



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:00 PM UTC

PDB ID : 2D3W / pdb_00002d3w
Title : Crystal Structure of Escherichia coli SufC, an ATPase component of the SUF iron-sulfur cluster assembly machinery
Authors : Kitaoka, S.; Wada, K.; Hasegawa, Y.; Minami, Y.; Takahashi, Y.; Fukuyama, K.
Deposited on : 2005-10-03
Resolution : 2.50 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

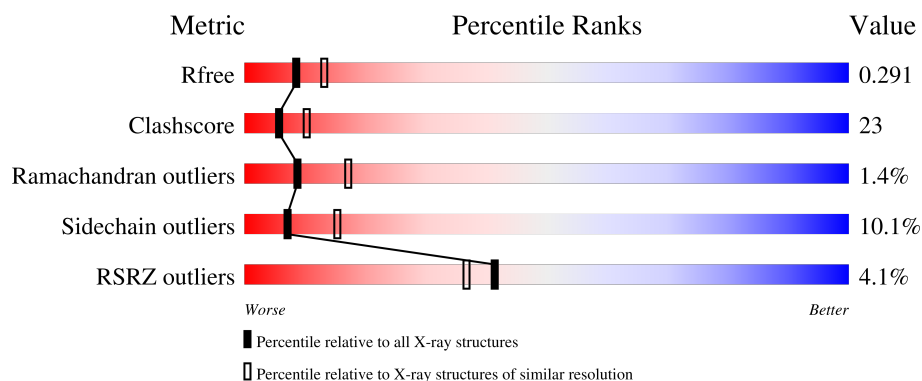
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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	248	
1	B	248	
1	C	248	
1	D	248	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7480 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 Probable ATP-dependent transporter sufC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1875	1188	316	364	7			
1	B	244	Total	C	N	O	S	0	0	0
			1871	1185	317	362	7			
1	C	241	Total	C	N	O	S	0	0	0
			1856	1181	311	357	7			
1	D	243	Total	C	N	O	S	0	0	0
			1844	1167	312	358	7			

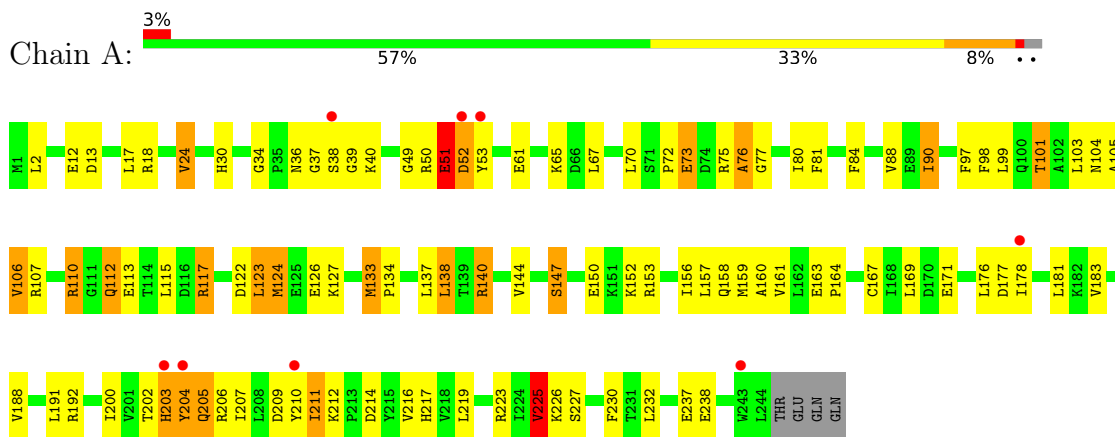
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	9	Total	O	0	0
			9	9		
2	C	8	Total	O	0	0
			8	8		
2	D	8	Total	O	0	0
			8	8		

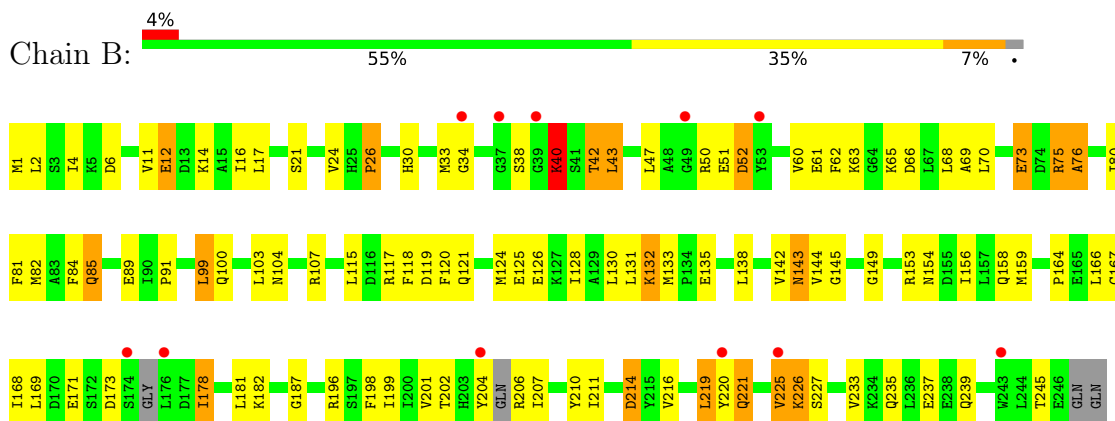
3 Residue-property plots

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.

