



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:54 AM GMT

PDB ID : 3GGZ
Title : Crystal Structure of S.cerevisiae Ist1 N-terminal domain in complex with Did2
MIM motif
Authors : Xiao, J.; Xu, Z.
Deposited on : 2009-03-02
Resolution : 3.80 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

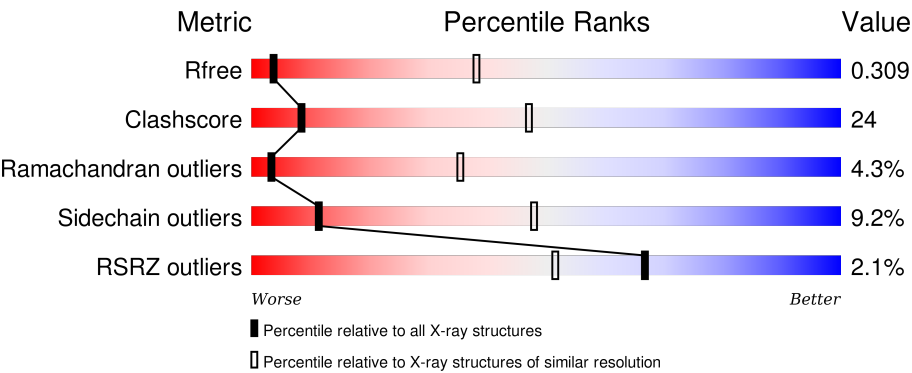
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	193	<div><div>2%</div><div></div><div>52%</div><div>39%</div><div>5%</div><div>• •</div></div>
1	B	193	<div><div>3%</div><div></div><div>49%</div><div>40%</div><div>7%</div><div>• •</div></div>
1	C	193	<div><div>2%</div><div></div><div>52%</div><div>39%</div><div>•</div><div>6%</div></div>
1	D	193	<div><div>2%</div><div></div><div>56%</div><div>32%</div><div>9%</div><div>• •</div></div>
2	E	29	<div><div></div><div>28%</div><div>24%</div><div>7%</div><div>41%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	29	
2	G	29	
2	H	29	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6595 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 Increased sodium tolerance protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1513	972	252	282	7			
1	B	186	Total	C	N	O	S	0	0	0
			1517	973	253	284	7			
1	C	182	Total	C	N	O	S	0	0	0
			1486	955	248	276	7			
1	D	188	Total	C	N	O	S	0	0	0
			1531	982	255	287	7			

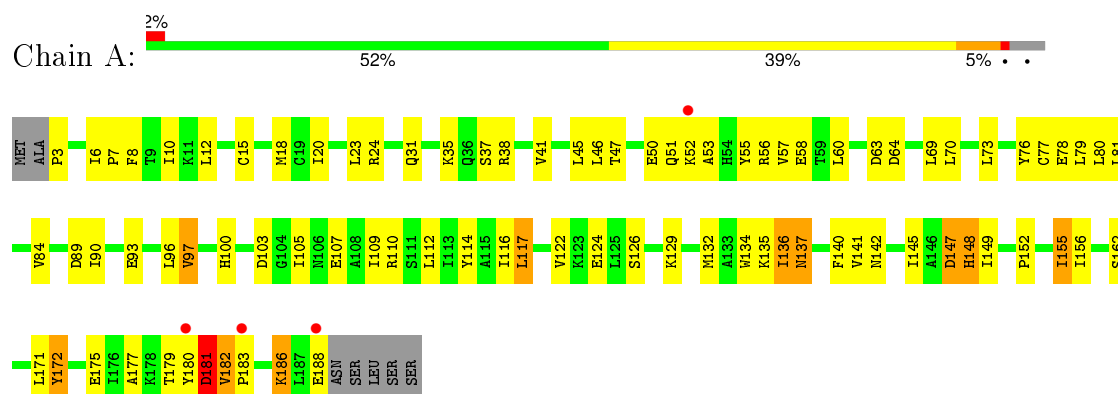
- Molecule 2 is a protein called Vacuolar protein-sorting-associated protein 46.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	0	0	0
			137	82	29	26			
2	F	17	Total	C	N	O	0	0	0
			137	82	29	26			
2	G	16	Total	C	N	O	0	0	0
			132	79	28	25			
2	H	18	Total	C	N	O	0	0	0
			142	85	30	27			

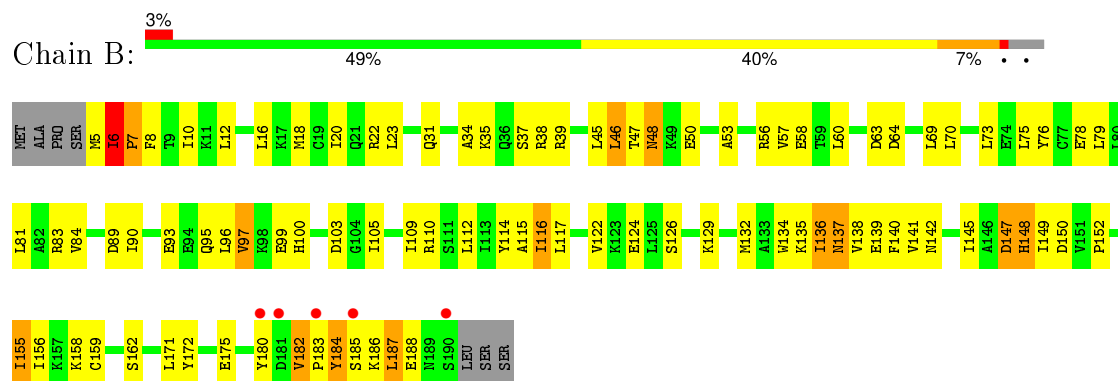
3 Residue-property plots [i](#)

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.

