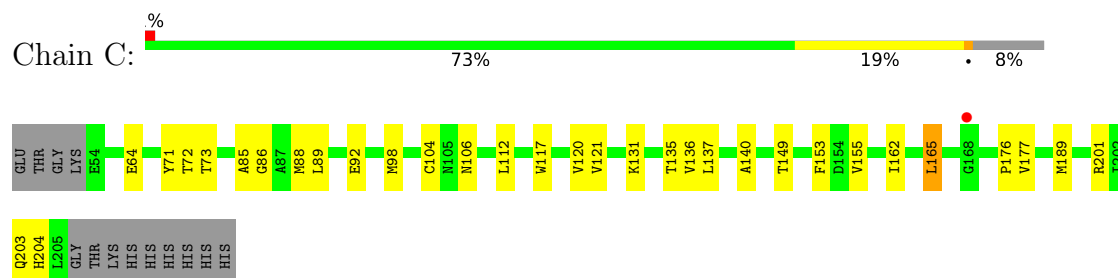
3 Residue-property plots [i](#)

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.

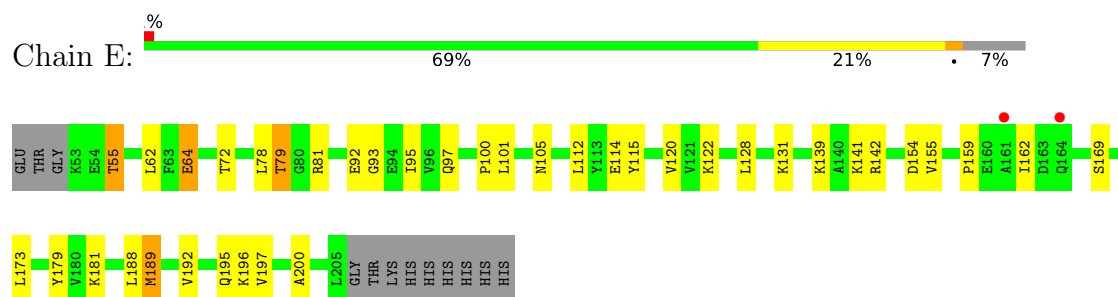
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



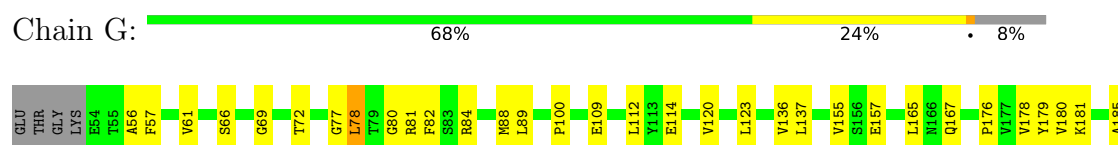
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3





- Molecule 2: R-SPONDIN-2

Chain B: 70% 14% 14%



- Molecule 2: R-SPONDIN-2

Chain D: 70% 14% 14%



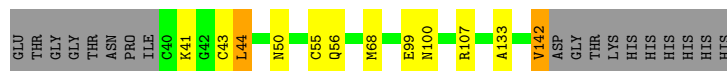
- Molecule 2: R-SPONDIN-2

Chain F: 69% 15% 15%



- Molecule 2: R-SPONDIN-2

Chain H: 75% 8% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.99Å 71.28Å 72.11Å 69.29° 61.48° 84.31°	Depositor
Resolution (Å)	35.37 – 3.00 35.37 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.37-3.00) 98.0 (35.37-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.245 , 0.334 0.247 , 0.329	Depositor DCC
R_{free} test set	1178 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7644	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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

