



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:18 AM UTC

PDB ID : 4C8Q / pdb_00004c8q
Title : Crystal structure of the yeast Lsm1-7-Pat1 complex
Authors : Sharif, H.; Conti, E.
Deposited on : 2013-10-01
Resolution : 3.70 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:

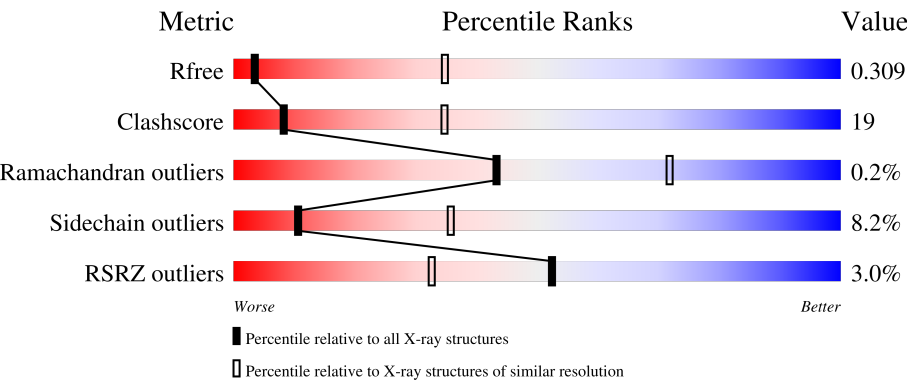
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	101	9% 62% 25% 5% 7%
2	B	105	% 63% 29% 7% ..
3	C	89	61% 21% 6% 11%
4	D	114	5% 52% 16% 29%
5	E	93	3% 60% 25% 11%

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Mol	Chain	Length	Quality of chain
6	F	86	62%26%10%2%
7	G	115	40%15%5%40%2%
8	H	328	51%30%15%2%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6280 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 SM-LIKE PROTEIN LSM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			673	428	115	125	5			

- Molecule 2 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			796	505	134	154	3			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	expression tag	UNP P38203
B	-8	GLU	-	expression tag	UNP P38203
B	-7	ASN	-	expression tag	UNP P38203
B	-6	LEU	-	expression tag	UNP P38203
B	-5	TYR	-	expression tag	UNP P38203
B	-4	PHE	-	expression tag	UNP P38203
B	-3	GLN	-	expression tag	UNP P38203
B	-2	GLY	-	expression tag	UNP P38203
B	-1	SER	-	expression tag	UNP P38203
B	0	GLY	-	expression tag	UNP P38203
B	1	SER	-	expression tag	UNP P38203

- Molecule 3 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	79	Total	C	N	O	S	0	0	0
			589	369	105	112	3			

- Molecule 4 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	81	Total	C	N	O	S	0	0	0
			504	321	85	97	1			

- Molecule 5 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	83	Total	C	N	O	S	0	0	0
			600	383	104	111	2			

- Molecule 6 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	77	Total	C	N	O	S	0	0	0
			571	361	95	113	2			

- Molecule 7 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	69	Total	C	N	O	S	0	0	0
			456	289	79	87	1			

- Molecule 8 is a protein called DNA TOPOISOMERASE 2-ASSOCIATED PROTEIN PAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	279	Total	C	N	O	S	0	0	0
			2089	1366	332	384	7			

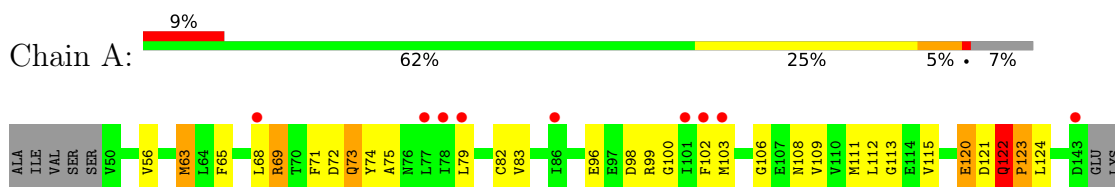
- Molecule 9 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Co	0	0
			1	1		
9	H	1	Total	Co	0	0
			1	1		

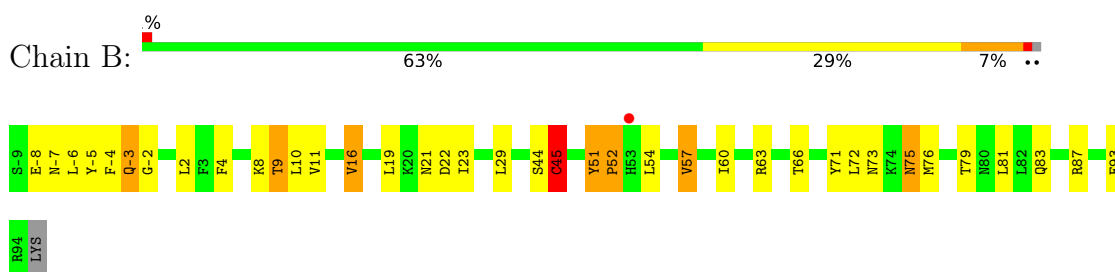
3 Residue-property plots [i](#)

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.