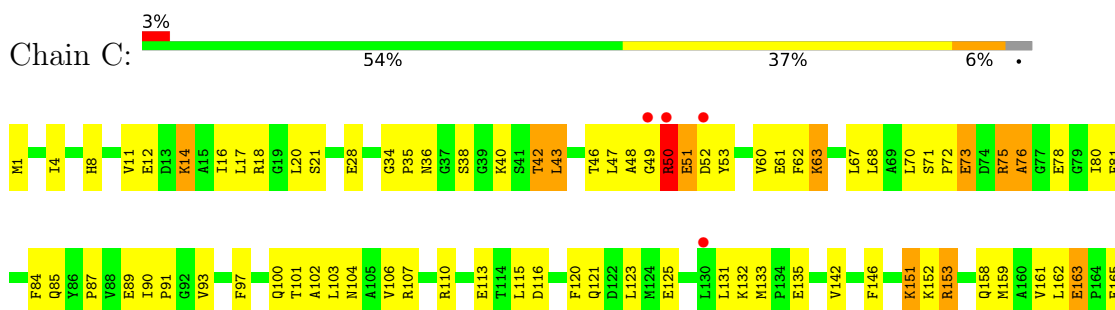
• Molecule 1: Probable ATP-dependent transporter sufC



• Molecule 1: Probable ATP-dependent transporter sufC

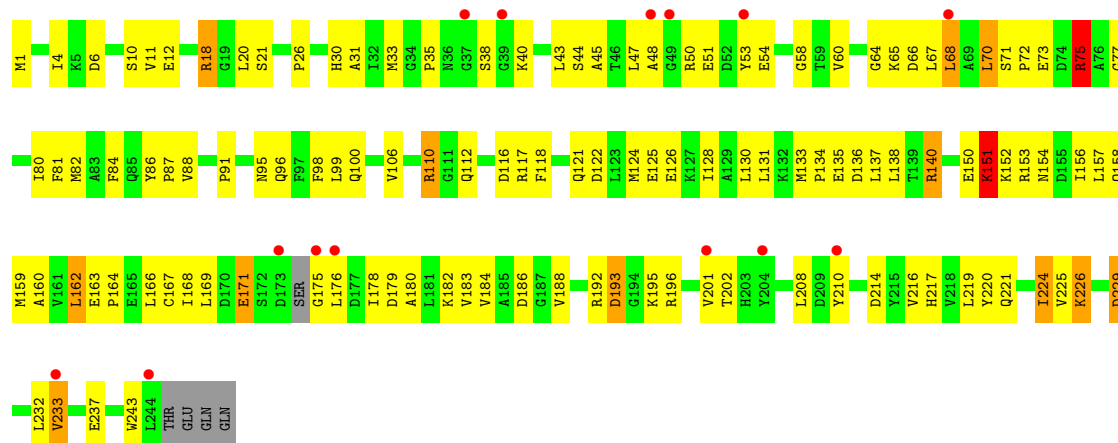


• Molecule 1: Probable ATP-dependent transporter sufC





- Molecule 1: Probable ATP-dependent transporter sufC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.53Å 46.68Å 149.32Å 90.00° 91.79° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 90.6 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.293 0.223 , 0.291	Depositor DCC
R_{free} test set	3585 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7480	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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](#)

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	0.67	1/1905 (0.1%)	1.12	15/2575 (0.6%)
1	B	0.55	0/1900	0.98	5/2566 (0.2%)
1	C	0.54	0/1887	1.06	14/2549 (0.5%)
1	D	0.50	0/1873	0.96	7/2533 (0.3%)
All	All	0.57	1/7565 (0.0%)	1.03	41/10223 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	MET	SD-CE	5.30	1.92	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLN	N-CA-C	12.96	124.78	108.45
1	A	211	ILE	N-CA-C	10.94	123.66	112.83
1	C	50	ARG	N-CA-C	10.49	125.36	109.41
1	C	206	ARG	N-CA-C	9.76	121.68	111.14
1	B	40	LYS	N-CA-C	-9.49	101.02	111.36
1	A	238	GLU	N-CA-C	-7.57	104.65	114.04
1	C	51	GLU	N-CA-C	-7.21	106.39	114.62
1	C	214	ASP	N-CA-C	-7.20	102.44	112.45
1	C	76	ALA	N-CA-C	-6.97	103.61	111.07
1	C	205	GLN	N-CA-C	6.86	125.41	110.80
1	A	203	HIS	N-CA-C	-6.79	105.15	113.50
1	B	81	PHE	N-CA-C	6.72	119.64	109.23
1	C	75	ARG	N-CA-C	-6.33	104.46	111.36
1	C	68	LEU	N-CA-C	6.30	119.81	111.75
1	C	70	LEU	N-CA-C	6.27	119.56	110.28
1	A	161	VAL	N-CA-C	6.26	117.05	110.72
1	C	161	VAL	N-CA-C	6.11	116.27	110.53
1	C	48	ALA	N-CA-C	6.02	118.75	111.40
1	A	18	ARG	N-CA-C	6.00	116.99	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	N-CA-C	5.97	117.36	108.23
1	A	76	ALA	N-CA-C	-5.83	104.89	112.23
1	D	88	VAL	N-CA-C	5.80	116.21	107.80
1	C	81	PHE	N-CA-C	5.70	118.75	109.06
1	D	51	GLU	N-CA-C	-5.70	103.18	110.53
1	A	204	TYR	N-CA-C	-5.67	106.20	113.01
1	B	76	ALA	N-CA-C	-5.67	105.10	111.28
1	D	214	ASP	N-CA-C	-5.66	105.49	112.90
1	A	90	ILE	N-CA-C	-5.56	101.54	107.77
1	A	123	LEU	N-CA-C	-5.55	105.13	111.07
1	D	162	LEU	N-CA-C	5.55	120.04	113.16
1	A	53	TYR	CA-C-O	5.55	121.16	117.94
1	B	12	GLU	N-CA-C	-5.50	103.04	110.68
1	C	208	LEU	N-CA-C	-5.47	106.56	113.18
1	D	75	ARG	N-CA-C	-5.34	105.51	112.23
1	A	178	ILE	N-CA-C	-5.23	105.23	112.50
1	A	214	ASP	N-CA-C	-5.20	106.09	112.90
1	D	151	LYS	N-CA-C	-5.17	105.54	111.07
1	A	225	VAL	N-CA-C	5.13	115.80	110.82
1	B	99	LEU	N-CA-C	-5.07	105.75	111.28
1	D	224	ILE	N-CA-C	-5.04	102.19	108.84
1	C	67	LEU	N-CA-C	5.02	116.56	111.14

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	1875	0	1856	88	0
1	B	1871	0	1846	91	0
1	C	1856	0	1835	80	0
1	D	1844	0	1800	93	0
2	A	9	0	0	1	0
2	B	9	0	0	1	0
2	C	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	8	0	0	0	0
All	All	7480	0	7337	344	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 23.