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	0.83	0/1181	1.06	4/1602 (0.2%)
1	C	0.76	0/1176	1.04	0/1596
1	E	0.81	0/1186	1.08	1/1609 (0.1%)
1	G	0.74	0/1170	1.00	1/1588 (0.1%)
2	B	0.64	0/745	0.92	0/1000
2	D	0.58	0/789	0.86	0/1055
2	F	0.62	0/750	0.90	1/1007 (0.1%)
2	H	0.65	0/784	0.90	0/1048
All	All	0.73	0/7781	0.99	7/10505 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	GLY	N-CA-C	6.56	120.19	110.42
1	G	66	SER	N-CA-C	-6.20	102.06	110.36
1	A	61	VAL	CB-CA-C	-5.88	103.35	110.99
2	F	104	CYS	N-CA-C	5.62	117.73	109.24
1	A	186	ILE	CB-CA-C	-5.52	104.91	111.97
1	A	141	LYS	N-CA-C	5.27	117.71	111.33
1	A	63	PHE	N-CA-C	5.08	117.11	109.23

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	1161	0	1153	33	0
1	C	1156	0	1146	20	0
1	E	1166	0	1159	26	0
1	G	1150	0	1138	30	0
2	B	732	0	625	30	0
2	D	774	0	703	16	0
2	F	736	0	630	18	0
2	H	769	0	701	22	0
All	All	7644	0	7255	170	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 11.