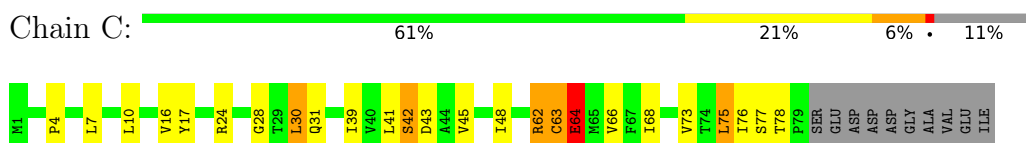
- Molecule 1: SM-LIKE PROTEIN LSM1



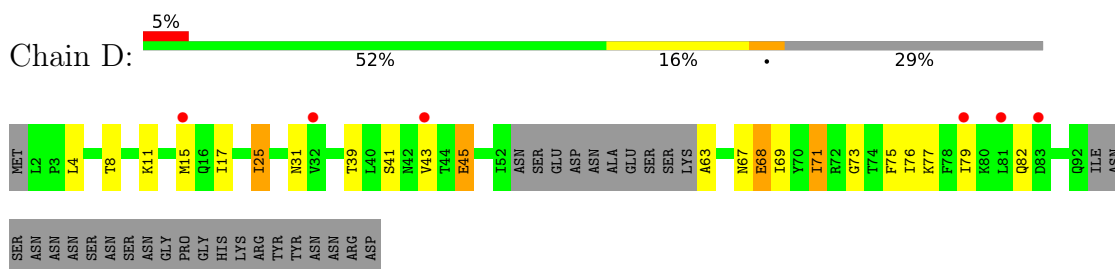
- Molecule 2: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM2



- Molecule 3: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM3



- Molecule 4: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM4



- Molecule 5: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM5

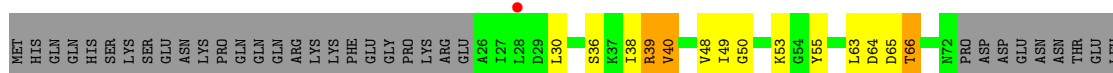
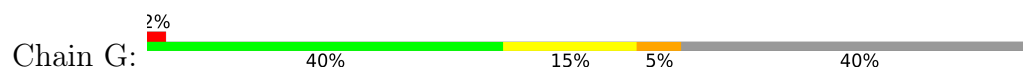




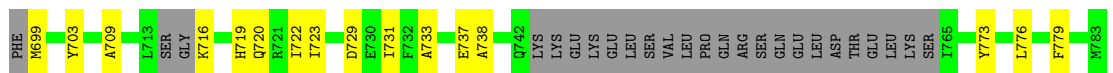
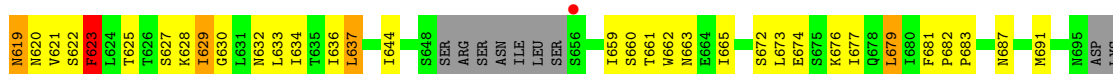
• Molecule 6: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM6



• Molecule 7: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM7



• Molecule 8: DNA TOPOISOMERASE 2-ASSOCIATED PROTEIN PAT1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	258.69Å 258.69Å 47.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.42 – 3.70 43.42 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.42-3.70) 99.2 (43.42-3.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.295 0.273 , 0.309	Depositor DCC
R_{free} test set	990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	135.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 125.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6280	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CO

