



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 8PK6 / pdb_00008pk6
Title : INTS13 complex with ZNF655
Authors : Sabath, K.; Jonas, S.
Deposited on : 2023-06-25
Resolution : 3.21 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:

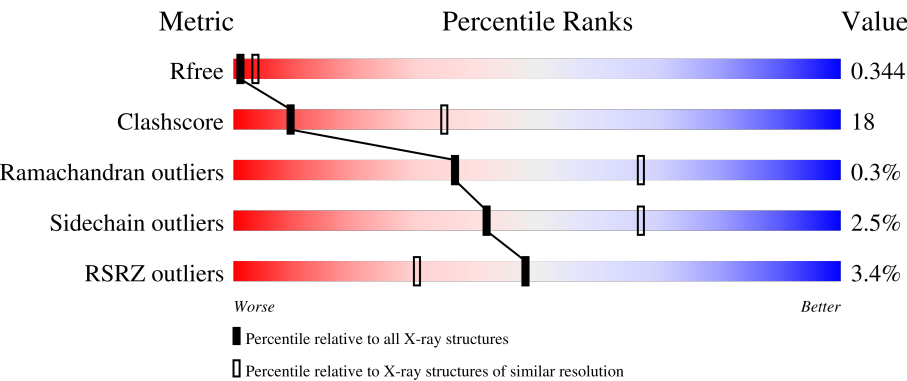
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	242	2% 53% 42% 5%
1	C	242	7% 62% 34% ..
1	E	242	2% 57% 33% 7%
2	B	30	67% 10% 23%
2	D	30	53% 17% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	30	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (57%), yellow (23%), and grey (17%). A small orange dot is located on the yellow segment. The percentages 57%, 23%, and 17% are labeled below the green, yellow, and grey segments respectively.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5874 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 Integrator complex subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1779	1114	311	338	16			
1	C	235	Total	C	N	O	S	0	0	0
			1802	1122	319	347	14			
1	E	226	Total	C	N	O	S	0	0	0
			1727	1078	306	329	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9NVM9
A	-4	PRO	-	expression tag	UNP Q9NVM9
A	-3	HIS	-	expression tag	UNP Q9NVM9
A	-2	MET	-	expression tag	UNP Q9NVM9
A	-1	LEU	-	expression tag	UNP Q9NVM9
A	0	GLU	-	expression tag	UNP Q9NVM9
C	-5	GLY	-	expression tag	UNP Q9NVM9
C	-4	PRO	-	expression tag	UNP Q9NVM9
C	-3	HIS	-	expression tag	UNP Q9NVM9
C	-2	MET	-	expression tag	UNP Q9NVM9
C	-1	LEU	-	expression tag	UNP Q9NVM9
C	0	GLU	-	expression tag	UNP Q9NVM9
E	-5	GLY	-	expression tag	UNP Q9NVM9
E	-4	PRO	-	expression tag	UNP Q9NVM9
E	-3	HIS	-	expression tag	UNP Q9NVM9
E	-2	MET	-	expression tag	UNP Q9NVM9
E	-1	LEU	-	expression tag	UNP Q9NVM9
E	0	GLU	-	expression tag	UNP Q9NVM9

- Molecule 2 is a protein called Zinc finger protein 655.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	0	0	0
			207	133	38	36			
2	D	21	Total	C	N	O	0	0	0
			167	108	32	27			
2	F	25	Total	C	N	O	0	0	0
			192	127	37	28			