All (344) 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:121:GLN:HG2	1:C:125:GLU:OE2	1.54	1.07
1:B:132:LYS:HE2	1:B:132:LYS:HA	1.36	1.05
1:A:133:MET:HE2	1:A:153:ARG:HG2	1.50	0.91
1:D:1:MET:HE3	1:D:26:PRO:HG3	1.52	0.90
1:D:70:LEU:HD12	1:D:70:LEU:H	1.36	0.90
1:B:104:ASN:HD21	1:B:115:LEU:H	1.20	0.86
1:A:97:PHE:O	1:A:101:THR:HG22	1.75	0.86
1:A:2:LEU:HB3	1:A:24:VAL:HG13	1.60	0.83
1:C:11:VAL:HG12	1:C:12:GLU:HG3	1.61	0.83
1:C:49:GLY:HA3	1:C:72:PRO:HG3	1.59	0.82
1:A:159:MET:HE1	1:A:169:LEU:HD21	1.63	0.80
1:C:46:THR:HG23	1:C:50:ARG:HH12	1.46	0.79
1:C:104:ASN:HD21	1:C:115:LEU:H	1.28	0.77
1:D:40:LYS:O	1:D:201:VAL:HG11	1.85	0.76
1:A:207:ILE:HA	1:A:210:TYR:HD2	1.49	0.76
1:D:171:GLU:OE1	1:D:184:VAL:HG21	1.85	0.76
1:A:223:ARG:HB3	1:A:223:ARG:HH21	1.51	0.75
1:B:107:ARG:HH22	1:B:115:LEU:HD21	1.51	0.74
1:B:84:PHE:H	1:B:158:GLN:HE22	1.35	0.74
1:D:229:ASP:N	1:D:229:ASP:OD2	2.20	0.74
1:D:195:LYS:NZ	1:D:195:LYS:HB3	2.03	0.73
1:C:14:LYS:HB2	1:C:14:LYS:NZ	2.04	0.72
1:A:207:ILE:HA	1:A:210:TYR:CD2	2.24	0.72
1:B:225:VAL:HG12	1:B:226:LYS:HD2	1.70	0.72
1:C:97:PHE:O	1:C:101:THR:HG23	1.91	0.71
1:C:181:LEU:HB3	1:C:207:ILE:HG22	1.72	0.71
1:D:188:VAL:O	1:D:192:ARG:HG3	1.90	0.70
1:C:75:ARG:HB3	1:C:80:ILE:CG2	2.22	0.70
1:A:67:LEU:CD1	1:A:75:ARG:HG2	2.22	0.69
1:C:104:ASN:ND2	1:C:115:LEU:H	1.89	0.69
1:D:180:ALA:O	1:D:183:VAL:HG22	1.92	0.69
1:A:30:HIS:ND1	1:A:217:HIS:HE1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:H	1:B:73:GLU:CD	1.99	0.68
1:C:84:PHE:H	1:C:158:GLN:HE22	1.41	0.68
1:C:133:MET:CE	1:C:153:ARG:HG3	2.24	0.68
1:A:223:ARG:HB3	1:A:223:ARG:NH2	2.08	0.67
1:B:107:ARG:HH22	1:B:115:LEU:CD2	2.07	0.67
1:B:214:ASP:OD2	1:B:214:ASP:N	2.28	0.66
1:C:16:ILE:HG21	1:C:42:THR:HG21	1.77	0.66
1:D:47:LEU:HD12	1:D:168:ILE:HD12	1.78	0.66
1:A:123:LEU:HD11	1:A:127:LYS:HE2	1.75	0.66
1:B:11:VAL:CG2	1:B:16:ILE:HD12	2.26	0.66
1:A:67:LEU:HD11	1:A:75:ARG:HG2	1.79	0.65
1:C:46:THR:HG23	1:C:50:ARG:NH1	2.10	0.65
1:C:104:ASN:HD21	1:C:115:LEU:N	1.94	0.65
1:D:110:ARG:HB3	1:D:112:GLN:HE21	1.59	0.65
1:B:126:GLU:O	1:B:130:LEU:HG	1.97	0.65
1:B:104:ASN:ND2	1:B:115:LEU:H	1.94	0.65
1:A:50:ARG:HH21	1:A:50:ARG:HG3	1.63	0.65
1:D:84:PHE:CE2	1:D:98:PHE:HE1	2.14	0.64
1:B:107:ARG:NH2	1:B:115:LEU:HG	2.13	0.64
1:B:76:ALA:HA	1:B:80:ILE:O	1.98	0.64
1:C:90:ILE:HG13	1:C:93:VAL:HB	1.79	0.63
1:D:20:LEU:HD23	1:D:21:SER:N	2.14	0.63
1:D:84:PHE:H	1:D:158:GLN:HE22	1.45	0.63
1:D:136:ASP:O	1:D:140:ARG:HB2	1.98	0.63
1:D:133:MET:HG2	1:D:137:LEU:HD22	1.81	0.63
1:B:38:SER:OG	1:B:219:LEU:HB3	1.99	0.63
1:B:4:ILE:HD11	1:B:47:LEU:HD21	1.80	0.62
1:A:133:MET:HE2	1:A:153:ARG:CG	2.25	0.62
1:C:212:LYS:HG3	1:C:230:PHE:HD2	1.63	0.62
1:C:135:GLU:HG3	2:C:254:HOH:O	1.98	0.62
1:C:42:THR:HB	1:C:53:TYR:HE1	1.64	0.62
1:B:107:ARG:HH21	1:B:115:LEU:HG	1.64	0.62
1:D:64:GLY:O	1:D:65:LYS:HD3	2.00	0.62
1:A:181:LEU:HD21	1:A:205:GLN:OE1	2.00	0.61
1:D:121:GLN:O	1:D:125:GLU:HG2	2.00	0.61
1:A:159:MET:HE1	1:A:169:LEU:CD2	2.30	0.61
1:B:38:SER:CB	1:B:219:LEU:HB3	2.31	0.61
1:B:181:LEU:HD12	1:B:207:ILE:HB	1.83	0.60
1:C:73:GLU:CD	1:C:73:GLU:H	2.05	0.59
1:B:168:ILE:HD13	1:B:199:ILE:HB	1.84	0.59
1:D:33:MET:HE3	1:D:216:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:H	1:A:158:GLN:HE22	1.51	0.58
1:A:177:ASP:O	1:A:181:LEU:HG	2.01	0.58
1:C:71:SER:O	1:C:75:ARG:HG3	2.04	0.58
1:A:36:ASN:C	1:A:38:SER:H	2.10	0.58
1:C:102:ALA:HB1	1:D:91:PRO:HG2	1.85	0.58
1:A:124:MET:HE1	1:A:138:LEU:HD22	1.86	0.58
1:A:232:LEU:HD13	1:A:232:LEU:O	2.04	0.57
1:A:105:ALA:HB1	1:B:91:PRO:O	2.04	0.57
1:C:185:ALA:HB1	1:C:210:TYR:HB3	1.86	0.57
1:D:179:ASP:O	1:D:183:VAL:HG13	2.04	0.57
1:A:123:LEU:CD1	1:A:127:LYS:HE2	2.34	0.57
1:A:212:LYS:HE2	1:A:230:PHE:CD1	2.39	0.57
1:B:11:VAL:HG21	1:B:16:ILE:HD12	1.87	0.57
1:A:50:ARG:O	1:A:52:ASP:N	2.37	0.57
1:A:237:GLU:HG3	1:A:237:GLU:O	2.05	0.57
1:D:124:MET:O	1:D:128:ILE:HG13	2.04	0.57
1:A:76:ALA:HA	1:A:80:ILE:O	2.04	0.56
1:A:104:ASN:HD21	1:A:115:LEU:H	1.52	0.56
1:C:46:THR:CG2	1:C:50:ARG:HH12	2.15	0.56
1:B:61:GLU:HA	1:B:65:LYS:O	2.06	0.56
1:B:207:ILE:HD11	1:B:211:ILE:HD11	1.88	0.56
1:A:202:THR:HG23	1:A:202:THR:O	2.05	0.56
1:B:33:MET:HE2	1:B:245:THR:HB	1.88	0.56
1:C:107:ARG:NH2	1:C:113:GLU:O	2.38	0.56
1:B:50:ARG:HH11	1:B:82:MET:HE2	1.69	0.56
1:A:164:PRO:HG2	1:A:167:CYS:SG	2.47	0.55
1:B:178:ILE:H	1:B:178:ILE:HD12	1.71	0.55
1:C:212:LYS:HG3	1:C:230:PHE:CD2	2.40	0.55
1:D:33:MET:HE3	1:D:216:VAL:CG1	2.35	0.55
1:D:100:GLN:HE22	1:D:117:ARG:HA	1.70	0.55
1:B:80:ILE:HD13	1:B:166:LEU:HB3	1.89	0.55
1:A:30:HIS:ND1	1:A:217:HIS:CE1	2.74	0.55
1:A:133:MET:HG2	1:A:137:LEU:HD22	1.90	0.54
1:D:162:LEU:C	1:D:163:GLU:HG2	2.31	0.54
1:C:181:LEU:HD22	1:C:207:ILE:CG2	2.37	0.54
1:B:2:LEU:HD22	1:B:166:LEU:HD21	1.89	0.54
1:D:162:LEU:O	1:D:163:GLU:HG2	2.07	0.54
1:B:40:LYS:HB3	1:B:201:VAL:HG13	1.89	0.54
1:B:38:SER:HB2	1:B:219:LEU:HB3	1.90	0.54
1:C:63:LYS:HD3	1:C:165:GLU:OE2	2.07	0.54
1:B:24:VAL:HG13	1:B:30:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:CD2	1:A:39:GLY:HA3	2.38	0.54
1:A:232:LEU:HD13	1:A:232:LEU:C	2.34	0.53
1:B:178:ILE:H	1:B:178:ILE:CD1	2.21	0.53
