



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:22 PM GMT

PDB ID : 4C9E
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

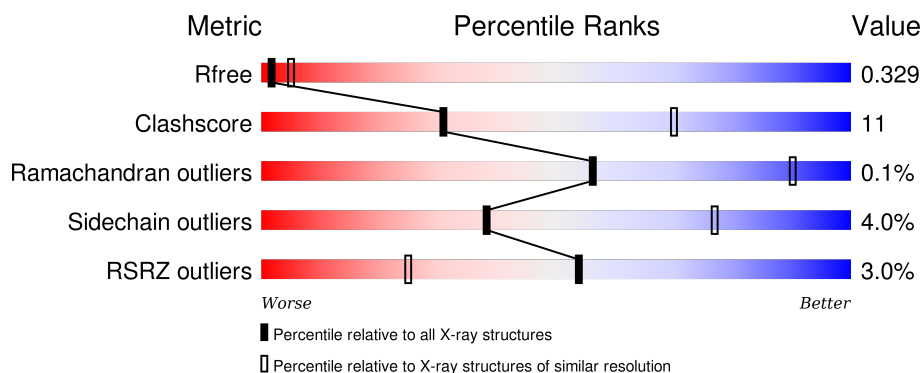
1 Overall quality at a glance

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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 $\leq 5\%$. 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	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 21% 7% </div> </div>
1	C	165	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 73% 19% 8% </div> </div>
1	E	165	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 73% 19% • 7% </div> </div>
1	G	165	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 69% 22% • 8% </div> </div>
2	B	121	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 4% </div> <div style="display: flex; justify-content: space-between; width: 100%;"> 70% 14% • 14% </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	121	<div><div><div></div><div></div><div></div></div><div>7%70%15%•14%</div></div>
2	F	121	<div><div><div></div><div></div><div></div></div><div>3%69%16%•15%</div></div>
2	H	121	<div><div><div></div><div></div><div></div></div><div>2%75%8%•15%</div></div>

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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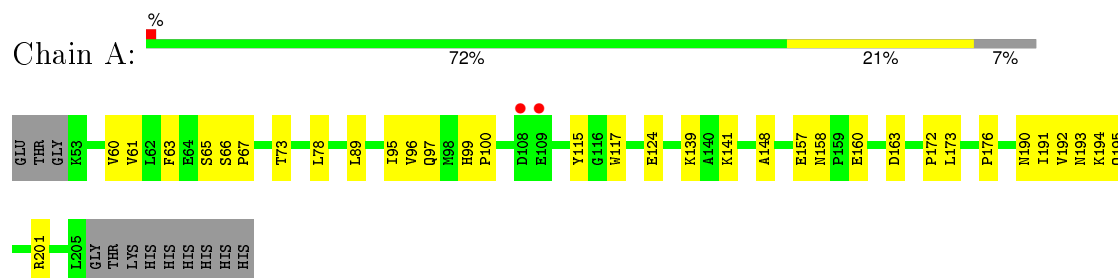
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Chain	Residue	Modelled	Actual	Comment	Reference
H	152	HIS	-	EXPRESSION TAG	UNP Q5M7L6

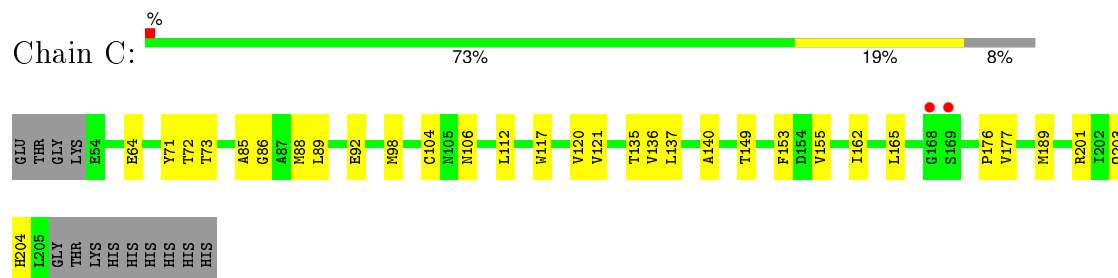
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