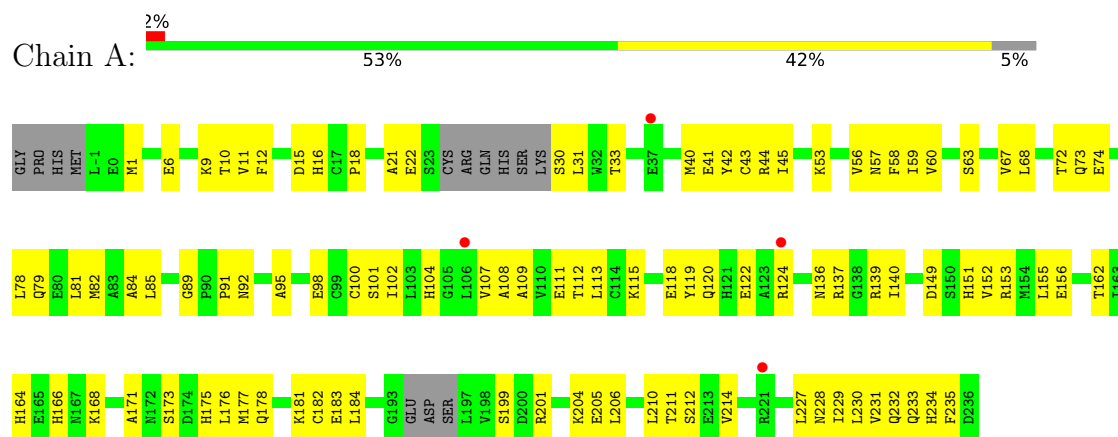
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	90	GLY	-	expression tag	UNP Q8N720
B	91	HIS	-	expression tag	UNP Q8N720
B	92	MET	-	expression tag	UNP Q8N720
D	90	GLY	-	expression tag	UNP Q8N720
D	91	HIS	-	expression tag	UNP Q8N720
D	92	MET	-	expression tag	UNP Q8N720
F	90	GLY	-	expression tag	UNP Q8N720
F	91	HIS	-	expression tag	UNP Q8N720
F	92	MET	-	expression tag	UNP Q8N720

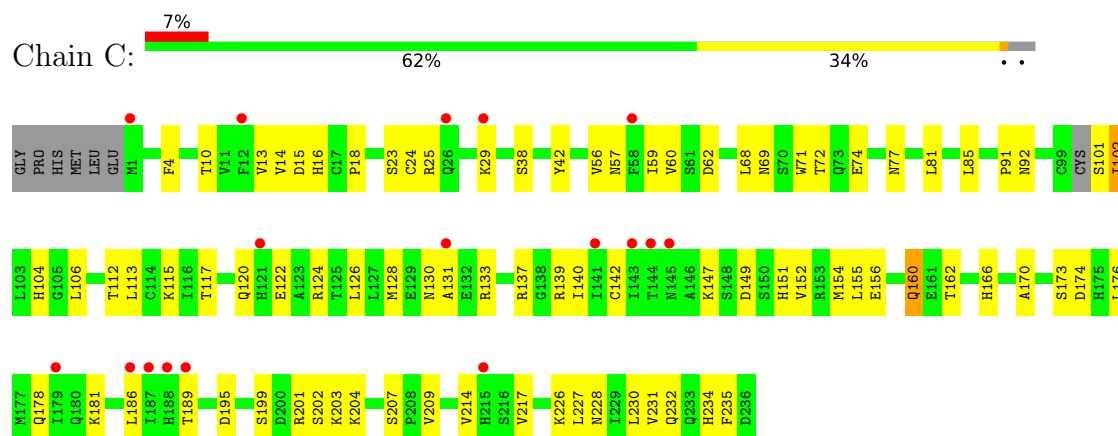
3 Residue-property plots [i](#)

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.

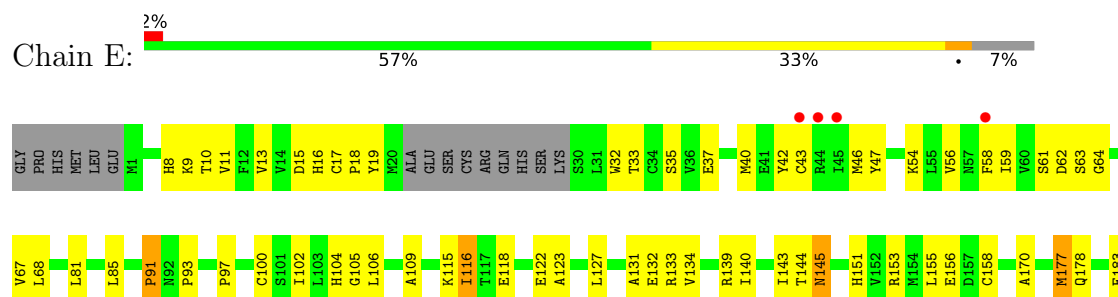
• Molecule 1: Integrator complex subunit 13