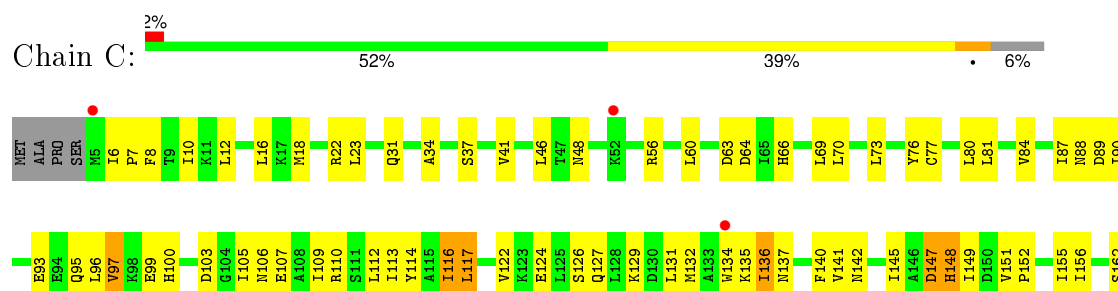
- Molecule 1: Increased sodium tolerance protein 1



- Molecule 1: Increased sodium tolerance protein 1

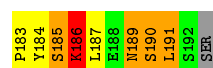
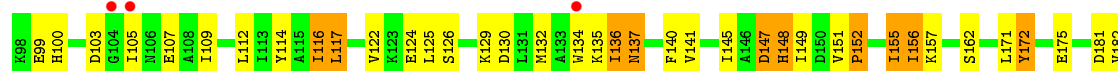


- Molecule 1: Increased sodium tolerance protein 1

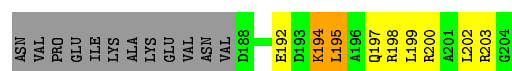
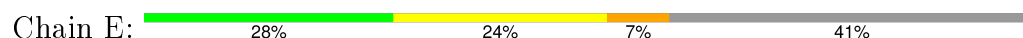




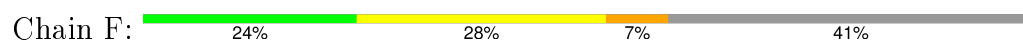
- Molecule 1: Increased sodium tolerance protein 1



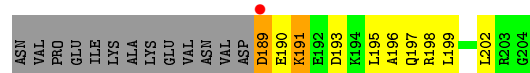
- Molecule 2: Vacuolar protein-sorting-associated protein 46



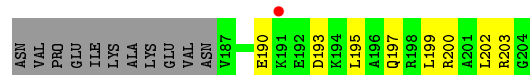
- Molecule 2: Vacuolar protein-sorting-associated protein 46



- Molecule 2: Vacuolar protein-sorting-associated protein 46



- Molecule 2: Vacuolar protein-sorting-associated protein 46



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	165.92Å 165.92Å 121.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.80 49.03 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.03-3.80) 99.6 (49.03-3.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.289 , 0.307 0.300 , 0.309	Depositor DCC
R_{free} test set	869 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	130.9	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.0	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 17212 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6595	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.375 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	0.49	0/1534	0.61	1/2071 (0.0%)
1	B	0.52	1/1538 (0.1%)	0.59	0/2076
1	C	0.52	0/1507	0.60	0/2034
1	D	0.53	0/1552	0.61	0/2095
2	E	0.44	0/136	0.52	0/178
2	F	0.43	0/136	0.54	0/178
2	G	0.49	0/131	0.70	0/171
2	H	0.52	0/141	0.64	0/185
All	All	0.51	1/6675 (0.0%)	0.60	1/8988 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	CYS	CB-SG	-5.55	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-CB	5.38	109.76	103.30

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	1513	0	1571	85	0
1	B	1517	0	1578	84	0
1	C	1486	0	1550	60	0
1	D	1531	0	1594	73	0
2	E	137	0	140	9	0
2	F	137	0	140	13	0
2	G	132	0	138	13	0
2	H	142	0	142	14	0
All	All	6595	0	6853	323	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 24.