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	0.51	1/684 (0.1%)	1.23	6/929 (0.6%)
2	B	0.46	0/806	1.12	6/1093 (0.5%)
3	C	0.63	0/594	1.21	3/807 (0.4%)
4	D	0.53	0/509	1.38	6/698 (0.9%)
5	E	0.52	0/609	1.24	5/831 (0.6%)
6	F	0.49	0/578	1.18	3/784 (0.4%)
7	G	0.46	0/456	1.39	7/618 (1.1%)
8	H	0.49	0/2120	0.96	12/2881 (0.4%)
All	All	0.51	1/6356 (0.0%)	1.15	48/8641 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	PRO	N-CD	5.16	1.54	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	497	ARG	N-CA-C	-9.07	97.71	110.50
3	C	42	SER	N-CA-C	8.71	124.22	113.50
4	D	41	SER	N-CA-C	8.59	121.79	111.82
6	F	56	TYR	N-CA-C	8.58	120.41	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	39	THR	N-CA-C	8.36	120.16	111.14
4	D	69	ILE	N-CA-C	8.31	119.31	108.35
5	E	82	VAL	N-CA-C	8.05	116.12	108.15
6	F	44	PHE	N-CA-C	-7.88	103.77	113.15
8	H	623	PHE	N-CA-C	-7.38	103.32	111.36
4	D	43	VAL	N-CA-C	7.27	120.24	108.97
2	B	45	CYS	N-CA-C	6.90	119.56	109.07
8	H	679	LEU	N-CA-C	-6.79	104.81	113.23
2	B	51	TYR	N-CA-C	6.65	119.15	109.04
8	H	499	GLY	N-CA-C	-6.60	99.61	110.56
5	E	64	VAL	N-CA-C	6.55	118.53	111.58
7	G	100	VAL	N-CA-C	6.42	117.10	111.90
1	A	98	ASP	N-CA-C	6.39	120.29	110.20
3	C	78	THR	N-CA-C	6.26	117.78	109.83
2	B	2	LEU	N-CA-C	6.25	118.64	111.02
5	E	7	LEU	CA-C-N	6.21	125.70	119.24
5	E	7	LEU	C-N-CA	6.21	125.70	119.24
7	G	89	LEU	N-CA-C	-6.19	106.70	114.56
8	H	619	ASN	N-CA-C	6.12	118.15	108.79
7	G	91	LEU	N-CA-C	6.08	119.43	109.76
4	D	82	GLN	N-CA-C	6.05	119.00	110.23
8	H	573	THR	CA-C-N	5.98	125.36	118.85
8	H	573	THR	C-N-CA	5.98	125.36	118.85
8	H	547	GLN	N-CA-C	-5.96	105.67	113.12
2	B	57	VAL	N-CA-C	5.83	117.18	108.54
6	F	39	GLU	N-CA-C	5.78	121.64	113.02
1	A	96	GLU	N-CA-C	5.72	118.39	109.52
1	A	106	GLY	N-CA-C	5.66	120.65	113.24
8	H	681	PHE	CA-C-N	5.64	123.72	119.66
8	H	681	PHE	C-N-CA	5.64	123.72	119.66
5	E	44	ILE	N-CA-C	5.60	116.16	107.99
8	H	476	LYS	N-CA-C	-5.46	104.97	111.69
1	A	73	GLN	N-CA-C	-5.42	105.37	111.28
2	B	-4	PHE	N-CA-C	5.40	117.01	107.61
1	A	122	GLN	CA-C-N	-5.38	113.08	119.05
1	A	122	GLN	C-N-CA	-5.38	113.08	119.05
2	B	-6	LEU	N-CA-C	5.37	117.89	111.71
4	D	71	ILE	N-CA-C	5.31	116.12	108.48
7	G	66	THR	N-CA-C	5.24	117.78	109.24
3	C	64	GLU	N-CA-C	5.18	116.74	111.14
7	G	92	THR	N-CA-C	5.15	116.64	108.96
8	H	738	ALA	N-CA-C	-5.12	102.76	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	36	SER	N-CA-C	-5.07	101.84	109.85
7	G	40	VAL	N-CA-C	5.04	115.23	107.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	496	LEU	Peptide

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	673	0	558	39	0
2	B	796	0	755	25	0
3	C	589	0	565	23	0
4	D	504	0	370	17	0
5	E	600	0	558	25	0
6	F	571	0	530	16	0
7	G	456	0	428	25	0
8	H	2089	0	1978	82	0
9	C	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6280	0	5742	232	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 19.