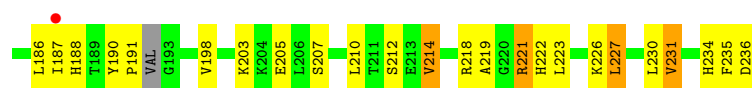


• Molecule 1: Integrator complex subunit 13



• Molecule 1: Integrator complex subunit 13





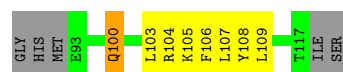
- Molecule 2: Zinc finger protein 655



- Molecule 2: Zinc finger protein 655



- Molecule 2: Zinc finger protein 655



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.00Å 188.10Å 52.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.21 48.72 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.72-3.21) 99.7 (48.72-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.299 , 0.333 0.301 , 0.344	Depositor DCC
R_{free} test set	1095 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	131.6	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 148.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5874	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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	0.23	0/1812	0.49	0/2457
1	C	0.19	0/1837	0.47	0/2494
1	E	0.23	0/1759	0.49	0/2391
2	B	0.20	0/209	0.51	0/277
2	D	0.20	0/169	0.42	0/225
2	F	0.20	0/194	0.42	0/260
All	All	0.21	0/5980	0.48	0/8104

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1779	0	1732	73	0
1	C	1802	0	1717	59	0
1	E	1727	0	1654	72	0
2	B	207	0	205	2	0
2	D	167	0	147	4	0
2	F	192	0	180	5	0
All	All	5874	0	5635	207	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 18.