All (323) 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:F:194:LYS:HA	2:F:197:GLN:HB2	1.52	0.91
1:D:37:SER:HB3	1:D:60:LEU:HD21	1.60	0.82
1:D:189:ASN:N	1:D:189:ASN:HD22	1.76	0.82
1:B:38:ARG:HD2	2:F:195:LEU:HD21	1.61	0.82
1:B:37:SER:HB3	1:B:60:LEU:HD21	1.62	0.80
1:A:73:LEU:HD22	1:A:112:LEU:HD23	1.64	0.79
1:A:180:TYR:O	1:A:181:ASP:HB2	1.81	0.78
2:E:200:ARG:HG3	2:E:203:ARG:NH2	1.98	0.78
2:F:196:ALA:HA	2:F:199:LEU:HD12	1.64	0.78
1:C:179:THR:HG21	2:G:195:LEU:HB2	1.66	0.78
2:G:202:LEU:HD23	2:G:202:LEU:O	1.85	0.77
1:C:81:LEU:O	1:C:84:VAL:HG23	1.85	0.76
1:A:7:PRO:HB2	1:A:10:ILE:CD1	2.17	0.75
1:A:109:ILE:HD11	1:A:132:MET:SD	2.27	0.74
1:D:69:LEU:O	1:D:69:LEU:HD12	1.87	0.74
1:D:6:ILE:HG22	1:D:7:PRO:HD2	1.69	0.74
1:D:171:LEU:HD21	2:H:202:LEU:HD11	1.69	0.74
1:B:50:GLU:OE2	1:B:186:LYS:HA	1.88	0.73
2:H:199:LEU:O	2:H:203:ARG:HG3	1.88	0.73
2:F:194:LYS:H	2:F:194:LYS:HD3	1.51	0.73
1:C:37:SER:HB3	1:C:60:LEU:HD21	1.70	0.72
1:D:189:ASN:HD22	1:D:189:ASN:H	1.34	0.72
1:D:190:SER:O	1:D:191:LEU:HB2	1.88	0.72
1:C:181:ASP:O	1:C:182:VAL:HG13	1.90	0.71
1:A:152:PRO:HB2	1:A:155:ILE:HG12	1.71	0.70
1:A:37:SER:HB3	1:A:60:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:VAL:HG23	1:D:183:PRO:HD2	1.74	0.70
1:B:114:TYR:CE2	1:B:156:ILE:HG22	2.27	0.69
1:A:172:TYR:CZ	2:E:199:LEU:HD22	2.27	0.69
1:B:73:LEU:HD22	1:B:112:LEU:HD23	1.72	0.69
1:B:184:TYR:CD1	1:B:187:LEU:HD21	2.27	0.69
1:C:179:THR:OG1	2:G:195:LEU:HD13	1.94	0.68
1:A:171:LEU:HG	2:E:202:LEU:HD21	1.75	0.68
1:A:50:GLU:OE1	1:A:186:LYS:HG2	1.93	0.68
2:F:198:ARG:O	2:F:202:LEU:HD13	1.94	0.68
1:D:152:PRO:HB2	1:D:155:ILE:HG12	1.75	0.67
1:B:7:PRO:HB2	1:B:10:ILE:HD12	1.77	0.67
1:A:81:LEU:O	1:A:84:VAL:HG23	1.95	0.67
1:A:69:LEU:O	1:A:69:LEU:HD12	1.95	0.66
2:H:197:GLN:O	2:H:200:ARG:HG2	1.96	0.66
1:C:73:LEU:HD22	1:C:112:LEU:HD23	1.77	0.66
1:A:6:ILE:HG23	1:A:7:PRO:HD2	1.78	0.65
1:D:18:MET:HG2	1:D:124:GLU:HG2	1.77	0.65
1:D:116:ILE:HD13	1:D:126:SER:HA	1.78	0.65
1:C:177:ALA:HB1	1:C:182:VAL:O	1.97	0.65
1:A:181:ASP:O	1:A:182:VAL:HG22	1.97	0.65
1:D:172:TYR:CE2	2:H:199:LEU:HD22	2.32	0.64
1:D:93:GLU:O	1:D:97:VAL:HG23	1.96	0.64
1:A:116:ILE:HD13	1:A:126:SER:HA	1.79	0.64
1:D:65:ILE:HG12	2:H:203:ARG:HH21	1.62	0.64
1:D:90:ILE:O	1:D:135:LYS:HE3	1.97	0.64
2:G:195:LEU:HA	2:G:198:ARG:HD3	1.80	0.63
1:C:18:MET:HG2	1:C:124:GLU:HG2	1.79	0.63
1:A:76:TYR:HE2	1:A:155:ILE:HD11	1.63	0.63
1:B:18:MET:HG2	1:B:124:GLU:HG2	1.81	0.62
1:C:116:ILE:HD13	1:C:126:SER:HA	1.81	0.62
1:A:52:LYS:HA	1:B:75:LEU:HD12	1.82	0.62
1:B:81:LEU:O	1:B:84:VAL:HG23	2.00	0.62
1:D:45:LEU:HB2	1:D:182:VAL:HG21	1.83	0.61
1:D:65:ILE:HG12	2:H:203:ARG:NH2	2.15	0.61
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.16	0.61
1:B:105:ILE:O	1:B:109:ILE:HG22	2.01	0.61
1:C:152:PRO:HB2	1:C:155:ILE:HG12	1.81	0.61
1:A:180:TYR:O	1:A:181:ASP:CB	2.48	0.60
2:F:198:ARG:NH1	2:F:198:ARG:HB2	2.17	0.60
1:B:69:LEU:HD12	1:B:69:LEU:O	2.02	0.60
1:A:78:GLU:OE2	1:D:56:ARG:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASN:OD1	1:C:110:ARG:HD2	2.01	0.59
1:C:8:PHE:CE1	1:C:135:LYS:HB2	2.37	0.59
1:C:12:LEU:HD11	1:C:16:LEU:HD11	1.85	0.59
1:A:117:LEU:HD11	1:A:145:ILE:HG23	1.84	0.59
1:B:183:PRO:HB2	1:B:186:LYS:HG2	1.83	0.59
1:D:6:ILE:HG22	1:D:7:PRO:CD	2.33	0.59
1:D:152:PRO:HB2	1:D:155:ILE:CG1	2.33	0.59
1:D:109:ILE:HD11	1:D:132:MET:SD	2.42	0.59
1:B:7:PRO:HB2	1:B:10:ILE:CD1	2.33	0.59
1:D:117:LEU:HD11	1:D:145:ILE:HG23	1.85	0.58
1:B:8:PHE:CE1	1:B:135:LYS:HB2	2.38	0.57
1:A:93:GLU:OE2	1:A:140:PHE:HD1	1.88	0.57
1:B:100:HIS:HB3	1:B:105:ILE:HD12	1.85	0.57
1:B:116:ILE:HD13	1:B:126:SER:HA	1.86	0.57
1:C:69:LEU:O	1:C:69:LEU:HD12	2.05	0.57
1:D:73:LEU:HD22	1:D:112:LEU:HD23	1.86	0.57
1:B:109:ILE:HD11	1:B:132:MET:SD	2.45	0.56
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.70	0.56
1:B:93:GLU:O	1:B:97:VAL:HG23	2.06	0.56
1:C:93:GLU:OE2	1:C:140:PHE:HD1	1.88	0.56
2:G:195:LEU:HA	2:G:198:ARG:CG	2.36	0.56
1:A:177:ALA:HB1	1:A:182:VAL:HG22	1.88	0.56
1:B:132:MET:O	1:B:136:ILE:N	2.34	0.56
2:G:195:LEU:HA	2:G:198:ARG:CD	2.36	0.56
1:A:18:MET:HG2	1:A:124:GLU:HG2	1.88	0.56
1:A:7:PRO:HD2	1:A:10:ILE:HD12	1.86	0.56
1:B:187:LEU:HD12	1:B:188:GLU:HG3	1.87	0.56
1:D:95:GLN:O	1:D:99:GLU:HB3	2.06	0.56
1:C:76:TYR:HE2	1:C:155:ILE:HD11	1.71	0.56
1:D:45:LEU:HD12	1:D:182:VAL:HG11	1.87	0.55
1:A:53:ALA:O	1:A:57:VAL:HG23	2.06	0.55
1:C:66:HIS:O	1:C:69:LEU:HB3	2.06	0.55
1:B:171:LEU:O	1:B:175:GLU:HG2	2.06	0.55
1:C:180:TYR:O	1:C:181:ASP:HB2	2.05	0.55
1:B:116:ILE:CD1	1:B:126:SER:HA	2.37	0.55
1:D:129:LYS:O	1:D:132:MET:HB2	2.07	0.55
2:G:195:LEU:HD12	2:G:198:ARG:HH11	1.71	0.55
1:D:171:LEU:O	1:D:175:GLU:HG2	2.07	0.54
1:A:172:TYR:CE1	2:E:199:LEU:HD22	2.41	0.54
1:A:171:LEU:O	1:A:175:GLU:HG2	2.07	0.54
2:H:190:GLU:O	2:H:193:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CE1	1:A:135:LYS:HB2	2.42	0.54