All (232) 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:A:72:ASP:HA	1:A:75:ALA:HA	1.29	1.07
5:E:73:LEU:HD13	5:E:78:ILE:HD11	1.27	1.05
1:A:72:ASP:HA	1:A:75:ALA:CA	1.92	0.99
3:C:30:LEU:HD12	3:C:31:GLN:N	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:PRO:HG3	6:F:40:SER:CB	1.96	0.95
5:E:73:LEU:HD12	5:E:73:LEU:O	1.73	0.89
3:C:42:SER:O	3:C:43:ASP:OD1	1.95	0.84
5:E:43:VAL:HB	5:E:73:LEU:HD11	1.61	0.82
6:F:47:VAL:HG23	6:F:73:LEU:HB2	1.62	0.80
2:B:16:VAL:HG13	2:B:71:TYR:HB2	1.63	0.79
5:E:45:LEU:HD13	5:E:73:LEU:HD23	1.65	0.79
7:G:39:ARG:HG2	7:G:39:ARG:HH11	1.49	0.78
8:H:495:ASN:O	8:H:496:LEU:HD12	1.84	0.77
4:D:17:ILE:HG23	4:D:79:ILE:HG22	1.66	0.77
7:G:39:ARG:HG2	7:G:39:ARG:NH1	2.01	0.75
1:A:72:ASP:HA	1:A:75:ALA:N	2.02	0.74
1:A:74:TYR:O	1:A:75:ALA:HB3	1.88	0.73
8:H:539:ILE:O	8:H:543:LEU:HD23	1.88	0.73
3:C:73:VAL:O	6:F:74:ARG:HG3	1.87	0.73
1:A:121:ASP:O	1:A:124:LEU:HB2	1.88	0.73
6:F:25:ASN:HB3	6:F:33:LEU:HD11	1.69	0.73
8:H:632:ASN:HD21	8:H:703:TYR:HB2	1.55	0.71
5:E:21:LEU:HD13	5:E:86:LYS:CB	2.20	0.71
8:H:621:VAL:O	8:H:622:SER:HB3	1.92	0.70
3:C:45:VAL:HG12	3:C:62:ARG:HB3	1.72	0.70
8:H:605:PHE:HD2	8:H:644:ILE:HD12	1.55	0.69
7:G:38:ILE:O	7:G:49:ILE:HA	1.92	0.69
4:D:11:LYS:HE3	4:D:31:ASN:HA	1.74	0.69
7:G:38:ILE:HG22	7:G:40:VAL:HG23	1.75	0.69
1:A:68:LEU:HD21	1:A:71:PHE:CB	2.23	0.68
3:C:30:LEU:HD12	3:C:31:GLN:H	1.54	0.68
8:H:659:ILE:O	8:H:663:ASN:ND2	2.27	0.68
8:H:489:ILE:HG21	8:H:535:ILE:HD11	1.76	0.66
7:G:38:ILE:HB	7:G:50:GLY:O	1.95	0.66
5:E:21:LEU:HD12	5:E:31:GLU:HB3	1.78	0.65
1:A:121:ASP:HA	1:A:124:LEU:HD12	1.78	0.65
5:E:73:LEU:HD13	5:E:78:ILE:CD1	2.16	0.65
2:B:73:ASN:OD1	2:B:73:ASN:N	2.30	0.64
1:A:63:MET:HE1	2:B:52:PRO:CG	2.27	0.64
8:H:515:ASP:OD1	8:H:517:SER:HB3	1.97	0.63
8:H:533:ILE:HG21	8:H:587:PHE:HA	1.81	0.62
1:A:120:GLU:O	1:A:123:PRO:HG2	2.00	0.62
8:H:495:ASN:C	8:H:496:LEU:HD12	2.25	0.61
1:A:72:ASP:C	1:A:75:ALA:H	2.09	0.61
5:E:73:LEU:CD1	5:E:78:ILE:HD11	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:ILE:HD12	4:D:25:ILE:O	2.01	0.60
7:G:39:ARG:HH11	7:G:39:ARG:CG	2.15	0.59
1:A:72:ASP:HA	1:A:75:ALA:H	1.65	0.59
8:H:492:LEU:HB3	8:H:542:PHE:CE2	2.38	0.59
8:H:568:SER:HB2	8:H:627:SER:HB2	1.83	0.59
1:A:72:ASP:CA	1:A:75:ALA:HA	2.19	0.59
3:C:30:LEU:HD12	3:C:30:LEU:C	2.28	0.59
3:C:24:ARG:HG2	3:C:48:ILE:HG12	1.86	0.58
8:H:511:LEU:HD11	8:H:539:ILE:HD11	1.86	0.58
8:H:622:SER:HA	8:H:625:THR:HG23	1.84	0.58
8:H:731:ILE:HG23	8:H:776:LEU:HD11	1.86	0.58
7:G:39:ARG:HA	7:G:49:ILE:HG13	1.85	0.58
7:G:66:THR:H	7:G:90:GLY:HA2	1.68	0.58
1:A:108:ASN:HD21	4:D:77:LYS:HA	1.69	0.58
3:C:75:LEU:HD11	6:F:67:PHE:HE2	1.69	0.58
4:D:17:ILE:HG12	4:D:79:ILE:HB	1.86	0.58
4:D:73:GLY:O	4:D:76:ILE:HG12	2.03	0.58