All (207) 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:C:62:ASP:O	1:C:101:SER:N	2.09	0.85
1:E:10:THR:HB	1:E:56:VAL:HG22	1.60	0.83
1:A:59:ILE:HG12	1:A:67:VAL:HG22	1.66	0.78
1:A:149:ASP:HB2	1:A:153:ARG:HH21	1.50	0.77
1:E:170:ALA:HB3	1:E:178:GLN:HG3	1.66	0.76
1:A:9:LYS:NZ	1:A:115:LYS:O	2.21	0.74
1:E:8:HIS:HA	1:E:54:LYS:HA	1.69	0.73
1:E:191:PRO:HD2	1:E:219:ALA:H	1.54	0.73
1:E:143:ILE:HG12	1:E:187:ILE:HD12	1.73	0.70
1:E:42:TYR:HD1	1:E:231:VAL:HG22	1.56	0.69
1:E:123:ALA:O	1:E:127:LEU:N	2.25	0.69
1:A:16:HIS:NE2	1:A:89:GLY:O	2.26	0.68
1:A:171:ALA:HB2	1:A:178:GLN:HE21	1.58	0.68
1:C:137:ARG:HG2	1:C:181:LYS:HB3	1.76	0.68
1:A:227:LEU:O	1:A:231:VAL:HG23	1.93	0.68
1:E:9:LYS:NZ	1:E:115:LYS:O	2.25	0.67
1:C:24:CYS:H	1:C:29:LYS:HB2	1.58	0.67
1:C:57:ASN:ND2	1:C:69:ASN:OD1	2.28	0.67
1:C:71:TRP:HE1	1:C:115:LYS:HB2	1.59	0.66
1:C:72:THR:HG22	1:C:74:GLU:H	1.60	0.66
1:A:1:MET:HG2	1:A:137:ARG:HH12	1.61	0.66
1:E:35:SER:HA	1:E:223:LEU:HD21	1.77	0.65
1:C:42:TYR:HB2	1:C:227:LEU:HD13	1.78	0.65
2:F:100:GLN:O	2:F:104:ARG:HG2	1.97	0.65
1:E:8:HIS:HD1	1:E:9:LYS:HG3	1.60	0.64
1:E:42:TYR:CD1	1:E:231:VAL:HG22	2.35	0.62
1:E:186:LEU:HD12	1:E:214:VAL:HB	1.83	0.61
1:E:221:ARG:HD2	1:E:222:HIS:H	1.65	0.61
1:C:139:ARG:NH1	1:C:234:HIS:O	2.33	0.61
1:A:68:LEU:HD23	1:C:202:SER:HB3	1.83	0.60
1:C:15:ASP:HB3	1:C:102:ILE:HG12	1.82	0.60
1:C:232:GLN:HA	1:C:235:PHE:CE2	2.36	0.60
1:E:18:PRO:HB2	1:E:93:PRO:HA	1.84	0.59
1:A:231:VAL:HG12	1:A:235:PHE:CE1	2.38	0.59
1:A:184:LEU:HB3	1:A:212:SER:HA	1.84	0.59
1:E:8:HIS:ND1	1:E:9:LYS:HG3	2.18	0.59
1:C:147:LYS:HB3	2:D:113:PHE:CZ	2.38	0.58
1:C:162:THR:O	1:C:166:HIS:ND1	2.34	0.58
1:A:73:GLN:OE1	1:A:73:GLN:N	2.32	0.58
1:A:72:THR:HG21	1:C:149:ASP:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:NZ	1:C:199:SER:OG	2.25	0.57
1:A:151:HIS:O	1:A:155:LEU:HG	2.04	0.57
1:A:11:VAL:HG11	1:A:109:ALA:HB1	1.86	0.57
1:A:58:PHE:HD2	1:A:68:LEU:HD12	1.70	0.56
2:D:100:GLN:O	2:D:104:ARG:HG2	2.05	0.56
1:C:60:VAL:HG22	1:C:68:LEU:HD11	1.86	0.56
1:A:68:LEU:HD22	1:A:84:ALA:HB1	1.86	0.56
1:C:81:LEU:O	1:C:85:LEU:HG	2.05	0.56
1:A:152:VAL:O	1:A:156:GLU:HG3	2.06	0.56
1:C:14:VAL:HB	1:C:60:VAL:HG12	1.86	0.56
1:E:10:THR:HA	1:E:139:ARG:O	2.06	0.56
1:E:153:ARG:O	1:E:156:GLU:HG2	2.06	0.56
1:E:207:SER:HB3	1:E:210:LEU:H	1.71	0.56
1:C:226:LYS:O	1:C:230:LEU:HG	2.06	0.55
1:E:81:LEU:O	1:E:85:LEU:HG	2.05	0.55
1:E:59:ILE:HG12	1:E:67:VAL:HA	1.89	0.55
1:C:124:ARG:NH1	1:C:130:ASN:O	2.39	0.55
1:A:137:ARG:HG2	1:A:181:LYS:HB3	1.88	0.55
1:C:181:LYS:N	1:C:209:VAL:HG13	2.21	0.55
1:A:201:ARG:HH21	1:A:204:LYS:HB2	1.70	0.55
1:E:226:LYS:O	1:E:230:LEU:HG	2.07	0.54
1:C:186:LEU:HB2	1:C:214:VAL:HG12	1.88	0.54
1:A:108:ALA:O	1:A:112:THR:HG23	2.07	0.54
1:E:32:TRP:NE1	1:E:91:PRO:HG3	2.22	0.54
1:E:118:GLU:O	1:E:122:GLU:HG3	2.08	0.54
1:A:18:PRO:HA	1:A:91:PRO:HB2	1.90	0.53
1:C:38:SER:HB3	1:C:227:LEU:CD2	2.39	0.53
1:A:137:ARG:HA	1:A:181:LYS:O	2.08	0.53
1:E:42:TYR:HB2	1:E:227:LEU:HD11	1.92	0.52
1:E:143:ILE:HA	1:E:187:ILE:HB	1.91	0.52
1:A:41:GLU:O	1:A:45:ILE:HG13	2.09	0.52
1:C:122:GLU:O	1:C:126:LEU:HG	2.10	0.52