1:A:100:HIS:HB3	1:A:105:ILE:HD12	1.89	0.54
1:D:148:HIS:HB2	1:D:151:VAL:CG2	2.37	0.54
1:A:114:TYR:CE2	1:A:156:ILE:HG22	2.42	0.54
1:A:58:GLU:OE2	1:B:83:ARG:NH2	2.40	0.54
1:D:18:MET:CG	1:D:124:GLU:HG2	2.37	0.54
2:G:195:LEU:HA	2:G:198:ARG:HG2	1.89	0.54
1:C:109:ILE:HD11	1:C:132:MET:SD	2.48	0.54
1:C:171:LEU:O	1:C:175:GLU:HG2	2.08	0.54
1:D:81:LEU:O	1:D:84:VAL:HG23	2.08	0.53
1:A:56:ARG:HD2	1:B:78:GLU:OE2	2.09	0.53
1:D:172:TYR:CZ	2:H:199:LEU:HD22	2.43	0.53
1:D:23:LEU:HD23	1:D:122:VAL:HG21	1.90	0.53
1:A:152:PRO:HB2	1:A:155:ILE:CG1	2.38	0.53
1:A:7:PRO:HB2	1:A:10:ILE:HD12	1.89	0.53
1:D:8:PHE:CE1	1:D:135:LYS:HB2	2.43	0.53
1:C:106:ASN:OD1	1:C:110:ARG:CD	2.57	0.53
1:D:116:ILE:CD1	1:D:126:SER:HA	2.39	0.53
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.74	0.53
1:B:183:PRO:HB2	1:B:186:LYS:CG	2.39	0.52
1:A:171:LEU:HG	2:E:202:LEU:CD2	2.40	0.52
1:A:12:LEU:HD12	1:A:12:LEU:O	2.10	0.52
1:C:100:HIS:HB3	1:C:105:ILE:HD12	1.90	0.52
1:D:53:ALA:O	1:D:57:VAL:HG23	2.10	0.52
1:C:7:PRO:HD2	1:C:10:ILE:HD12	1.91	0.52
1:B:45:LEU:HD12	1:B:182:VAL:HG21	1.91	0.52
1:A:55:TYR:CZ	1:B:79:LEU:HD12	2.44	0.52
1:A:56:ARG:HG3	1:A:56:ARG:HH11	1.74	0.52
1:A:147:ASP:O	1:A:148:HIS:C	2.47	0.52
2:F:196:ALA:O	2:F:199:LEU:HB2	2.09	0.52
1:B:152:PRO:HB2	1:B:155:ILE:HG12	1.92	0.52
1:C:90:ILE:O	1:C:135:LYS:HE3	2.09	0.52
1:A:7:PRO:HB2	1:A:10:ILE:HG13	1.92	0.52
1:D:190:SER:O	1:D:191:LEU:CB	2.57	0.51
1:D:23:LEU:CD2	1:D:122:VAL:HG21	2.40	0.51
2:H:195:LEU:HG	2:H:199:LEU:HD11	1.92	0.51
1:D:20:ILE:HD13	1:D:78:GLU:HG2	1.93	0.51
1:A:105:ILE:O	1:A:109:ILE:HG22	2.10	0.51
1:C:37:SER:O	1:C:41:VAL:HG23	2.10	0.51
1:B:183:PRO:HB3	1:B:186:LYS:HZ1	1.76	0.51
2:F:194:LYS:HD3	2:F:194:LYS:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ASP:C	1:D:90:ILE:HG13	2.31	0.51
1:D:148:HIS:HB2	1:D:151:VAL:HG21	1.91	0.51
1:D:189:ASN:N	1:D:189:ASN:ND2	2.50	0.51
1:A:129:LYS:HD3	1:A:145:ILE:HD11	1.93	0.51
1:D:105:ILE:O	1:D:109:ILE:HG22	2.10	0.51
1:B:45:LEU:O	1:B:186:LYS:HG3	2.12	0.50
1:C:107:GLU:HG3	1:C:152:PRO:HG3	1.94	0.50
1:C:96:LEU:HD12	1:C:100:HIS:HB2	1.94	0.50
1:B:147:ASP:O	1:B:148:HIS:C	2.50	0.50
1:C:148:HIS:HB2	1:C:151:VAL:CG2	2.42	0.50
1:B:184:TYR:HA	1:B:187:LEU:HD21	1.94	0.49
1:D:155:ILE:O	1:D:157:LYS:N	2.45	0.49
1:D:136:ILE:HG22	1:D:137:ASN:OD1	2.12	0.49
1:B:53:ALA:O	1:B:57:VAL:HG23	2.12	0.49
2:E:200:ARG:O	2:E:203:ARG:HG2	2.13	0.49
1:B:46:LEU:HA	1:B:183:PRO:HG2	1.95	0.49
1:B:184:TYR:HA	1:B:187:LEU:HG	1.94	0.49
1:B:93:GLU:OE2	1:B:140:PHE:HD1	1.96	0.49
1:A:7:PRO:HB2	1:A:10:ILE:CG1	2.42	0.49
1:A:116:ILE:CD1	1:A:126:SER:HA	2.42	0.49
1:D:96:LEU:HD12	1:D:100:HIS:HB2	1.95	0.49
1:D:129:LYS:HD3	1:D:145:ILE:HD11	1.95	0.49
1:A:177:ALA:HB1	1:A:182:VAL:CG2	2.43	0.49
2:G:191:LYS:HE2	2:G:191:LYS:O	2.12	0.49
1:B:184:TYR:HA	1:B:187:LEU:CD2	2.43	0.48
1:C:152:PRO:HB2	1:C:155:ILE:CG1	2.42	0.48
1:C:147:ASP:O	1:C:148:HIS:C	2.51	0.48
1:B:95:GLN:O	1:B:99:GLU:HB3	2.13	0.48
1:C:148:HIS:HB2	1:C:151:VAL:HG21	1.96	0.48
2:E:194:LYS:HG3	2:E:198:ARG:NE	2.27	0.48
1:D:65:ILE:CG1	2:H:203:ARG:HH21	2.27	0.48
1:A:90:ILE:O	1:A:135:LYS:HE3	2.14	0.48
1:B:38:ARG:HH11	1:B:38:ARG:HG2	1.79	0.48
1:A:38:ARG:HH11	1:A:38:ARG:HG2	1.79	0.48
1:D:145:ILE:O	1:D:145:ILE:HG22	2.14	0.48
1:A:181:ASP:HB3	1:A:182:VAL:H	1.38	0.48
1:B:138:VAL:HG21	1:C:7:PRO:HA	1.95	0.48
1:D:136:ILE:HG22	1:D:137:ASN:CG	2.33	0.48
1:C:95:GLN:O	1:C:99:GLU:HB3	2.14	0.48
1:D:147:ASP:O	1:D:149:ILE:N	2.47	0.47
1:B:23:LEU:CD2	1:B:70:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:CYS:O	1:A:78:GLU:C	2.52	0.47
1:D:171:LEU:HG	2:H:202:LEU:HD21	1.97	0.47
1:C:110:ARG:NH1	1:C:110:ARG:HG2	2.29	0.47
1:D:84:VAL:HA	1:D:87:ILE:HD12	1.96	0.47
1:B:38:ARG:HD3	2:F:195:LEU:HD11	1.96	0.47
1:B:56:ARG:HG3	1:B:56:ARG:HH11	1.78	0.47
1:D:38:ARG:HG2	1:D:38:ARG:HH11	1.80	0.47
1:A:24:ARG:HD3	1:D:40:GLN:HE22	1.80	0.47
1:A:136:ILE:HG22	1:A:137:ASN:CG	2.35	0.47
1:D:182:VAL:CG2	1:D:183:PRO:HD2	2.44	0.47
1:D:56:ARG:HH11	1:D:56:ARG:HG3	1.80	0.47
1:B:46:LEU:HD12	1:B:182:VAL:HG12	1.96	0.46
1:C:109:ILE:O	1:C:113:ILE:HG13	2.15	0.46
1:C:129:LYS:HD3	1:C:145:ILE:HD11	1.96	0.46
1:B:34:ALA:O	1:B:38:ARG:HG3	2.16	0.46
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.81	0.46
1:A:107:GLU:O	1:A:107:GLU:HG2	2.16	0.46
1:B:129:LYS:HD3	1:B:145:ILE:HD11	1.97	0.46
2:F:194:LYS:HB2	2:F:198:ARG:NH1	2.31	0.45
1:D:186:LYS:HG2	1:D:186:LYS:H	1.47	0.45
1:A:57:VAL:O	1:A:60:LEU:N	2.49	0.45
1:B:46:LEU:HG	1:B:183:PRO:HD3	1.97	0.45
1:B:129:LYS:O	1:B:132:MET:HB2	2.16	0.45
2:G:189:ASP:C	2:G:191:LYS:H	2.20	0.45
1:C:177:ALA:HA	1:C:182:VAL:HG23	1.98	0.45
1:B:141:VAL:HG23	1:B:142:ASN:N	2.31	0.45
1:B:5:MET:C	1:B:6:ILE:HG12	2.35	0.45
1:A:89:ASP:C	1:A:90:ILE:HG13	2.36	0.45
1:B:75:LEU:HD23	1:B:76:TYR:N	2.31	0.45
1:A:107:GLU:HG3	1:A:152:PRO:HG3	1.98	0.45
1:A:147:ASP:O	1:A:149:ILE:N	2.50	0.45