1:A:61:GLU:HA	1:A:65:LYS:O	2.07	0.53
1:C:49:GLY:CA	1:C:72:PRO:HG3	2.34	0.53
1:D:71:SER:HB2	1:D:72:PRO:HD2	1.90	0.53
1:D:80:ILE:HD13	1:D:166:LEU:HD23	1.91	0.53
1:B:132:LYS:HA	1:B:132:LYS:CE	2.22	0.53
1:B:17:LEU:HD11	1:B:43:LEU:HA	1.91	0.52
1:C:103:LEU:HD13	1:C:107:ARG:HD2	1.92	0.52
1:D:81:PHE:CE2	1:D:159:MET:HG3	2.45	0.52
1:D:195:LYS:HB3	1:D:195:LYS:HZ3	1.71	0.52
1:D:95:ASN:HB3	1:D:138:LEU:HD12	1.91	0.52
1:A:188:VAL:O	1:A:192:ARG:HB2	2.08	0.52
1:D:48:ALA:C	1:D:50:ARG:H	2.18	0.52
1:D:70:LEU:H	1:D:70:LEU:CD1	2.16	0.52
1:A:117:ARG:NH2	2:A:250:HOH:O	2.43	0.52
1:A:207:ILE:HD12	1:A:207:ILE:C	2.35	0.52
1:C:80:ILE:HG23	1:C:80:ILE:O	2.10	0.52
1:D:96:GLN:HG3	1:D:124:MET:SD	2.50	0.52
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.75	0.52
1:C:133:MET:HE2	1:C:153:ARG:HG3	1.91	0.52
1:A:144:VAL:O	1:A:147:SER:HB3	2.10	0.52
1:A:216:VAL:O	1:A:227:SER:HA	2.10	0.52
1:A:123:LEU:O	1:A:126:GLU:HB3	2.10	0.52
1:D:124:MET:HE3	1:D:128:ILE:HD11	1.91	0.52
1:D:226:LYS:HB2	1:D:226:LYS:NZ	2.24	0.52
1:D:131:LEU:HD13	1:D:156:ILE:HG22	1.91	0.51
1:D:232:LEU:C	1:D:232:LEU:HD13	2.35	0.51
1:C:28:GLU:HA	1:C:214:ASP:OD2	2.10	0.51
1:A:49:GLY:O	1:A:72:PRO:HG3	2.11	0.51
1:D:175:GLY:O	1:D:176:LEU:HB3	2.11	0.51
1:A:17:LEU:HD21	1:A:39:GLY:HA3	1.91	0.51
1:B:73:GLU:CD	1:B:73:GLU:N	2.68	0.51
1:D:35:PRO:O	1:D:38:SER:HB2	2.11	0.51
1:D:4:ILE:HG23	1:D:60:VAL:HG22	1.93	0.51
1:C:14:LYS:HB2	1:C:14:LYS:HZ3	1.75	0.51
1:D:217:HIS:HB3	1:D:224:ILE:HD12	1.93	0.51
1:A:12:GLU:O	1:A:13:ASP:HB2	2.12	0.50
1:A:110:ARG:HB3	1:A:112:GLN:HG3	1.93	0.50
1:C:14:LYS:HB2	1:C:14:LYS:HZ2	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:HD12	1:B:178:ILE:N	2.25	0.50
1:C:62:PHE:HE1	1:C:78:GLU:O	1.94	0.50
1:D:137:LEU:HD23	1:D:157:LEU:HD22	1.93	0.50
1:D:50:ARG:HD2	1:D:82:MET:HE2	1.92	0.50
1:D:31:ALA:O	1:D:216:VAL:HA	2.11	0.50
1:C:230:PHE:O	1:C:230:PHE:CD1	2.65	0.50
1:D:159:MET:HE1	1:D:169:LEU:HD21	1.93	0.50
1:A:40:LYS:HA	1:A:219:LEU:HD13	1.93	0.50
1:A:225:VAL:HG12	1:A:226:LYS:N	2.25	0.50
1:D:122:ASP:O	1:D:126:GLU:HG2	2.12	0.50
1:A:104:ASN:ND2	1:A:115:LEU:H	2.09	0.49
1:B:171:GLU:C	1:B:173:ASP:H	2.20	0.49
1:C:75:ARG:HB3	1:C:80:ILE:HG23	1.93	0.49
1:B:225:VAL:HG12	1:B:226:LYS:N	2.27	0.49
1:A:67:LEU:HD11	1:A:80:ILE:HD12	1.94	0.49
1:B:235:GLN:O	1:B:239:GLN:HG3	2.11	0.49
1:C:91:PRO:N	1:D:73:GLU:HB2	2.27	0.49
1:B:85:GLN:OE1	1:B:85:GLN:HA	2.11	0.49
1:A:81:PHE:C	1:A:81:PHE:CD2	2.90	0.49
1:C:42:THR:HB	1:C:53:TYR:CE1	2.45	0.49
1:A:137:LEU:HD23	1:A:157:LEU:HD22	1.93	0.49
1:A:36:ASN:O	1:A:38:SER:N	2.46	0.49
1:A:38:SER:OG	1:A:39:GLY:N	2.45	0.49
1:C:21:SER:O	1:C:224:ILE:HD12	2.13	0.49
1:D:208:LEU:C	1:D:210:TYR:H	2.18	0.49
1:C:181:LEU:HD22	1:C:207:ILE:HG21	1.95	0.49
1:C:87:PRO:HB3	1:D:87:PRO:HB3	1.94	0.48
1:C:103:LEU:CD1	1:C:107:ARG:HD2	2.43	0.48
1:C:191:LEU:O	1:C:196:ARG:NH1	2.43	0.48
1:A:50:ARG:O	1:A:51:GLU:C	2.56	0.48
1:A:205:GLN:HG2	1:A:206:ARG:HH21	1.78	0.48
1:D:81:PHE:HE2	1:D:159:MET:HG3	1.78	0.48
1:B:11:VAL:HG12	1:B:12:GLU:N	2.28	0.48
1:C:142:VAL:HB	1:C:146:PHE:HB2	1.96	0.48
1:D:86:TYR:CD1	1:D:95:ASN:ND2	2.82	0.48
1:C:123:LEU:C	1:C:123:LEU:HD23	2.39	0.48
1:C:238:GLU:C	1:C:240:GLY:H	2.21	0.48
1:D:30:HIS:ND1	1:D:217:HIS:HE1	2.12	0.48
1:A:98:PHE:HA	1:A:101:THR:CG2	2.44	0.48
1:B:107:ARG:NH2	1:B:115:LEU:CD2	2.75	0.48
1:D:44:SER:HB2	1:D:168:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD12	1:A:75:ARG:HG2	1.96	0.47
1:B:1:MET:HB2	1:B:26:PRO:HD3	1.96	0.47
1:A:117:ARG:H	1:A:117:ARG:HD3	1.80	0.47
1:C:4:ILE:O	1:C:21:SER:HA	2.14	0.47
1:A:36:ASN:C	1:A:38:SER:N	2.72	0.47
1:B:107:ARG:NH2	1:B:115:LEU:CG	2.77	0.47
1:C:100:GLN:HA	1:C:120:PHE:CE1	2.50	0.47
1:A:50:ARG:HG3	1:A:50:ARG:NH2	2.27	0.47
1:B:121:GLN:O	1:B:125:GLU:HG2	2.13	0.47
1:B:168:ILE:C	1:B:169:LEU:HD23	2.40	0.47
1:C:35:PRO:O	1:C:36:ASN:C	2.57	0.47
1:A:152:LYS:O	1:A:156:ILE:HG12	2.15	0.47
1:B:34:GLY:O	1:B:40:LYS:HD2	2.14	0.47
1:B:131:LEU:HD13	1:B:133:MET:HE3	1.96	0.47
1:D:6:ASP:O	1:D:58:GLY:HA3	2.14	0.47
1:A:192:ARG:NH2	1:A:211:ILE:O	2.46	0.47
1:B:117:ARG:HD2	1:B:118:PHE:CE1	2.50	0.47
1:C:106:VAL:CG1	1:C:110:ARG:NH2	2.78	0.47
1:B:216:VAL:O	1:B:227:SER:HA	2.14	0.47
1:C:34:GLY:O	1:C:40:LYS:NZ	2.48	0.47
1:D:195:LYS:HB3	1:D:195:LYS:HZ2	1.79	0.46
1:B:60:VAL:HG21	1:B:68:LEU:HD21	1.97	0.46
1:B:149:GLY:O	1:B:153:ARG:HG3	2.15	0.46
1:A:107:ARG:NH2	1:A:113:GLU:O	2.47	0.46
1:B:4:ILE:O	1:B:21:SER:HA	2.15	0.46
1:C:4:ILE:HD11	1:C:47:LEU:HD21	1.98	0.46
1:D:152:LYS:HB2	1:D:183:VAL:HG21	1.97	0.46
1:B:167:CYS:HB2	1:B:198:PHE:CD1	2.50	0.46
1:D:220:TYR:CE2	1:D:221:GLN:HG3	2.51	0.46
1:B:80:ILE:CD1	1:B:166:LEU:HD23	2.45	0.46
1:B:206:ARG:NH1	1:B:210:TYR:OH	2.46	0.46
1:C:167:CYS:HB2	1:C:198:PHE:CD1	2.50	0.46
1:A:103:LEU:HD12	1:A:103:LEU:O	2.16	0.46
1:C:133:MET:SD	1:C:153:ARG:HG3	2.56	0.46
1:D:77:GLY:HA2	1:D:106:VAL:HG13	1.98	0.46
1:D:193:ASP:OD2	1:D:196:ARG:HD3	2.16	0.46
1:A:204:TYR:O	1:A:205:GLN:HG3	2.16	0.45
1:B:171:GLU:HA	1:B:173:ASP:OD1	2.16	0.45
1:C:116:ASP:OD2	1:C:116:ASP:C	2.59	0.45
1:A:181:LEU:HB3	1:A:207:ILE:HG22	1.98	0.45