1:A:231:VAL:HA	1:A:234:HIS:HB2	1.91	0.52
1:E:42:TYR:HB2	1:E:227:LEU:HD21	1.92	0.52
1:C:201:ARG:NH1	1:C:204:LYS:HD2	2.25	0.52
1:E:16:HIS:HB3	1:E:62:ASP:HB3	1.92	0.52
1:E:43:CYS:HA	1:E:46:MET:HG2	1.92	0.52
1:E:140:ILE:N	1:E:183:GLU:O	2.29	0.52
1:A:78:LEU:O	1:A:82:MET:HG3	2.10	0.52
1:E:188:HIS:CG	1:E:198:VAL:HG21	2.44	0.52
1:C:174:ASP:N	1:C:174:ASP:OD1	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ARG:HD2	1:E:222:HIS:N	2.24	0.52
1:C:189:THR:HA	1:C:217:VAL:O	2.10	0.51
2:D:111:ARG:O	2:D:114:ARG:HB2	2.10	0.51
1:E:227:LEU:O	1:E:231:VAL:HG23	2.09	0.51
1:C:13:VAL:HA	1:C:59:ILE:O	2.09	0.51
1:E:11:VAL:HG11	1:E:109:ALA:HB1	1.93	0.51
1:A:205:GLU:HA	1:A:211:THR:HA	1.92	0.51
1:E:61:SER:OG	1:E:102:ILE:HG13	2.11	0.51
2:F:105:LYS:O	2:F:109:LEU:HG	2.11	0.51
1:C:4:PHE:CE1	1:C:120:GLN:HG2	2.45	0.51
1:E:58:PHE:CD2	1:E:68:LEU:HD12	2.46	0.51
1:C:142:CYS:HB3	1:C:186:LEU:HD23	1.93	0.51
1:E:47:TYR:OH	1:E:56:VAL:N	2.42	0.51
1:E:102:ILE:HD12	1:E:144:THR:HB	1.93	0.51
1:E:118:GLU:CD	1:E:118:GLU:H	2.19	0.50
1:A:53:LYS:HE3	1:A:119:TYR:HE2	1.77	0.50
1:E:63:SER:OG	1:E:64:GLY:N	2.45	0.50
1:C:59:ILE:HD11	1:C:112:THR:HG21	1.94	0.50
1:C:170:ALA:HB2	1:C:178:GLN:CB	2.42	0.50
1:E:205:GLU:CD	1:E:205:GLU:H	2.20	0.49
1:A:10:THR:HB	1:A:56:VAL:HG22	1.94	0.49
1:A:41:GLU:HA	1:A:44:ARG:HD2	1.94	0.49
1:C:201:ARG:H	1:C:214:VAL:CG2	2.25	0.49
1:A:12:PHE:HZ	1:A:42:TYR:CD1	2.31	0.49
1:A:40:MET:O	1:A:44:ARG:HG3	2.13	0.48
1:E:230:LEU:HB3	1:E:234:HIS:CE1	2.48	0.48
1:E:15:ASP:CG	1:E:144:THR:HA	2.38	0.48
1:E:230:LEU:O	1:E:234:HIS:ND1	2.46	0.48
1:A:42:TYR:OH	1:A:234:HIS:ND1	2.29	0.48
1:C:151:HIS:O	1:C:155:LEU:HG	2.12	0.48
1:A:228:ASN:O	1:A:232:GLN:HG3	2.14	0.48
1:C:186:LEU:O	1:C:214:VAL:HA	2.14	0.48
1:A:107:VAL:O	1:A:111:GLU:HG3	2.13	0.48
1:C:151:HIS:ND1	1:C:154:MET:HE3	2.29	0.48
1:E:177:MET:HE2	1:E:177:MET:HB3	1.71	0.48
1:A:104:HIS:CE1	2:B:107:LEU:HD11	2.48	0.47
1:C:147:LYS:HB3	2:D:113:PHE:CE2	2.48	0.47
1:A:79:GLN:HA	1:A:82:MET:HE2	1.96	0.47
1:A:101:SER:O	1:A:104:HIS:HD2	1.98	0.47
1:A:119:TYR:HA	1:A:122:GLU:HG2	1.96	0.47
1:C:160:GLN:CD	1:C:207:SER:HB2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:PRO:HD2	1:E:100:CYS:SG	2.55	0.47
1:A:199:SER:O	1:A:201:ARG:N	2.47	0.47
1:E:10:THR:O	1:E:56:VAL:HA	2.15	0.47
1:E:63:SER:O	1:E:104:HIS:ND1	2.47	0.47
1:E:16:HIS:HD1	1:E:62:ASP:CG	2.23	0.47
1:A:206:LEU:HB2	1:A:210:LEU:HD23	1.96	0.47
1:E:190:TYR:HB2	1:E:218:ARG:HG2	1.96	0.46
1:A:22:GLU:H	1:A:31:LEU:HD13	1.81	0.46
1:C:102:ILE:H	1:C:102:ILE:HG13	1.49	0.46
1:E:17:CYS:O	1:E:19:TYR:N	2.42	0.46
1:A:15:ASP:HB3	1:A:102:ILE:HD12	1.97	0.46
1:C:228:ASN:O	1:C:231:VAL:HG12	2.15	0.46
1:A:58:PHE:CD2	1:A:68:LEU:HD12	2.49	0.46
1:A:229:ILE:HG22	1:A:233:GLN:HE21	1.80	0.46
1:E:15:ASP:OD1	1:E:15:ASP:N	2.49	0.46
1:E:116:ILE:H	1:E:116:ILE:HG13	1.33	0.46
1:A:43:CYS:SG	1:A:56:VAL:HG11	2.56	0.46
1:A:139:ARG:NH2	1:A:234:HIS:CD2	2.84	0.45
1:C:14:VAL:O	1:C:60:VAL:HA	2.16	0.45
1:E:186:LEU:HB2	1:E:214:VAL:HA	1.98	0.45
1:C:77:ASN:O	1:C:81:LEU:HG	2.17	0.45
1:E:132:GLU:O	1:E:133:ARG:HB2	2.17	0.45
1:E:151:HIS:O	1:E:155:LEU:HG	2.16	0.45