1:B:5:MET:O	1:B:6:ILE:HG12	2.17	0.45
1:B:47:THR:O	1:B:47:THR:HG22	2.17	0.45
1:B:57:VAL:O	1:B:60:LEU:N	2.50	0.45
1:B:184:TYR:HA	1:B:187:LEU:CG	2.47	0.45
1:A:37:SER:O	1:A:41:VAL:HG23	2.17	0.44
1:A:8:PHE:HE1	1:A:135:LYS:HB2	1.81	0.44
1:D:171:LEU:CG	2:H:202:LEU:HD21	2.46	0.44
1:B:185:SER:C	1:B:186:LYS:HE3	2.38	0.44
1:B:185:SER:HB3	1:B:186:LYS:HE3	1.99	0.44
1:B:22:ARG:HG3	1:B:124:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLN:O	1:C:131:LEU:HG	2.16	0.44
1:B:187:LEU:HD12	1:B:188:GLU:N	2.33	0.44
1:C:56:ARG:HH11	1:C:56:ARG:HG3	1.82	0.44
1:C:77:CYS:O	1:C:80:LEU:N	2.51	0.44
1:B:39:ARG:HG3	1:B:180:TYR:CE1	2.53	0.44
1:A:45:LEU:C	1:A:47:THR:H	2.21	0.44
2:F:194:LYS:HB2	2:F:198:ARG:HH12	1.83	0.44
1:C:141:VAL:HG23	1:C:142:ASN:N	2.33	0.44
1:D:22:ARG:HH11	1:D:22:ARG:HG3	1.82	0.44
1:A:129:LYS:O	1:A:132:MET:HB2	2.17	0.44
1:A:23:LEU:HD23	1:A:122:VAL:HG21	2.00	0.44
1:C:89:ASP:C	1:C:90:ILE:HG13	2.38	0.43
1:A:15:CYS:O	1:A:18:MET:HB3	2.18	0.43
1:B:57:VAL:O	1:B:58:GLU:C	2.55	0.43
1:B:8:PHE:HE1	1:B:135:LYS:HB2	1.82	0.43
1:D:15:CYS:O	1:D:18:MET:HB3	2.18	0.43
1:B:96:LEU:HD12	1:B:100:HIS:HB2	2.01	0.43
1:A:77:CYS:O	1:A:80:LEU:N	2.52	0.43
2:G:195:LEU:HG	2:G:199:LEU:HD12	2.01	0.43
1:A:6:ILE:HA	1:A:7:PRO:HD3	1.76	0.43
1:D:114:TYR:CE2	1:D:156:ILE:HG22	2.53	0.43
1:D:93:GLU:OE2	1:D:140:PHE:HD1	2.01	0.43
1:C:122:VAL:HG12	1:C:122:VAL:O	2.17	0.43
2:G:193:ASP:O	2:G:196:ALA:HB3	2.18	0.43
1:B:184:TYR:CG	1:B:187:LEU:HD11	2.54	0.43
1:A:79:LEU:C	1:A:79:LEU:HD23	2.39	0.43
1:A:181:ASP:C	1:A:182:VAL:HG13	2.38	0.43
1:B:22:ARG:HH11	1:B:22:ARG:HG3	1.84	0.43
1:B:129:LYS:HG3	1:B:141:VAL:HB	2.01	0.43
1:C:87:ILE:HA	1:C:90:ILE:HD12	2.01	0.43
1:D:147:ASP:O	1:D:148:HIS:C	2.57	0.43
1:B:12:LEU:HD11	1:B:16:LEU:HD11	2.01	0.43
1:C:34:ALA:O	1:C:37:SER:HB2	2.19	0.43
1:B:76:TYR:HE2	1:B:155:ILE:HD11	1.83	0.43
1:A:93:GLU:O	1:A:97:VAL:HG23	2.18	0.43
1:A:23:LEU:CD2	1:A:70:LEU:HD22	2.49	0.43
1:B:149:ILE:O	1:B:150:ASP:HB2	2.18	0.43
1:C:168:LEU:HD11	2:G:202:LEU:HD23	2.01	0.43
1:B:122:VAL:HG12	1:B:122:VAL:O	2.19	0.43
2:F:197:GLN:O	2:F:200:ARG:HG2	2.18	0.42
1:A:110:ARG:HD3	1:A:149:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD13	1:A:78:GLU:HG2	2.00	0.42
1:A:129:LYS:HG3	1:A:141:VAL:HB	2.00	0.42
1:A:57:VAL:O	1:A:58:GLU:C	2.58	0.42
1:A:55:TYR:HD2	1:B:75:LEU:HD11	1.84	0.42
1:C:114:TYR:CE2	1:C:156:ILE:HG22	2.54	0.42
1:D:122:VAL:HG12	1:D:125:LEU:HG	2.02	0.42
1:A:6:ILE:HD13	1:A:6:ILE:HA	1.76	0.42
1:C:93:GLU:O	1:C:97:VAL:HG23	2.20	0.42
1:D:81:LEU:HD12	1:D:81:LEU:O	2.20	0.42
1:B:137:ASN:CG	1:B:139:GLU:HG3	2.40	0.42
1:A:179:THR:HG21	2:E:195:LEU:HB2	2.01	0.42
1:A:73:LEU:CD2	1:A:112:LEU:HD23	2.44	0.42
1:A:186:LYS:HB2	1:A:186:LYS:HZ3	1.85	0.42
1:C:22:ARG:HG3	1:C:22:ARG:NH1	2.35	0.42
1:B:89:ASP:C	1:B:90:ILE:HG13	2.40	0.42
1:A:141:VAL:HG23	1:A:142:ASN:N	2.35	0.42
1:B:115:ALA:O	1:B:116:ILE:C	2.58	0.42
1:A:8:PHE:C	1:A:8:PHE:CD2	2.94	0.42
1:B:145:ILE:O	1:B:145:ILE:HG22	2.20	0.41
1:D:184:TYR:CD1	1:D:185:SER:N	2.88	0.41
1:D:83:ARG:O	1:D:87:ILE:HG13	2.20	0.41
1:B:35:LYS:NZ	1:B:35:LYS:HB3	2.35	0.41
2:H:195:LEU:HG	2:H:199:LEU:CD1	2.49	0.41
1:D:129:LYS:HG3	1:D:141:VAL:HB	2.02	0.41
1:D:185:SER:O	1:D:187:LEU:N	2.45	0.41
1:A:109:ILE:CD1	1:A:132:MET:SD	3.04	0.41
1:A:23:LEU:CD2	1:A:122:VAL:HG21	2.50	0.41
1:A:35:LYS:HE2	2:E:192:GLU:OE1	2.21	0.41
1:C:180:TYR:O	1:C:181:ASP:CB	2.69	0.41
1:B:187:LEU:HD12	1:B:188:GLU:H	1.86	0.41
1:C:88:ASN:HA	1:C:135:LYS:HE2	2.03	0.41
1:D:171:LEU:HG	2:H:202:LEU:CD2	2.51	0.41
1:C:105:ILE:O	1:C:109:ILE:HG22	2.21	0.41
1:C:117:LEU:HD11	1:C:145:ILE:HG23	2.03	0.41
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.85	0.41
1:B:45:LEU:C	1:B:47:THR:H	2.23	0.41
1:D:107:GLU:HG3	1:D:152:PRO:HG3	2.02	0.41
1:D:130:ASP:C	1:D:132:MET:H	2.23	0.41
1:C:132:MET:O	1:C:136:ILE:N	2.45	0.41
1:C:129:LYS:O	1:C:132:MET:HB2	2.20	0.41
2:F:194:LYS:H	2:F:194:LYS:CD	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:VAL:CG1	1:D:125:LEU:HG	2.51	0.41
1:A:132:MET:O	1:A:136:ILE:N	2.45	0.40
1:B:155:ILE:O	1:B:158:LYS:N	2.54	0.40
1:C:23:LEU:CD2	1:C:70:LEU:HD22	2.50	0.40
1:B:48:ASN:HA	1:B:186:LYS:HD2	2.03	0.40
1:B:187:LEU:CD1	1:B:188:GLU:HG3	2.51	0.40
1:C:147:ASP:O	1:C:149:ILE:N	2.55	0.40
1:B:20:ILE:HD13	1:B:78:GLU:HG2	2.04	0.40
1:A:96:LEU:HD12	1:A:100:HIS:HB2	2.04	0.40
1:C:116:ILE:CD1	1:C:126:SER:HA	2.51	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	184/193 (95%)	146 (79%)	32 (17%)	6 (3%)	5	43
1	B	184/193 (95%)	146 (79%)	30 (16%)	8 (4%)	3	35
1	C	180/193 (93%)	143 (79%)	31 (17%)	6 (3%)	5	43
1	D	186/193 (96%)	149 (80%)	25 (13%)	12 (6%)	1	25
2	E	15/29 (52%)	12 (80%)	3 (20%)	0	100	100
2	F	15/29 (52%)	13 (87%)	1 (7%)	1 (7%)	1	25
2	G	14/29 (48%)	9 (64%)	4 (29%)	1 (7%)	1	23
2	H	16/29 (55%)	11 (69%)	5 (31%)	0	100	100
All	All	794/888 (89%)	629 (79%)	131 (16%)	34 (4%)	3	35