8:H:520:VAL:HG12	8:H:561:HIS:ND1	2.18	0.58
3:C:63:CYS:SG	3:C:66:VAL:HG11	2.45	0.57
3:C:76:ILE:HB	6:F:72:PHE:HB3	1.86	0.57
1:A:68:LEU:HD11	1:A:71:PHE:CB	2.35	0.56
1:A:111:MET:HE3	2:B:60:ILE:HG21	1.87	0.56
2:B:10:LEU:HD11	2:B:72:LEU:HD21	1.86	0.56
1:A:74:TYR:O	1:A:75:ALA:CB	2.52	0.55
1:A:103:MET:HB2	4:D:79:ILE:HG12	1.89	0.55
8:H:507:MET:HE1	8:H:543:LEU:HD21	1.87	0.55
6:F:35:SER:O	6:F:52:ALA:HA	2.05	0.55
6:F:56:TYR:CD1	6:F:56:TYR:C	2.85	0.54
2:B:54:LEU:O	2:B:57:VAL:HG12	2.06	0.54
7:G:89:LEU:HD11	7:G:92:THR:HG22	1.88	0.54
5:E:28:ARG:NH2	6:F:57:GLU:OE2	2.40	0.54
7:G:89:LEU:HD11	7:G:92:THR:CG2	2.38	0.54
8:H:623:PHE:C	8:H:623:PHE:CD1	2.85	0.53
3:C:16:VAL:N	3:C:28:GLY:O	2.32	0.53
5:E:46:GLU:HG3	5:E:70:ARG:HG2	1.89	0.53
8:H:543:LEU:HD12	8:H:547:GLN:HB3	1.90	0.53
8:H:552:LEU:HD22	8:H:598:PHE:CD2	2.44	0.53
8:H:673:LEU:O	8:H:676:LYS:N	2.41	0.53
2:B:19:LEU:HD22	2:B:66:THR:HG23	1.89	0.52
3:C:30:LEU:HA	3:C:41:LEU:HD23	1.92	0.52
8:H:536:MET:HA	8:H:539:ILE:HG22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:729:ASP:O	8:H:733:ALA:N	2.42	0.52
4:D:25:ILE:HG12	4:D:71:ILE:CD1	2.39	0.52
6:F:75:GLY:O	6:F:78:VAL:HG22	2.10	0.52
6:F:43:GLY:C	6:F:45:MET:H	2.15	0.52
8:H:475:LYS:O	8:H:479:LEU:HD23	2.08	0.52
1:A:72:ASP:CA	1:A:75:ALA:H	2.22	0.52
8:H:482:ILE:HG21	8:H:531:LYS:HD3	1.91	0.52
1:A:120:GLU:O	1:A:123:PRO:CG	2.58	0.52
7:G:64:ASP:OD1	7:G:65:ASP:N	2.43	0.52
8:H:474:GLY:C	8:H:476:LYS:H	2.17	0.51
8:H:495:ASN:C	8:H:497:ARG:O	2.53	0.51
2:B:73:ASN:OD1	2:B:76:MET:HE3	2.10	0.51
5:E:73:LEU:HD12	5:E:73:LEU:C	2.33	0.51
8:H:474:GLY:O	8:H:475:LYS:HB3	2.11	0.51
5:E:41:VAL:HG11	7:G:95:ARG:HD2	1.93	0.51
7:G:30:LEU:HD11	7:G:55:TYR:CD1	2.45	0.51
7:G:38:ILE:HG22	7:G:40:VAL:CG2	2.39	0.51
7:G:38:ILE:CB	7:G:50:GLY:O	2.58	0.51
2:B:63:ARG:O	2:B:66:THR:HG22	2.11	0.51
8:H:682:PRO:HG2	8:H:687:ASN:HD21	1.77	0.50
2:B:-5:TYR:HE1	2:B:9:THR:HG21	1.76	0.50
2:B:44:SER:C	2:B:45:CYS:SG	2.94	0.50
2:B:79:THR:HB	3:C:31:GLN:OE1	2.12	0.50
8:H:588:GLN:HG3	8:H:592:LEU:HD12	1.94	0.50
1:A:121:ASP:O	1:A:124:LEU:N	2.45	0.50
8:H:568:SER:HB3	8:H:628:LYS:H	1.77	0.50
1:A:82:CYS:SG	1:A:102:PHE:HB2	2.51	0.50
8:H:479:LEU:HD21	8:H:529:PHE:CE2	2.46	0.50
8:H:486:TYR:CD2	8:H:535:ILE:HD12	2.47	0.49
8:H:488:GLU:HG2	8:H:507:MET:HA	1.94	0.49
2:B:21:ASN:O	2:B:22:ASP:HB2	2.11	0.49
3:C:10:LEU:HD22	8:H:479:LEU:HB3	1.95	0.49
5:E:45:LEU:HD13	5:E:73:LEU:CD2	2.38	0.49
1:A:82:CYS:N	1:A:99:ARG:O	2.46	0.49
4:D:75:PHE:CD1	7:G:100:VAL:HG22	2.47	0.49
8:H:568:SER:HB3	8:H:628:LYS:N	2.27	0.49
1:A:113:GLY:HA3	2:B:60:ILE:HD13	1.94	0.49
3:C:39:ILE:O	3:C:68:ILE:HG22	2.13	0.49
8:H:543:LEU:HD12	8:H:547:GLN:CB	2.42	0.48
8:H:683:PRO:O	8:H:687:ASN:ND2	2.45	0.48