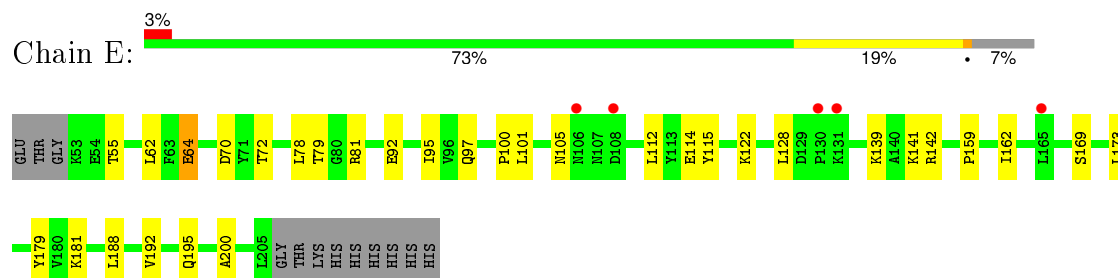
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



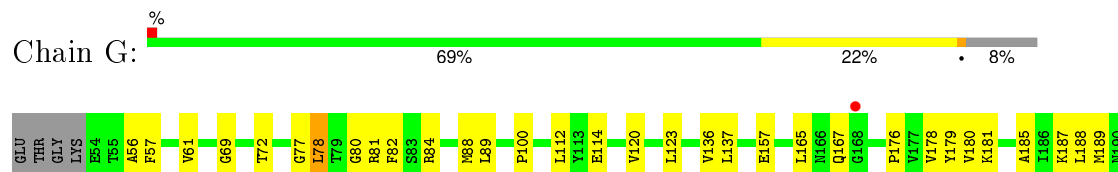
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3





• Molecule 2: R-SPONDIN-2



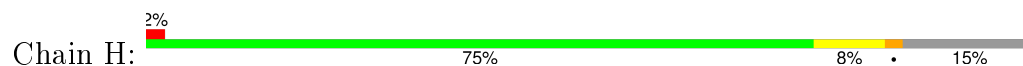
• Molecule 2: R-SPONDIN-2



• Molecule 2: R-SPONDIN-2



• Molecule 2: R-SPONDIN-2



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 35.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.37-3.00) 87.0 (35.34-3.00)	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 (5.47%)	DCC
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 22716 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 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		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/1181	0.79	0/1602
1	C	0.56	0/1176	0.77	0/1596
1	E	0.59	0/1186	0.78	0/1609
1	G	0.55	0/1170	0.75	0/1588
2	B	0.44	0/745	0.68	0/1000
2	D	0.42	0/789	0.67	0/1055
2	F	0.45	0/750	0.71	0/1007
2	H	0.54	1/784 (0.1%)	0.70	0/1048
All	All	0.53	1/7781 (0.0%)	0.74	0/10505

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	43	CYS	CB-SG	-7.48	1.69	1.82