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ASP
1	A	183	PRO
1	B	7	PRO
1	D	148	HIS
1	D	185	SER
1	D	186	LYS
1	D	190	SER
1	D	191	LEU
1	A	148	HIS
1	B	148	HIS
1	C	148	HIS
1	D	156	ILE
1	B	48	ASN
1	B	116	ILE
1	C	48	ASN
1	C	183	PRO
1	D	116	ILE
2	F	189	ASP
2	G	190	GLU
1	D	181	ASP
1	D	155	ILE
1	A	155	ILE
1	C	97	VAL
1	C	116	ILE
1	D	152	PRO
1	B	155	ILE
1	C	136	ILE
1	D	97	VAL
1	A	136	ILE
1	B	136	ILE
1	D	136	ILE
1	A	97	VAL
1	B	97	VAL
1	B	6	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	170/179 (95%)	154 (91%)	16 (9%)	11	47
1	B	172/179 (96%)	157 (91%)	15 (9%)	13	50
1	C	168/179 (94%)	155 (92%)	13 (8%)	16	56
1	D	174/179 (97%)	159 (91%)	15 (9%)	13	51
2	E	13/25 (52%)	10 (77%)	3 (23%)	1	8
2	F	13/25 (52%)	10 (77%)	3 (23%)	1	8
2	G	13/25 (52%)	10 (77%)	3 (23%)	1	8
2	H	13/25 (52%)	13 (100%)	0	100	100
All	All	736/816 (90%)	668 (91%)	68 (9%)	11	48