1:B:38:SER:O	1:B:219:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ILE:HD13	1:B:187:GLY:HA3	1.99	0.45
1:C:179:ASP:OD2	1:C:179:ASP:N	2.50	0.45
1:D:133:MET:HG3	1:D:134:PRO:HD2	1.98	0.45
1:D:217:HIS:HB3	1:D:224:ILE:HG23	1.99	0.45
1:B:207:ILE:O	1:B:211:ILE:HG13	2.17	0.45
1:C:243:TRP:H	1:C:243:TRP:CD1	2.33	0.45
1:A:117:ARG:N	1:A:117:ARG:CD	2.80	0.45
1:D:131:LEU:HD11	1:D:160:ALA:HB2	1.98	0.45
1:B:142:VAL:HG22	1:B:143:ASN:H	1.82	0.45
1:C:4:ILE:HG12	1:C:60:VAL:HG22	1.98	0.45
1:A:98:PHE:O	1:A:101:THR:HG23	2.16	0.45
1:C:89:GLU:N	1:C:89:GLU:CD	2.75	0.45
1:C:102:ALA:HA	1:D:91:PRO:O	2.17	0.45
1:B:118:PHE:O	1:B:121:GLN:HB3	2.17	0.45
1:D:243:TRP:CD1	1:D:243:TRP:H	2.34	0.45
1:A:50:ARG:C	1:A:52:ASP:N	2.75	0.44
1:C:73:GLU:O	1:C:76:ALA:HB3	2.17	0.44
1:D:134:PRO:HG2	1:D:137:LEU:HD13	2.00	0.44
1:D:50:ARG:NH1	1:D:82:MET:O	2.50	0.44
1:A:73:GLU:HG2	1:B:89:GLU:HB3	2.00	0.44
1:A:169:LEU:HD13	1:A:200:ILE:HG12	1.98	0.44
1:B:103:LEU:O	1:B:107:ARG:HG3	2.17	0.44
1:B:178:ILE:HG23	1:B:182:LYS:HE3	2.00	0.44
1:C:131:LEU:O	1:C:132:LYS:C	2.61	0.44
1:C:8:HIS:HA	1:C:17:LEU:O	2.18	0.43
1:D:150:GLU:OE2	1:D:150:GLU:HA	2.18	0.43
1:C:226:LYS:HD3	1:C:236:LEU:HD11	2.00	0.43
1:D:100:GLN:NE2	1:D:117:ARG:HA	2.32	0.43
1:D:106:VAL:HG12	1:D:110:ARG:CZ	2.48	0.43
1:D:116:ASP:OD2	1:D:118:PHE:N	2.50	0.43
1:A:134:PRO:HG2	1:A:140:ARG:NH2	2.34	0.43
1:A:223:ARG:HH21	1:A:223:ARG:CB	2.25	0.43
1:B:12:GLU:C	1:B:14:LYS:H	2.26	0.43
1:B:100:GLN:HB2	1:B:120:PHE:CD2	2.54	0.43
1:B:164:PRO:HG2	1:B:167:CYS:SG	2.57	0.43
1:D:18:ARG:HD3	1:D:221:GLN:O	2.19	0.43
1:A:150:GLU:OE1	1:A:150:GLU:HA	2.17	0.43
1:A:152:LYS:HA	1:A:152:LYS:HD3	1.79	0.43
1:C:50:ARG:HD3	1:C:53:TYR:HB2	1.99	0.43
1:B:12:GLU:C	1:B:14:LYS:N	2.73	0.43
1:B:142:VAL:HG22	1:B:143:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:HD13	1:C:236:LEU:HD22	2.01	0.43
1:D:11:VAL:HG22	1:D:53:TYR:CD1	2.54	0.43
1:D:30:HIS:ND1	1:D:217:HIS:CE1	2.86	0.43
1:D:154:ASN:O	1:D:158:GLN:HG3	2.18	0.43
1:A:206:ARG:H	1:A:206:ARG:HD2	1.84	0.43
1:C:85:GLN:HE21	1:C:151:LYS:HZ3	1.67	0.43
1:D:45:ALA:HB3	1:D:53:TYR:HE2	1.81	0.43
1:A:70:LEU:O	1:A:75:ARG:HD2	2.19	0.42
1:A:203:HIS:C	1:A:205:GLN:N	2.75	0.42
1:D:151:LYS:HE3	1:D:151:LYS:HB2	1.92	0.42
1:D:152:LYS:O	1:D:156:ILE:HD13	2.19	0.42
1:A:34:GLY:O	1:A:40:LYS:NZ	2.46	0.42
1:C:85:GLN:HE21	1:C:151:LYS:NZ	2.17	0.42
1:D:233:VAL:O	1:D:237:GLU:HG3	2.19	0.42
1:A:77:GLY:O	1:A:110:ARG:HD2	2.20	0.42
1:D:178:ILE:O	1:D:182:LYS:HB2	2.19	0.42
1:A:160:ALA:HB2	1:A:191:LEU:HD21	2.00	0.42
1:B:154:ASN:O	1:B:158:GLN:HG3	2.19	0.42
1:D:150:GLU:OE2	1:D:153:ARG:NH2	2.52	0.42
1:A:122:ASP:O	1:A:126:GLU:HB2	2.19	0.42
1:C:43:LEU:HD22	1:C:43:LEU:O	2.20	0.42
1:B:33:MET:HA	1:B:40:LYS:NZ	2.35	0.42
1:B:33:MET:CE	1:B:245:THR:HB	2.50	0.42
1:B:168:ILE:O	1:B:169:LEU:HD23	2.19	0.42
1:B:196:ARG:O	1:B:196:ARG:HG3	2.18	0.42
1:B:207:ILE:HG13	1:B:211:ILE:HD12	2.02	0.42
1:D:67:LEU:HA	1:D:70:LEU:CD1	2.49	0.42
1:C:18:ARG:O	1:C:223:ARG:HD2	2.20	0.42
1:D:163:GLU:N	1:D:164:PRO:HD3	2.35	0.42
1:B:11:VAL:HG23	1:B:16:ILE:HD12	2.01	0.41
1:D:110:ARG:CB	1:D:112:GLN:HE21	2.28	0.41
1:D:152:LYS:NZ	1:D:171:GLU:OE1	2.53	0.41
1:A:106:VAL:HG13	1:A:110:ARG:CZ	2.50	0.41
1:C:49:GLY:C	1:C:50:ARG:HG2	2.42	0.41
1:A:90:ILE:HG12	1:B:84:PHE:CD2	2.56	0.41
1:B:62:PHE:CE1	1:B:63:LYS:HE2	2.55	0.41
1:C:20:LEU:HG	1:C:224:ILE:HG13	2.02	0.41
1:C:152:LYS:HA	1:C:152:LYS:HD3	1.93	0.41
1:C:162:LEU:O	1:C:163:GLU:HG2	2.19	0.41
1:D:10:SER:HB2	1:D:54:GLU:CG	2.51	0.41
1:D:60:VAL:HB	1:D:68:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:HG2	1:D:112:GLN:HE21	1.85	0.41
1:D:195:LYS:NZ	1:D:195:LYS:CB	2.77	0.41
1:A:140:ARG:HD3	1:A:150:GLU:OE2	2.21	0.41
1:B:16:ILE:HG21	1:B:42:THR:HG21	2.01	0.41
1:B:69:ALA:HB2	2:B:257:HOH:O	2.19	0.41
1:B:124:MET:O	1:B:128:ILE:HG13	2.19	0.41
1:D:67:LEU:O	1:D:75:ARG:NH2	2.53	0.41
1:D:54:GLU:O	1:D:54:GLU:HG3	2.19	0.41
1:A:207:ILE:CA	1:A:210:TYR:HD2	2.27	0.41
1:C:87:PRO:HB2	1:D:98:PHE:CE2	2.55	0.41
1:D:66:ASP:OD2	1:D:66:ASP:C	2.62	0.41
1:B:181:LEU:HD13	1:B:181:LEU:HA	1.91	0.41
1:C:100:GLN:HG3	1:C:120:PHE:CG	2.56	0.41
1:D:164:PRO:O	1:D:196:ARG:HG2	2.21	0.41
1:B:89:GLU:OE1	1:B:89:GLU:N	2.52	0.41
1:B:128:ILE:HG21	1:B:135:GLU:HA	2.02	0.41
1:B:221:GLN:HE21	1:B:221:GLN:HB2	1.63	0.41
1:C:38:SER:O	1:C:219:LEU:HD21	2.21	0.41
1:B:80:ILE:HD11	1:B:166:LEU:HD23	2.02	0.40
1:B:220:TYR:O	1:B:221:GLN:C	2.63	0.40
1:B:70:LEU:O	1:B:75:ARG:NH2	2.38	0.40
1:C:232:LEU:HD13	1:C:232:LEU:C	2.46	0.40
1:A:203:HIS:C	1:A:205:GLN:H	2.29	0.40
1:B:66:ASP:OD2	1:B:66:ASP:C	2.64	0.40
1:B:143:ASN:CG	1:B:145:GLY:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	242/248 (98%)	219 (90%)	20 (8%)	3 (1%)	10 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	238/248 (96%)	216 (91%)	17 (7%)	5 (2%)	5	9
1	C	237/248 (96%)	216 (91%)	19 (8%)	2 (1%)	16	31
1	D	239/248 (96%)	210 (88%)	26 (11%)	3 (1%)	9	18
All	All	956/992 (96%)	861 (90%)	82 (9%)	13 (1%)	9	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	52	ASP
1	C	52	ASP
1	C	205	GLN
1	B	52	ASP
1	A	37	GLY
1	B	51	GLU
1	D	135	GLU
1	D	193	ASP
1	B	221	GLN
1	D	140	ARG
1	B	178	ILE
1	B	225	VAL