1:A:120:GLU:C	1:A:123:PRO:HD2	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:N	1:A:123:PRO:HD2	2.27	0.48
3:C:7:LEU:O	3:C:10:LEU:HB2	2.13	0.48
4:D:45:GLU:O	4:D:63:ALA:N	2.47	0.48
5:E:16:ILE:HG12	5:E:34:LEU:HD22	1.96	0.48
5:E:11:VAL:O	5:E:15:THR:HG23	2.14	0.48
1:A:108:ASN:ND2	4:D:77:LYS:HA	2.28	0.48
3:C:68:ILE:HG23	3:C:68:ILE:O	2.12	0.48
8:H:556:PHE:CZ	8:H:637:LEU:HD21	2.48	0.48
8:H:559:LEU:HD21	8:H:633:LEU:HD23	1.95	0.48
7:G:40:VAL:N	7:G:48:VAL:O	2.42	0.48
8:H:605:PHE:CD2	8:H:644:ILE:HD12	2.43	0.47
8:H:716:LYS:O	8:H:720:GLN:HG3	2.15	0.47
8:H:709:ALA:HB2	8:H:779:PHE:HA	1.95	0.47
1:A:73:GLN:C	1:A:74:TYR:HD1	2.22	0.47
1:A:121:ASP:OD1	1:A:124:LEU:HD12	2.15	0.47
8:H:733:ALA:O	8:H:737:GLU:N	2.48	0.47
1:A:65:PHE:O	1:A:82:CYS:HA	2.14	0.47
7:G:38:ILE:O	7:G:49:ILE:HG23	2.15	0.47
4:D:4:LEU:O	4:D:8:THR:OG1	2.31	0.47
8:H:536:MET:HG3	8:H:591:ILE:HD11	1.96	0.47
5:E:22:ILE:CG2	5:E:78:ILE:HD12	2.46	0.46
7:G:39:ARG:HB2	7:G:105:ALA:HB2	1.97	0.46
8:H:612:LEU:O	8:H:616:ILE:HG12	2.15	0.46
5:E:40:PHE:O	5:E:41:VAL:HG12	2.15	0.46
2:B:51:TYR:HA	2:B:52:PRO:HD2	1.73	0.46
8:H:632:ASN:O	8:H:636:ILE:HG13	2.16	0.46
1:A:103:MET:SD	4:D:79:ILE:HD11	2.55	0.46
8:H:674:GLU:HG3	8:H:722:ILE:HG21	1.98	0.46
2:B:73:ASN:HB2	2:B:75:ASN:OD1	2.15	0.46
1:A:63:MET:HE3	1:A:63:MET:HB2	1.66	0.46
1:A:121:ASP:O	1:A:124:LEU:CB	2.63	0.46
5:E:43:VAL:HG12	5:E:45:LEU:HD12	1.98	0.46
5:E:71:MET:CB	6:F:82:SER:HB2	2.45	0.46
8:H:630:GLY:O	8:H:634:ILE:HG12	2.15	0.45
1:A:120:GLU:O	1:A:124:LEU:HG	2.16	0.45
2:B:75:ASN:OD1	2:B:75:ASN:N	2.47	0.45
5:E:43:VAL:O	5:E:73:LEU:HG	2.17	0.45
7:G:55:TYR:CD2	7:G:55:TYR:C	2.93	0.45
8:H:546:GLN:HA	8:H:549:LEU:HB3	1.98	0.45
3:C:17:TYR:HB3	3:C:77:SER:O	2.17	0.45
8:H:719:HIS:O	8:H:723:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:47:VAL:CG2	6:F:73:LEU:HB2	2.42	0.45
8:H:604:ASN:CG	8:H:606:ILE:HG22	2.42	0.45
3:C:63:CYS:SG	3:C:66:VAL:CG1	3.05	0.44
8:H:622:SER:HA	8:H:625:THR:CG2	2.47	0.44
5:E:43:VAL:HB	5:E:73:LEU:CD1	2.40	0.44
8:H:546:GLN:O	8:H:550:LYS:HB2	2.17	0.44
8:H:482:ILE:HD11	8:H:532:GLY:CA	2.48	0.44
8:H:545:LYS:HD2	8:H:602:ASN:OD1	2.17	0.44
8:H:620:ASN:O	8:H:623:PHE:HB3	2.18	0.44
1:A:73:GLN:O	1:A:74:TYR:HD1	2.00	0.44
5:E:26:SER:OG	5:E:27:ASN:N	2.50	0.44
7:G:66:THR:N	7:G:90:GLY:HA2	2.32	0.44
1:A:82:CYS:HB2	1:A:99:ARG:CB	2.48	0.44
3:C:4:PRO:CG	6:F:40:SER:CB	2.84	0.44
5:E:57:ASP:O	5:E:60:ARG:N	2.48	0.44
8:H:527:LEU:HD12	8:H:527:LEU:HA	1.84	0.44
5:E:75:GLY:HA2	5:E:78:ILE:HG12	1.99	0.43
8:H:515:ASP:OD1	8:H:517:SER:N	2.50	0.43
8:H:533:ILE:O	8:H:590:ILE:HG21	2.18	0.43
8:H:612:LEU:HG	8:H:637:LEU:HB3	2.01	0.43
8:H:662:TRP:HA	8:H:665:ILE:HD12	2.00	0.43
8:H:673:LEU:O	8:H:677:ILE:HG13	2.18	0.43
8:H:623:PHE:HD1	8:H:623:PHE:O	2.01	0.43
3:C:42:SER:O	3:C:64:GLU:O	2.37	0.43