1:E:18:PRO:CB	1:E:93:PRO:HA	2.45	0.45
1:E:139:ARG:HD3	1:E:183:GLU:CD	2.41	0.45
1:A:63:SER:HA	1:A:100:CYS:HA	1.99	0.45
1:A:92:ASN:HB3	1:A:95:ALA:HB2	1.98	0.44
2:F:103:LEU:O	2:F:107:LEU:HG	2.16	0.44
1:A:81:LEU:O	1:A:85:LEU:HG	2.17	0.44
1:A:164:HIS:CE1	1:A:168:LYS:HD2	2.51	0.44
1:C:106:LEU:HD21	1:C:142:CYS:SG	2.57	0.44
1:E:61:SER:OG	1:E:102:ILE:HA	2.18	0.44
1:C:23:SER:HB2	1:C:29:LYS:H	1.82	0.44
1:C:101:SER:HB2	1:C:104:HIS:CE1	2.52	0.44
1:C:113:LEU:HD11	1:C:140:ILE:HD11	2.00	0.44
1:E:131:ALA:O	1:E:134:VAL:HB	2.17	0.44
1:E:191:PRO:HG2	1:E:219:ALA:HB3	1.99	0.44
1:A:11:VAL:HB	1:A:140:ILE:HA	1.99	0.44
1:A:181:LYS:HE3	1:A:211:THR:OG1	2.18	0.44
1:A:137:ARG:HG2	1:A:181:LYS:CB	2.48	0.43
1:A:120:GLN:O	1:A:124:ARG:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:HIS:C	1:C:62:ASP:HB3	2.43	0.43
2:B:96:LEU:O	2:B:99:LEU:HB3	2.17	0.43
1:C:15:ASP:OD1	1:C:15:ASP:N	2.50	0.43
1:A:136:ASN:HD22	1:A:177:MET:HB2	1.84	0.43
1:C:10:THR:O	1:C:56:VAL:HA	2.19	0.43
1:E:46:MET:SD	1:E:56:VAL:HG21	2.59	0.43
1:A:12:PHE:CB	1:A:58:PHE:HD1	2.32	0.42
1:A:30:SER:O	1:A:33:THR:HB	2.18	0.42
1:C:112:THR:HA	1:C:115:LYS:HG3	2.00	0.42
1:C:173:SER:HA	1:C:176:LEU:O	2.20	0.42
1:C:152:VAL:O	1:C:156:GLU:HG3	2.19	0.42
1:C:16:HIS:CE1	1:C:91:PRO:HA	2.55	0.42
1:A:6:GLU:OE2	1:A:6:GLU:N	2.48	0.42
1:A:56:VAL:O	1:A:57:ASN:ND2	2.52	0.42
1:A:21:ALA:HB2	1:A:91:PRO:HD2	2.01	0.41
1:E:221:ARG:H	1:E:221:ARG:HG3	1.44	0.41
1:A:74:GLU:H	1:A:74:GLU:CD	2.28	0.41
1:A:162:THR:O	1:A:166:HIS:HB2	2.20	0.41
1:C:18:PRO:HB3	1:C:92:ASN:O	2.20	0.41
1:C:201:ARG:HH11	1:C:204:LYS:HD2	1.84	0.41
1:E:19:TYR:CE2	1:E:145:ASN:HB3	2.54	0.41
1:A:118:GLU:O	1:A:122:GLU:HG2	2.19	0.41
1:C:124:ARG:NH1	1:C:131:ALA:HB2	2.35	0.41
1:C:202:SER:O	1:C:203:LYS:HG3	2.20	0.41
1:E:226:LYS:HD2	1:E:226:LYS:HA	1.90	0.41
1:A:230:LEU:HB3	1:A:234:HIS:CE1	2.55	0.41
1:E:158:CYS:HB2	2:F:106:PHE:CD2	2.55	0.41
1:E:40:MET:HE3	1:E:40:MET:HB3	1.91	0.41
1:A:98:GLU:C	1:A:100:CYS:H	2.29	0.41
1:E:13:VAL:HG11	1:E:106:LEU:HD23	2.02	0.41
1:E:203:LYS:HA	1:E:212:SER:O	2.20	0.41
1:E:235:PHE:CD1	1:E:236:ASP:N	2.89	0.41
1:A:182:CYS:SG	1:A:183:GLU:N	2.94	0.41
1:A:173:SER:OG	1:C:195:ASP:OD2	2.34	0.40
1:A:232:GLN:HA	1:A:235:PHE:CD2	2.56	0.40
1:E:33:THR:O	1:E:37:GLU:HG3	2.21	0.40
1:A:73:GLN:H	1:A:73:GLN:CD	2.24	0.40
1:A:232:GLN:HA	1:A:235:PHE:CE2	2.56	0.40
1:E:61:SER:HB3	1:E:105:GLY:HA3	2.03	0.40
1:E:134:VAL:HG11	1:E:177:MET:HE1	2.02	0.40
2:F:104:ARG:O	2:F:108:TYR:HD1	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LYS:HD2	1:C:226:LYS:HA	1.81	0.40
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.83	0.40
1:A:201:ARG:HB3	1:A:214:VAL:HB	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	223/242 (92%)	209 (94%)	14 (6%)	0	100	100
1	C	231/242 (96%)	222 (96%)	8 (4%)	1 (0%)	30	61
1	E	220/242 (91%)	206 (94%)	13 (6%)	1 (0%)	24	58
2	B	21/30 (70%)	20 (95%)	1 (5%)	0	100	100
2	D	19/30 (63%)	17 (90%)	2 (10%)	0	100	100
2	F	23/30 (77%)	23 (100%)	0	0	100	100
All	All	737/816 (90%)	697 (95%)	38 (5%)	2 (0%)	36	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	91	PRO
1	C	128	MET