All (170) 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:B:59:LEU:HD22	2:B:75:LEU:C	1.37	1.47
2:B:59:LEU:CD2	2:B:75:LEU:C	2.10	1.23
2:B:59:LEU:HD22	2:B:75:LEU:O	1.42	1.18
2:H:44:LEU:HD21	2:H:56:GLN:N	1.60	1.16
2:B:59:LEU:CD2	2:B:75:LEU:O	1.92	1.16
2:H:44:LEU:CD2	2:H:56:GLN:HG3	1.81	1.08
2:H:44:LEU:HD21	2:H:56:GLN:CA	1.85	1.05
2:H:44:LEU:HD22	2:H:56:GLN:HG3	1.49	0.92
2:B:59:LEU:HD21	2:B:76:GLN:CA	2.01	0.90
2:B:59:LEU:CD2	2:B:76:GLN:HA	2.01	0.90
2:B:59:LEU:CD2	2:B:76:GLN:N	2.35	0.90
1:C:120:VAL:HG11	1:C:189:MET:HE1	1.54	0.88
2:H:44:LEU:CD2	2:H:56:GLN:N	2.38	0.86
2:B:59:LEU:CD2	2:B:76:GLN:CA	2.54	0.85
2:B:59:LEU:HD23	2:B:75:LEU:O	1.75	0.85
1:G:120:VAL:HG11	1:G:189:MET:HE1	1.58	0.83
1:A:192:VAL:HG22	2:B:68:MSE:HE2	1.59	0.83
2:B:98:ILE:HD12	2:B:108:ASP:HA	1.61	0.83
2:H:44:LEU:HD21	2:H:56:GLN:HG3	1.59	0.81
1:G:181:LYS:HA	1:G:185:ALA:HB2	1.63	0.81
2:B:59:LEU:HD21	2:B:76:GLN:HA	1.62	0.80
1:E:192:VAL:HG22	2:F:68:MSE:HE2	1.64	0.77
1:A:60:VAL:HG11	1:A:191:ILE:HD13	1.67	0.76
2:D:83:TYR:OH	2:D:107:ARG:HA	1.87	0.75
1:C:155:VAL:HG21	1:C:162:ILE:HD11	1.67	0.75
2:B:59:LEU:HD21	2:B:76:GLN:N	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:THR:HG23	1:E:79:THR:HG23	1.72	0.71
2:D:100:ASN:HA	2:D:114:LYS:HE3	1.73	0.71
2:H:44:LEU:HD21	2:H:56:GLN:HA	1.72	0.71
2:B:59:LEU:HD23	2:B:76:GLN:HA	1.72	0.70
2:D:82:TYR:OH	2:D:95:ARG:NH2	2.25	0.70
2:H:44:LEU:HD23	2:H:44:LEU:N	2.08	0.68
1:G:136:VAL:HG12	1:G:165:LEU:HD21	1.76	0.67
1:G:78:LEU:HD23	1:G:78:LEU:N	2.11	0.65
2:F:98:ILE:HG23	2:F:101:CYS:HB3	1.79	0.65
1:G:188:LEU:HG	1:G:189:MET:HE2	1.77	0.64
1:A:120:VAL:CG1	1:A:189:MET:HE1	2.28	0.63
1:C:136:VAL:HG12	1:C:165:LEU:HD13	1.80	0.63
1:G:89:LEU:HB2	1:G:176:PRO:HG3	1.80	0.63
1:C:120:VAL:CG1	1:C:189:MET:HE1	2.28	0.62
1:G:84:ARG:HA	1:G:88:MET:HE1	1.82	0.62
1:E:120:VAL:CG1	1:E:189:MET:HE1	2.30	0.61
1:A:89:LEU:O	1:A:176:PRO:HG3	2.00	0.61
1:A:158:ASN:OD1	1:A:160:GLU:HB2	2.00	0.61
1:A:95:ILE:CG2	2:B:68:MSE:HE3	2.31	0.60
2:H:44:LEU:HD21	2:H:56:GLN:CG	2.30	0.60
1:E:95:ILE:HG21	2:F:68:MSE:HE3	1.82	0.60
2:D:83:TYR:CD1	2:D:104:CYS:HB2	2.37	0.59
2:D:100:ASN:O	2:D:114:LYS:HG2	2.02	0.59
2:F:118:TYR:HA	2:F:139:MET:O	2.02	0.58
1:A:141:LYS:HA	1:A:173:LEU:HD11	1.84	0.58
1:G:57:PHE:CE2	1:G:205:LEU:HD12	2.38	0.58
1:G:61:VAL:HG21	1:G:201:ARG:HH11	1.69	0.58
2:D:64:ARG:NH1	2:D:71:TYR:OH	2.37	0.57
1:G:195:GLN:O	2:H:68:MSE:HE3	2.04	0.57
1:G:123:LEU:O	1:G:157:GLU:HB2	2.03	0.57
2:H:44:LEU:CD2	2:H:55:CYS:C	2.77	0.57
1:G:198:ALA:HB3	2:H:68:MSE:SE	2.54	0.56
1:A:120:VAL:HG13	1:A:189:MET:HE1	1.87	0.56
1:C:89:LEU:O	1:C:176:PRO:HG3	2.06	0.56