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	201/212 (95%)	182 (90%)	19 (10%)	8	17
1	B	200/212 (94%)	177 (88%)	23 (12%)	5	11
1	C	198/212 (93%)	179 (90%)	19 (10%)	8	17
1	D	194/212 (92%)	175 (90%)	19 (10%)	7	16
All	All	793/848 (94%)	713 (90%)	80 (10%)	7	15

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	51	GLU
1	A	73	GLU
1	A	99	LEU
1	A	101	THR
1	A	106	VAL
1	A	110	ARG
1	A	112	GLN
1	A	117	ARG
1	A	133	MET
1	A	138	LEU
1	A	140	ARG
1	A	147	SER
1	A	163	GLU
1	A	171	GLU
1	A	176	LEU
1	A	183	VAL
1	A	209	ASP
1	A	225	VAL
1	B	6	ASP
1	B	26	PRO
1	B	40	LYS
1	B	42	THR
1	B	43	LEU
1	B	52	ASP
1	B	73	GLU
1	B	75	ARG
1	B	85	GLN
1	B	99	LEU
1	B	119	ASP
1	B	132	LYS
1	B	138	LEU
1	B	143	ASN
1	B	144	VAL
1	B	159	MET
1	B	202	THR
1	B	204	TYR
1	B	214	ASP
1	B	219	LEU
1	B	226	LYS
1	B	233	VAL
1	B	237	GLU
1	C	1	MET