7:G:53:LYS:HG3	7:G:64:ASP:HB2	1.98	0.43
8:H:564:ILE:HD11	8:H:584:VAL:HA	2.01	0.43
8:H:578:LEU:HA	8:H:581:LEU:HD12	2.00	0.43
8:H:564:ILE:HG21	8:H:587:PHE:CD2	2.54	0.43
8:H:620:ASN:OD1	8:H:623:PHE:HB2	2.19	0.43
2:B:11:VAL:HA	2:B:29:LEU:HD23	2.01	0.42
8:H:691:MET:HE1	8:H:699:MET:N	2.33	0.42
1:A:56:VAL:HG22	1:A:112:LEU:HB3	2.00	0.42
8:H:661:THR:HG22	8:H:665:ILE:HD11	2.01	0.42
6:F:42:ASP:CB	6:F:46:ASN:HB2	2.49	0.42
1:A:74:TYR:N	1:A:74:TYR:CD1	2.86	0.42
3:C:75:LEU:HD11	6:F:67:PHE:CE2	2.53	0.42
8:H:660:SER:HA	8:H:663:ASN:HD22	1.84	0.42
2:B:19:LEU:HD12	2:B:23:ILE:HB	2.01	0.42
8:H:544:ASP:O	8:H:545:LYS:C	2.63	0.42
1:A:68:LEU:HD12	1:A:69:ARG:H	1.85	0.42
2:B:57:VAL:HG21	2:B:60:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:63:LEU:HD13	7:G:94:ILE:HG12	2.00	0.42
8:H:475:LYS:HG3	8:H:529:PHE:HZ	1.84	0.42
8:H:570:TYR:OH	8:H:679:LEU:O	2.23	0.41
8:H:629:ILE:HD13	8:H:629:ILE:HA	1.78	0.41
4:D:45:GLU:OE2	7:G:39:ARG:NH2	2.52	0.41
2:B:4:PHE:O	2:B:8:LYS:HG3	2.19	0.41
7:G:89:LEU:HD12	7:G:89:LEU:C	2.45	0.41
4:D:67:ASN:C	4:D:68:GLU:HG2	2.46	0.41
5:E:71:MET:HE3	5:E:71:MET:HB2	1.97	0.41
8:H:495:ASN:O	8:H:497:ARG:O	2.39	0.41
8:H:623:PHE:C	8:H:623:PHE:HD1	2.29	0.41
8:H:632:ASN:HD22	8:H:632:ASN:HA	1.76	0.41
2:B:-3:GLN:HG2	2:B:-2:GLY:N	2.36	0.41
8:H:604:ASN:OD1	8:H:605:PHE:N	2.54	0.41
8:H:482:ILE:HD12	8:H:526:MET:HB2	2.03	0.40
2:B:8:LYS:HE2	2:B:8:LYS:HB3	1.63	0.40
4:D:15:MET:HE2	4:D:15:MET:HB3	1.94	0.40
4:D:17:ILE:HB	4:D:25:ILE:CD1	2.50	0.40
2:B:83:GLN:O	2:B:87:ARG:HG3	2.22	0.40
8:H:525:SER:O	8:H:528:SER:OG	2.35	0.40
1:A:79:LEU:HB2	1:A:82:CYS:SG	2.61	0.40
8:H:511:LEU:HD11	8:H:539:ILE:CD1	2.51	0.40
2:B:-7:ASN:CB	2:B:81:LEU:HD21	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	92/101 (91%)	88 (96%)	3 (3%)	1 (1%)	11	42
2	B	102/105 (97%)	93 (91%)	8 (8%)	1 (1%)	12	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	77/89 (86%)	75 (97%)	2 (3%)	0	100	100
4	D	77/114 (68%)	73 (95%)	4 (5%)	0	100	100
5	E	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
6	F	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
7	G	65/115 (56%)	62 (95%)	3 (5%)	0	100	100
8	H	269/328 (82%)	253 (94%)	16 (6%)	0	100	100
All	All	838/1031 (81%)	792 (94%)	44 (5%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLY
2	B	52	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	53/91 (58%)	46 (87%)	7 (13%)	4	20
2	B	84/99 (85%)	77 (92%)	7 (8%)	10	35
3	C	59/81 (73%)	54 (92%)	5 (8%)	10	35
4	D	29/104 (28%)	26 (90%)	3 (10%)	7	29
5	E	58/84 (69%)	54 (93%)	4 (7%)	14	41
6	F	58/75 (77%)	54 (93%)	4 (7%)	14	41
7	G	39/103 (38%)	37 (95%)	2 (5%)	21	47
8	H	204/307 (66%)	188 (92%)	16 (8%)	11	37
All	All	584/944 (62%)	536 (92%)	48 (8%)	10	36