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	1161	0	1153	30	0
1	C	1156	0	1146	20	0
1	E	1166	0	1159	23	0
1	G	1150	0	1138	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	163	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 (163) 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	1.42
2:B:59:LEU:CD2	2:B:75:LEU:C	2.10	1.18
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:158:ASN:OD1	1:A:160:GLU:HB2	2.00	0.61
1:A:89:LEU:O	1:A:176:PRO:HG3	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:B:59:LEU:HD22	2:B:75:LEU:CA	2.31	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
1:G:198:ALA:HB3	2:H:68:MSE:SE	2.54	0.56
1:C:89:LEU:O	1:C:176:PRO:HG3	2.06	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
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
2:H:44:LEU:CD2	2:H:55:CYS:C	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:LEU:CB	2:F:138:THR:CB	2.88	0.51
2:F:98:ILE:CG2	2:F:101:CYS:HB3	2.39	0.51
1:A:141:LYS:CA	1:A:173:LEU:HD11	2.40	0.51
2:D:83:TYR:OH	2:D:107:ARG:CA	2.57	0.51
2:H:44:LEU:HD21	2:H:55:CYS:C	2.28	0.50
1:A:141:LYS:HA	1:A:173:LEU:CD1	2.40	0.50
1:G:120:VAL:HG11	1:G:189:MET:CE	2.41	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
1:E:95:ILE:HG21	2:F:68:MSE:CE	2.42	0.49
1:C:98:MET:SD	2:D:65:ARG:NH2	2.83	0.49
1:A:61:VAL:HG21	1:A:201:ARG:NH1	2.28	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:140:ALA:HB2	1:C:153:PHE:CE2	2.49	0.48
2:H:44:LEU:CD2	2:H:56:GLN:CG	2.73	0.48
1:E:112:LEU:HD13	1:G:69:GLY:HA2	1.96	0.48
1:A:63:PHE:HB3	1:A:73:THR:HG22	1.94	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
2:H:44:LEU:HG	2:H:55:CYS:O	2.15	0.47
1:A:60:VAL:HG11	1:A:191:ILE:HG21	1.96	0.47
1:C:120:VAL:HG11	1:C:189:MET:HE1	1.97	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:G:137:LEU:HD21	1:G:165:LEU:O	2.14	0.46
1:A:141:LYS:CB	1:A:173:LEU:HD11	2.46	0.46
1:G:188:LEU:HG	1:G:189:MET:HE2	1.98	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:F:98:ILE:HG23	2:F:101:CYS:CB	2.46	0.45
2:D:138:THR:OG1	2:D:140:VAL:HG22	2.16	0.45
1:E:142:ARG:HD2	1:E:142:ARG:HA	1.81	0.45
2:B:65:ARG:NH1	2:B:68:MSE:O	2.50	0.45
2:H:44:LEU:HG	2:H:55:CYS:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:81:ARG:O	1:G:178:VAL:HG13	2.16	0.45
1:E:141:LYS:CG	1:E:173:LEU:HD21	2.46	0.45
1:G:84:ARG:HA	1:G:88:MET:CE	2.47	0.45
1:G:120:VAL:HG11	1:G:189:MET:HE1	1.98	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
1:C:104:CYS:C	1:C:106:ASN:H	2.21	0.44
2:H:133:ALA:O	2:H:142:VAL:HG22	2.18	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:44:LEU:HD11	2:H:56:GLN:HA	1.98	0.44
2:F:134:PRO:HA	2:F:141:CYS:HA	1.99	0.44
1:A:124:GLU:HA	1:A:157:GLU:HG3	1.99	0.44
1:A:157:GLU:HA	1:A:157:GLU:OE1	2.17	0.44
2:H:44:LEU:HD23	2:H:44:LEU:H	1.81	0.43
1:E:101:LEU:HD12	2:F:61:PHE:CZ	2.52	0.43
1:E:62:LEU:HD21	1:E:195:GLN:HG3	2.00	0.43
1:G:89:LEU:O	1:G:176:PRO:HG2	2.18	0.43
2:B:58:LYS:N	2:B:58:LYS:HD2	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
2:D:83:TYR:CG	2:D:104:CYS:HB2	2.54	0.43
1:A:141:LYS:HG3	1:A:173:LEU:HD11	2.00	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
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: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:G:100:PRO:HD3	2:H:50:ASN:ND2	2.35	0.41
1:G:77:GLY:C	1:G:78:LEU:HD23	2.40	0.41
1:G:188:LEU:HG	1:G:189:MET:CE	2.51	0.41
2:B:100:ASN:CB	2:B:117:PHE:CE2	3.04	0.41
1:C:120:VAL:HG11	1:C:189:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ARG:O	2:B:70:GLN:HA	2.21	0.40
2:D:114:LYS:HB2	2:D:117:PHE:CE2	2.56	0.40
1:C:117:TRP:O	1:C:149:THR:HG22	2.21	0.40
1:A:195:GLN:OE1	1:E:64:GLU:HG3	2.21	0.40
1:G:114:GLU:H	1:G:114:GLU:CD	2.19	0.40
2:D:64:ARG:HD2	2:D:73:GLU:CD	2.42	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:G:136:VAL:CG1	1:G:165:LEU:HD21	2.49	0.40
1:A:66:SER:HB2	1:A:67:PRO:HD2	2.04	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	151/165 (92%)	146 (97%)	4 (3%)	1 (1%)	26	70
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
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%)	56	90