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Mol	Chain	Res	Type
1	C	14	LYS
1	C	42	THR
1	C	43	LEU
1	C	50	ARG
1	C	51	GLU
1	C	61	GLU
1	C	63	LYS
1	C	73	GLU
1	C	151	LYS
1	C	153	ARG
1	C	159	MET
1	C	163	GLU
1	C	179	ASP
1	C	182	LYS
1	C	183	VAL
1	C	202	THR
1	C	225	VAL
1	C	236	LEU
1	D	12	GLU
1	D	18	ARG
1	D	43	LEU
1	D	68	LEU
1	D	70	LEU
1	D	75	ARG
1	D	99	LEU
1	D	110	ARG
1	D	130	LEU
1	D	151	LYS
1	D	167	CYS
1	D	171	GLU
1	D	186	ASP
1	D	202	THR
1	D	219	LEU
1	D	225	VAL
1	D	226	LYS
1	D	229	ASP
1	D	233	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	158	GLN
1	A	189	ASN
1	A	217	HIS
1	A	221	GLN
1	B	100	GLN
1	B	104	ASN
1	B	154	ASN
1	B	158	GLN
1	B	189	ASN
1	B	203	HIS
1	B	217	HIS
1	B	221	GLN
1	C	85	GLN
1	C	104	ASN
1	C	112	GLN
1	C	158	GLN
1	C	189	ASN
1	C	203	HIS
1	D	8	HIS
1	D	95	ASN
1	D	100	GLN
1	D	112	GLN
1	D	154	ASN
1	D	158	GLN
1	D	189	ASN
1	D	217	HIS