2:H:44:LEU:HD21	2:H:55:CYS:C	2.28	0.56
2:F:128:CYS:HB2	2:F:134:PRO:HD3	1.89	0.55
1:A:65:SER:CB	1:C:112:LEU:HD21	2.36	0.55
1:A:193:ASN:OD1	2:B:69:ARG:NH1	2.40	0.55
1:C:98:MET:HB2	1:C:121:VAL:HG22	1.89	0.55
1:C:140:ALA:HB2	1:C:153:PHE:HE2	1.73	0.54
1:E:81:ARG:HB2	1:E:179:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:VAL:CG1	1:G:189:MET:HE1	2.34	0.54
2:B:59:LEU:HD21	2:B:76:GLN:CG	2.38	0.54
1:C:155:VAL:HG21	1:C:162:ILE:CD1	2.37	0.54
2:D:114:LYS:HB2	2:D:117:PHE:CD2	2.43	0.54
1:G:181:LYS:HA	1:G:185:ALA:CB	2.35	0.53
1:G:178:VAL:HG12	1:G:179:TYR:N	2.22	0.53
1:A:97:GLN:O	2:B:65:ARG:NH2	2.40	0.53
1:A:117:TRP:CH2	1:A:148:ALA:HB2	2.44	0.53
1:E:101:LEU:HD11	2:F:53:LEU:O	2.09	0.52
1:A:115:TYR:HB2	1:C:71:TYR:CE2	2.45	0.52
2:B:62:TYR:CE2	2:B:64:ARG:HB2	2.45	0.52
1:A:100:PRO:O	1:A:139:LYS:HE3	2.10	0.52
2:F:135:LEU:CB	2:F:138:THR:CB	2.88	0.51
1:A:141:LYS:CA	1:A:173:LEU:HD11	2.40	0.51
2:F:98:ILE:CG2	2:F:101:CYS:HB3	2.39	0.51
2:D:83:TYR:OH	2:D:107:ARG:CA	2.57	0.51
1:A:141:LYS:HA	1:A:173:LEU:CD1	2.40	0.50
1:E:100:PRO:O	1:E:139:LYS:CE	2.60	0.50
1:C:136:VAL:CG1	1:C:165:LEU:HD13	2.41	0.50
2:H:44:LEU:HG	2:H:55:CYS:C	2.36	0.50
1:E:95:ILE:HG21	2:F:68:MSE:CE	2.42	0.49
1:A:61:VAL:HG21	1:A:201:ARG:NH1	2.28	0.49
1:C:98:MET:SD	2:D:65:ARG:NH2	2.83	0.49
1:A:190:ASN:HB3	1:A:194:LYS:CE	2.42	0.49
1:E:92:GLU:HA	1:E:200:ALA:O	2.13	0.49
2:B:59:LEU:HD21	2:B:76:GLN:HG3	1.94	0.49
1:C:104:CYS:C	1:C:106:ASN:H	2.21	0.48
1:C:140:ALA:HB2	1:C:153:PHE:CE2	2.49	0.48
1:A:63:PHE:HB3	1:A:73:THR:HG22	1.94	0.48
1:E:112:LEU:HD13	1:G:69:GLY:HA2	1.96	0.48
2:H:44:LEU:CD2	2:H:56:GLN:CG	2.73	0.48
1:A:95:ILE:HG21	2:B:68:MSE:HE3	1.95	0.47
1:C:92:GLU:HG3	1:C:201:ARG:HG2	1.95	0.47
1:E:95:ILE:CG2	2:F:68:MSE:HE3	2.44	0.47
1:E:122:LYS:HE2	2:F:49:ASP:OD2	2.14	0.47
1:E:78:LEU:HD21	1:E:188:LEU:HB2	1.95	0.47
1:A:60:VAL:HG11	1:A:191:ILE:HG21	1.96	0.47
2:H:44:LEU:HG	2:H:55:CYS:O	2.15	0.47
2:H:44:LEU:CD2	2:H:44:LEU:N	2.76	0.47
1:E:114:GLU:HG2	1:E:115:TYR:O	2.15	0.46
1:A:141:LYS:CB	1:A:173:LEU:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:LEU:HD21	1:G:165:LEU:O	2.14	0.46
2:B:59:LEU:HD22	2:B:75:LEU:CA	2.31	0.46
1:G:80:GLY:HA3	1:G:180:VAL:HG12	1.97	0.46
2:D:113:CYS:HB3	2:D:117:PHE:HB2	1.98	0.46
2:H:99:GLU:O	2:H:100:ASN:HB2	2.16	0.46
2:B:98:ILE:HG23	2:B:101:CYS:HB3	1.98	0.45
2:D:138:THR:OG1	2:D:140:VAL:HG22	2.16	0.45
2:F:98:ILE:HG23	2:F:101:CYS:CB	2.46	0.45
1:E:142:ARG:HA	1:E:142:ARG:HD2	1.81	0.45
2:B:65:ARG:NH1	2:B:68:MSE:O	2.50	0.45
1:A:96:VAL:HG12	2:B:65:ARG:NH2	2.31	0.45
1:A:141:LYS:CG	1:A:173:LEU:HD11	2.46	0.45
2:D:64:ARG:HD2	2:D:73:GLU:CD	2.42	0.45