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%)	70	92
1	C	124/138 (90%)	119 (96%)	5 (4%)	38	77
1	E	125/138 (91%)	119 (95%)	6 (5%)	31	71
1	G	122/138 (88%)	117 (96%)	5 (4%)	37	76
2	B	71/106 (67%)	66 (93%)	5 (7%)	19	55
2	D	83/106 (78%)	81 (98%)	2 (2%)	57	87
2	F	73/106 (69%)	70 (96%)	3 (4%)	37	76
2	H	83/106 (78%)	79 (95%)	4 (5%)	31	71
All	All	804/976 (82%)	772 (96%)	32 (4%)	38	77

All (32) 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
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	135	THR
1	C	203	GLN
2	D	43	CYS
2	D	107	ARG
1	E	64	GLU

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Mol	Chain	Res	Type
1	E	70	ASP
1	E	72	THR
1	E	105	ASN
1	E	169	SER
1	E	181	LYS
2	F	43	CYS
2	F	94	SER
2	F	103	SER
1	G	72	THR
1	G	78	LEU
1	G	112	LEU
1	G	167	GLN
1	G	193	ASN
2	H	41	LYS
2	H	43	CYS
2	H	44	LEU
2	H	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	HIS
1	C	145	GLN
1	C	167	GLN
1	C	203	GLN
1	G	74	HIS
1	G	167	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 ⓘ

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	153/165 (92%)	-0.29	2 (1%) 79 53	34, 78, 144, 191	0
1	C	152/165 (92%)	-0.35	2 (1%) 79 53	37, 83, 129, 183	0
1	E	153/165 (92%)	-0.23	5 (3%) 50 22	34, 81, 138, 163	0
1	G	152/165 (92%)	-0.31	1 (0%) 89 70	40, 88, 140, 162	0
2	B	103/121 (85%)	-0.25	5 (4%) 33 13	66, 114, 148, 163	0
2	D	103/121 (85%)	0.23	9 (8%) 13 4	54, 131, 190, 242	0
2	F	102/121 (84%)	-0.13	4 (3%) 43 18	70, 121, 157, 194	0
2	H	102/121 (84%)	-0.14	3 (2%) 55 26	57, 116, 156, 186	0
All	All	1020/1144 (89%)	-0.20	31 (3%) 54 25	34, 100, 156, 242	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ASP	5.3
1	C	169	SER	4.7
2	H	141	CYS	4.3
2	D	105	PHE	3.9
2	D	134	PRO	3.9
1	E	106	ASN	3.6
2	D	120	HIS	3.3
2	F	129	PRO	3.1
2	B	142	VAL	3.0
2	D	141	CYS	3.0
2	D	131	GLY	2.9
1	C	168	GLY	2.9
2	D	136	ASP	2.8
1	A	109	GLU	2.7
2	H	138	THR	2.7
2	F	76	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	137	ASP	2.6
2	F	77	SER	2.6
2	D	108	ASP	2.5
2	F	56	GLN	2.4
1	E	130	PRO	2.3
1	G	168	GLY	2.3
2	B	57	PRO	2.3
2	D	41	LYS	2.2
1	E	165	LEU	2.2
1	E	108	ASP	2.1
2	H	142	VAL	2.1
2	B	88	PRO	2.1
2	B	129	PRO	2.1
2	B	95	ARG	2.0
1	E	131	LYS	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.