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

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	244/248 (98%)	0.10	8 (3%) 49 45	25, 42, 71, 86	0
1	B	244/248 (98%)	0.16	11 (4%) 38 33	23, 44, 75, 92	0
1	C	241/248 (97%)	0.25	7 (2%) 53 49	34, 51, 73, 97	0
1	D	243/248 (97%)	0.41	14 (5%) 29 25	30, 58, 85, 97	0
All	All	972/992 (97%)	0.23	40 (4%) 41 37	23, 50, 78, 97	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	HIS	5.1
1	C	205	GLN	4.7
1	C	204	TYR	4.4
1	D	49	GLY	3.9
1	C	52	ASP	3.3
1	B	204	TYR	3.3
1	D	173	ASP	3.3
1	D	210	TYR	3.3
1	A	204	TYR	3.2
1	D	244	LEU	3.1
1	B	176	LEU	3.1
1	B	39	GLY	3.1
1	A	52	ASP	3.1
1	B	220	TYR	3.0
1	D	48	ALA	2.9
1	A	210	TYR	2.9
1	D	176	LEU	2.8
1	D	37	GLY	2.8
1	D	175	GLY	2.8
1	A	38	SER	2.7
1	B	174	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	225	VAL	2.7
1	B	34	GLY	2.6
1	C	177	ASP	2.5
1	C	49	GLY	2.3
1	A	53	TYR	2.3
1	B	53	TYR	2.3
1	D	68	LEU	2.3
1	D	204	TYR	2.3
1	C	50	ARG	2.3
1	A	178	ILE	2.3
1	D	233	VAL	2.3
1	C	130	LEU	2.2
1	D	39	GLY	2.2
1	B	243	TRP	2.2
1	D	201	VAL	2.1
1	A	243	TRP	2.1
1	D	53	TYR	2.1
1	B	37	GLY	2.0
1	B	49	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.