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	46	LEU
1	A	51	GLN
1	A	63	ASP
1	A	64	ASP
1	A	103	ASP
1	A	117	LEU
1	A	134	TRP
1	A	137	ASN
1	A	147	ASP
1	A	162	SER
1	A	172	TYR
1	A	181	ASP
1	A	182	VAL
1	A	186	LYS
1	A	188	GLU
1	B	6	ILE
1	B	31	GLN
1	B	46	LEU
1	B	63	ASP
1	B	64	ASP
1	B	103	ASP
1	B	117	LEU
1	B	134	TRP
1	B	137	ASN
1	B	147	ASP
1	B	162	SER

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Mol	Chain	Res	Type
1	B	172	TYR
1	B	182	VAL
1	B	184	TYR
1	B	187	LEU
1	C	6	ILE
1	C	31	GLN
1	C	46	LEU
1	C	63	ASP
1	C	64	ASP
1	C	103	ASP
1	C	117	LEU
1	C	134	TRP
1	C	137	ASN
1	C	147	ASP
1	C	162	SER
1	C	172	TYR
1	C	182	VAL
1	D	6	ILE
1	D	31	GLN
1	D	46	LEU
1	D	63	ASP
1	D	64	ASP
1	D	83	ARG
1	D	103	ASP
1	D	117	LEU
1	D	134	TRP
1	D	137	ASN
1	D	147	ASP
1	D	162	SER
1	D	172	TYR
1	D	186	LYS
1	D	189	ASN
2	E	194	LYS
2	E	195	LEU
2	E	197	GLN
2	F	193	ASP
2	F	194	LYS
2	F	200	ARG
2	G	189	ASP
2	G	191	LYS
2	G	197	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	40	GLN
1	A	48	ASN
1	A	51	GLN
1	A	142	ASN
1	B	31	GLN
1	B	48	ASN
1	B	51	GLN
1	C	30	GLN
1	C	31	GLN
1	C	48	ASN
1	C	51	GLN
1	D	31	GLN
1	D	40	GLN
1	D	48	ASN
1	D	51	GLN
1	D	189	ASN