1:G:77:GLY:C	1:G:78:LEU:HD23	2.40	0.45
1:E:141:LYS:CG	1:E:173:LEU:HD21	2.46	0.45
1:G:81:ARG:O	1:G:178:VAL:HG13	2.16	0.45
1:G:84:ARG:CA	1:G:88:MET:HE1	2.47	0.44
2:F:50:ASN:HB2	2:F:53:LEU:HD21	1.99	0.44
2:D:99:GLU:O	2:D:100:ASN:HB2	2.16	0.44
2:D:59:LEU:CD2	2:D:76:GLN:HG3	2.48	0.44
1:E:97:GLN:HB3	2:F:69:ARG:HA	1.99	0.44
2:H:133:ALA:O	2:H:142:VAL:HG22	2.18	0.44
1:A:124:GLU:HA	1:A:157:GLU:HG3	1.99	0.44
2:F:134:PRO:HA	2:F:141:CYS:HA	1.99	0.44
2:H:44:LEU:HD11	2:H:56:GLN:HA	1.98	0.44
1:A:157:GLU:OE1	1:A:157:GLU:HA	2.17	0.44
1:G:114:GLU:H	1:G:114:GLU:CD	2.19	0.44
1:A:139:LYS:O	1:A:140:ALA:C	2.61	0.43
1:E:62:LEU:HD21	1:E:195:GLN:HG3	2.00	0.43
1:E:101:LEU:HD12	2:F:61:PHE:CZ	2.52	0.43
2:H:44:LEU:HD23	2:H:44:LEU:H	1.81	0.43
1:E:154:ASP:C	1:E:154:ASP:OD1	2.59	0.43
1:G:89:LEU:O	1:G:176:PRO:HG2	2.18	0.43
2:B:58:LYS:HD2	2:B:58:LYS:N	2.33	0.43
1:G:187:LYS:O	1:G:191:ILE:HG13	2.18	0.43
1:A:190:ASN:HB3	1:A:194:LYS:HE2	2.01	0.43
1:A:141:LYS:HG3	1:A:173:LEU:HD11	2.00	0.43
2:D:83:TYR:CG	2:D:104:CYS:HB2	2.54	0.43
2:F:40:CYS:SG	2:F:43:CYS:SG	3.18	0.42
1:E:128:LEU:HD22	2:F:45:SER:HB3	2.01	0.42
1:A:95:ILE:HB	2:B:68:MSE:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:LYS:HG2	1:E:173:LEU:HD21	2.01	0.42
1:G:178:VAL:CG1	1:G:179:TYR:N	2.83	0.42
1:C:88:MET:HB3	1:C:204:HIS:CD2	2.54	0.42
1:C:155:VAL:CG2	1:C:162:ILE:HD11	2.44	0.42
1:G:82:PHE:HB3	1:G:88:MET:SD	2.60	0.42
1:G:56:ALA:N	1:G:80:GLY:O	2.42	0.42
1:G:84:ARG:HA	1:G:88:MET:CE	2.47	0.41
1:E:159:PRO:O	1:E:162:ILE:HD12	2.21	0.41
1:C:86:GLY:HA3	1:C:177:VAL:HG23	2.02	0.41
1:E:196:LYS:C	1:E:197:VAL:HG13	2.45	0.41
1:G:100:PRO:HD3	2:H:50:ASN:ND2	2.35	0.41
2:B:100:ASN:CB	2:B:117:PHE:CE2	3.04	0.41
2:B:64:ARG:O	2:B:70:GLN:HA	2.21	0.40
1:A:195:GLN:OE1	1:E:64:GLU:HG3	2.21	0.40
1:C:117:TRP:O	1:C:149:THR:HG22	2.21	0.40
2:D:114:LYS:HB2	2:D:117:PHE:CE2	2.56	0.40
1:E:159:PRO:O	1:E:162:ILE:HG13	2.21	0.40
1:A:99:HIS:CD2	2:B:50:ASN:HB3	2.56	0.40
1:C:85:ALA:HB1	1:C:137:LEU:HD21	2.03	0.40
1:A:66:SER:HB2	1:A:67:PRO:HD2	2.04	0.40
1:G:136:VAL:CG1	1:G:165:LEU:HD21	2.49	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	151/165 (92%)	146 (97%)	4 (3%)	1 (1%)	18	53
1	C	150/165 (91%)	142 (95%)	8 (5%)	0	100	100
1	E	151/165 (92%)	143 (95%)	8 (5%)	0	100	100
1	G	150/165 (91%)	145 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	102/121 (84%)	95 (93%)	7 (7%)	0	100	100
2	D	102/121 (84%)	92 (90%)	10 (10%)	0	100	100
2	F	101/121 (84%)	94 (93%)	7 (7%)	0	100	100
2	H	101/121 (84%)	90 (89%)	11 (11%)	0	100	100
All	All	1008/1144 (88%)	947 (94%)	60 (6%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO