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	MET
1	A	69	ARG
1	A	83	VAL
1	A	109	VAL
1	A	115	VAL
1	A	120	GLU
1	A	122	GLN
2	B	-8	GLU
2	B	-3	GLN
2	B	9	THR
2	B	16	VAL
2	B	45	CYS
2	B	75	ASN
2	B	93	GLU
3	C	30	LEU
3	C	62	ARG
3	C	63	CYS
3	C	64	GLU
3	C	75	LEU
4	D	25	ILE
4	D	45	GLU
4	D	68	GLU
5	E	11	VAL
5	E	21	LEU
5	E	28	ARG
5	E	34	LEU
6	F	12	THR
6	F	17	SER
6	F	23	THR
6	F	47	VAL
7	G	39	ARG
7	G	103	SER
8	H	497	ARG
8	H	531	LYS
8	H	535	ILE
8	H	540	PHE
8	H	552	LEU
8	H	564	ILE
8	H	565	ILE
8	H	586	LEU
8	H	612	LEU
8	H	617	ARG
8	H	619	ASN

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Mol	Chain	Res	Type
8	H	623	PHE
8	H	629	ILE
8	H	637	LEU
8	H	672	SER
8	H	773	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
2	B	-3	GLN
2	B	80	ASN
2	B	83	GLN
3	C	11	ASN
6	F	61	ASN
6	F	84	GLN
8	H	588	GLN
8	H	632	ASN
8	H	663	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	94/101 (93%)	0.58	9 (9%) 13 13	102, 179, 212, 225	0
2	B	104/105 (99%)	0.13	1 (0%) 79 55	92, 125, 187, 198	0
3	C	79/89 (88%)	-0.01	0 100 100	50, 100, 192, 209	0
4	D	81/114 (71%)	0.77	6 (7%) 20 15	157, 181, 208, 213	0
5	E	83/93 (89%)	0.39	3 (3%) 46 29	71, 133, 177, 183	0
6	F	77/86 (89%)	0.15	0 100 100	79, 106, 145, 153	0
7	G	69/115 (60%)	0.62	2 (2%) 53 33	84, 157, 190, 219	0
8	H	279/328 (85%)	-0.03	5 (1%) 67 42	50, 95, 163, 231	0
All	All	866/1031 (83%)	0.24	26 (3%) 52 32	50, 126, 197, 231	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	73	LEU	4.6
7	G	92	THR	4.0
4	D	32	VAL	3.9
8	H	473	GLY	3.5
1	A	103	MET	3.4
4	D	15	MET	2.9
1	A	102	PHE	2.8
1	A	68	LEU	2.7
8	H	572	THR	2.7
8	H	656	SER	2.7
1	A	79	LEU	2.6
4	D	79	ILE	2.6
5	E	52	LEU	2.5
4	D	83	ASP	2.3
8	H	472	SER	2.3
1	A	101	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	86	ILE	2.2
1	A	78	ILE	2.2
2	B	53	HIS	2.1
4	D	81	LEU	2.1
4	D	43	VAL	2.1
1	A	143	ASP	2.1
7	G	28	LEU	2.1
5	E	78	ILE	2.1
8	H	474	GLY	2.0
1	A	77	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CO	C	1080	1/1	0.90	0.16	144,144,144,144	0
9	CO	H	1080	1/1	0.94	0.15	189,189,189,189	0

6.5 Other polymers [i](#)

There are no such residues in this entry.