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 carbohydrates 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 ⓘ

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	186/193 (96%)	-0.06	4 (2%) 65 50	104, 140, 180, 195	0
1	B	186/193 (96%)	-0.04	5 (2%) 58 42	104, 138, 184, 200	0
1	C	182/193 (94%)	0.02	3 (1%) 74 60	106, 141, 181, 198	0
1	D	188/193 (97%)	0.01	3 (1%) 74 60	105, 140, 178, 185	0
2	E	17/29 (58%)	-0.13	0 100 100	146, 170, 176, 177	0
2	F	17/29 (58%)	0.12	0 100 100	144, 171, 176, 179	0
2	G	16/29 (55%)	0.18	1 (6%) 23 14	152, 167, 184, 185	0
2	H	18/29 (62%)	0.17	1 (5%) 28 18	141, 160, 171, 172	0
All	All	810/888 (91%)	-0.01	17 (2%) 67 51	104, 144, 181, 200	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	SER	4.2
1	B	180	TYR	3.7
2	G	189	ASP	2.7
1	A	52	LYS	2.7
1	C	134	TRP	2.6
1	A	188	GLU	2.6
1	D	104	GLY	2.3
1	B	181	ASP	2.3
1	D	134	TRP	2.2
1	C	52	LYS	2.2
2	H	191	LYS	2.1
1	C	5	MET	2.1
1	A	183	PRO	2.1
1	B	183	PRO	2.1
1	B	185	SER	2.0
1	D	105	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	180	TYR	2.0

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 carbohydrates 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.