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	123/138 (89%)	121 (98%)	2 (2%)	55	79
1	C	124/138 (90%)	117 (94%)	7 (6%)	19	52
1	E	125/138 (91%)	115 (92%)	10 (8%)	11	38
1	G	122/138 (88%)	116 (95%)	6 (5%)	22	56
2	B	71/106 (67%)	66 (93%)	5 (7%)	14	44
2	D	83/106 (78%)	80 (96%)	3 (4%)	31	65
2	F	73/106 (69%)	70 (96%)	3 (4%)	27	61
2	H	83/106 (78%)	78 (94%)	5 (6%)	17	50
All	All	804/976 (82%)	763 (95%)	41 (5%)	21	55

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

Mol	Chain	Res	Type
1	A	78	LEU
1	A	163	ASP
2	B	43	CYS

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Mol	Chain	Res	Type
2	B	58	LYS
2	B	66	GLU
2	B	68	MSE
2	B	94	SER
1	C	64	GLU
1	C	72	THR
1	C	73	THR
1	C	131	LYS
1	C	135	THR
1	C	165	LEU
1	C	203	GLN
2	D	43	CYS
2	D	107	ARG
2	D	114	LYS
1	E	55	THR
1	E	64	GLU
1	E	72	THR
1	E	79	THR
1	E	105	ASN
1	E	131	LYS
1	E	155	VAL
1	E	169	SER
1	E	181	LYS
1	E	189	MET
2	F	43	CYS
2	F	68	MSE
2	F	103	SER
1	G	72	THR
1	G	78	LEU
1	G	109	GLU
1	G	112	LEU
1	G	155	VAL
1	G	167	GLN
2	H	41	LYS
2	H	43	CYS
2	H	44	LEU
2	H	107	ARG
2	H	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	HIS
1	C	166	ASN
1	C	167	GLN
1	C	193	ASN
1	C	203	GLN
2	D	120	HIS
1	E	125	GLN
2	F	100	ASN
1	G	74	HIS
1	G	166	ASN
1	G	167	GLN
1	G	193	ASN
1	G	203	GLN
1	G	204	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	153/165 (92%)	0.00	3 (1%) 65 41	34, 78, 144, 191	0
1	C	152/165 (92%)	-0.09	1 (0%) 84 66	37, 83, 129, 183	0
1	E	153/165 (92%)	0.02	2 (1%) 75 53	34, 81, 138, 163	0
1	G	152/165 (92%)	-0.01	0 100 100	40, 88, 140, 162	0
2	B	103/121 (85%)	0.08	0 100 100	66, 114, 148, 163	0
2	D	103/121 (85%)	0.18	0 100 100	54, 131, 190, 242	0
2	F	102/121 (84%)	0.14	1 (0%) 79 59	70, 121, 157, 194	0
2	H	102/121 (84%)	0.06	0 100 100	57, 116, 156, 186	0
All	All	1020/1144 (89%)	0.03	7 (0%) 84 66	34, 100, 156, 242	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ASN	2.9
1	A	132	PRO	2.5
1	C	168	GLY	2.5
1	E	161	ALA	2.3
2	F	50	ASN	2.3
1	E	164	GLN	2.3
1	A	163	ASP	2.2

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.