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/218 (91%)	196 (98%)	3 (2%)	57	74
1	C	197/218 (90%)	192 (98%)	5 (2%)	42	67
1	E	189/218 (87%)	182 (96%)	7 (4%)	30	60
2	B	21/29 (72%)	21 (100%)	0	100	100
2	D	13/29 (45%)	13 (100%)	0	100	100
2	F	15/29 (52%)	14 (93%)	1 (7%)	15	45
All	All	634/741 (86%)	618 (98%)	16 (2%)	42	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	175	HIS
1	A	176	LEU
1	C	25	ARG
1	C	102	ILE
1	C	117	THR
1	C	133	ARG
1	C	160	GLN
1	E	116	ILE
1	E	145	ASN
1	E	177	MET
1	E	214	VAL
1	E	221	ARG
1	E	227	LEU
1	E	231	VAL
2	F	100	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	104	HIS
1	A	164	HIS
1	A	178	GLN
1	A	222	HIS
1	A	233	GLN
1	C	66	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	160	GLN
1	E	57	ASN
1	E	121	HIS
1	E	145	ASN
1	E	164	HIS
1	E	233	GLN

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 ⓘ

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	229/242 (94%)	-0.02	4 (1%) 69 49	95, 164, 239, 355	0
1	C	235/242 (97%)	0.32	17 (7%) 21 14	129, 196, 283, 351	0
1	E	226/242 (93%)	0.03	5 (2%) 62 42	143, 204, 280, 384	0
2	B	23/30 (76%)	-0.24	0 100 100	95, 138, 216, 240	0
2	D	21/30 (70%)	-0.72	0 100 100	177, 207, 252, 279	0
2	F	25/30 (83%)	-0.33	0 100 100	111, 182, 213, 234	0
All	All	759/816 (93%)	0.06	26 (3%) 48 30	95, 189, 274, 384	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	44	ARG	4.1
1	C	143	ILE	4.1
1	A	37	GLU	4.0
1	C	145	ASN	4.0
1	C	187	ILE	3.7
1	A	221	ARG	3.4
1	C	141	ILE	3.3
1	C	58	PHE	3.2
1	C	131	ALA	2.9
1	C	189	THR	2.9
1	A	106	LEU	2.8
1	C	121	HIS	2.8
1	E	45	ILE	2.7
1	C	186	LEU	2.7
1	C	12	PHE	2.5
1	E	43	CYS	2.5
1	E	58	PHE	2.4
1	C	179	ILE	2.4
1	A	124	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.3
1	E	187	ILE	2.3
1	C	144	THR	2.2
1	C	188	HIS	2.2
1	C	215	HIS	2.1
1	C	29	LYS	2.1
1	C	26	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.