



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:01 PM UTC

PDB ID : 2RCV / pdb_00002rcv
Title : Crystal structure of the Bacillus subtilis superoxide dismutase
Authors : Liu, P.; Ewis, H.E.; Huang, Y.J.; Lu, C.D.; Tai, P.C.; Weber, I.T.
Deposited on : 2007-09-20
Resolution : 1.60 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:

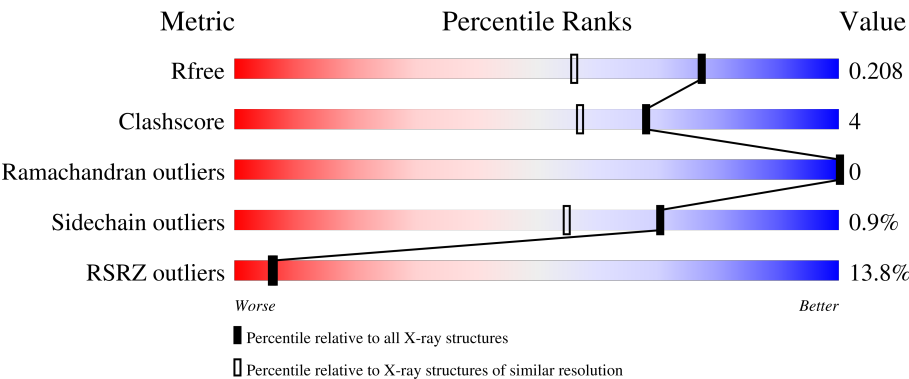
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.60 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.



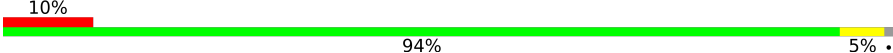
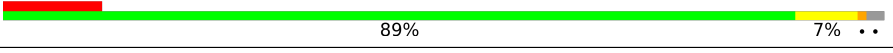
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	202	12% 93% 5% ..
1	B	202	16% 90% 7% .
1	C	202	16% 88% 9% ..
1	D	202	16% 85% 11% ..
1	E	202	13% 92% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	202	 10% 94% 5% •
1	G	202	 14% 89% 9% ••
1	H	202	 11% 89% 7% ••

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13464 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 Superoxide dismutase [Mn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1576	1000	270	305	1			
1	B	197	Total	C	N	O	S	0	0	0
			1555	989	266	299	1			
1	C	200	Total	C	N	O	S	0	0	0
			1576	1000	270	305	1			
1	D	197	Total	C	N	O	S	0	0	0
			1556	987	267	301	1			
1	E	200	Total	C	N	O	S	0	0	0
			1576	1000	270	305	1			
1	F	200	Total	C	N	O	S	0	0	0
			1576	1000	270	305	1			
1	G	200	Total	C	N	O	S	0	0	0
			1576	1000	270	305	1			
1	H	197	Total	C	N	O	S	0	0	0
			1555	989	266	299	1			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0

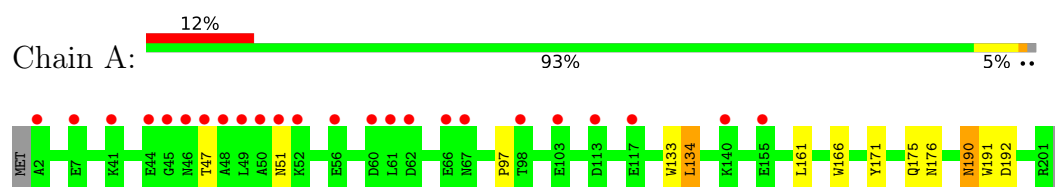
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total 115	O 115	0	0
3	B	114	Total 114	O 114	0	0
3	C	98	Total 98	O 98	0	0
3	D	103	Total 103	O 103	0	0
3	E	123	Total 123	O 123	0	0
3	F	117	Total 117	O 117	0	0
3	G	111	Total 111	O 111	0	0
3	H	129	Total 129	O 129	0	0

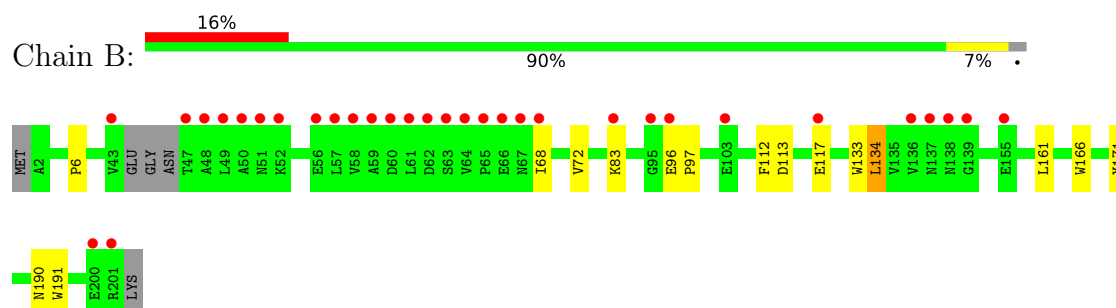
3 Residue-property plots [i](#)

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.

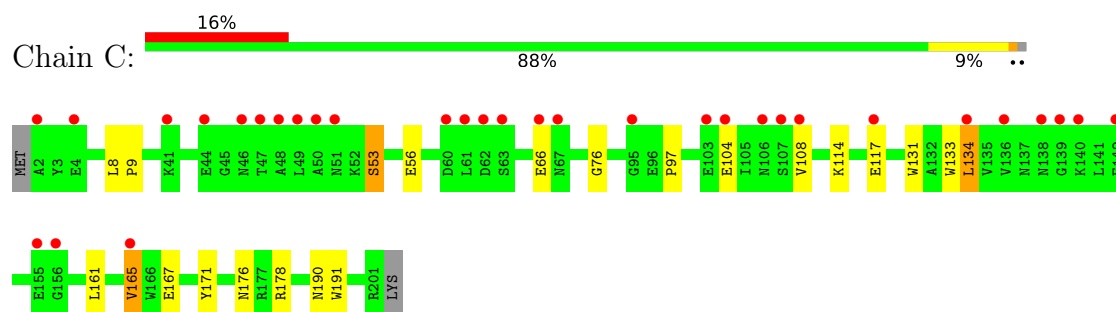
- Molecule 1: Superoxide dismutase [Mn]



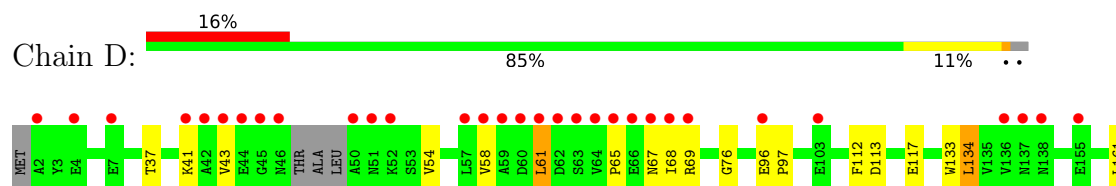
- Molecule 1: Superoxide dismutase [Mn]

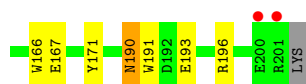


- Molecule 1: Superoxide dismutase [Mn]

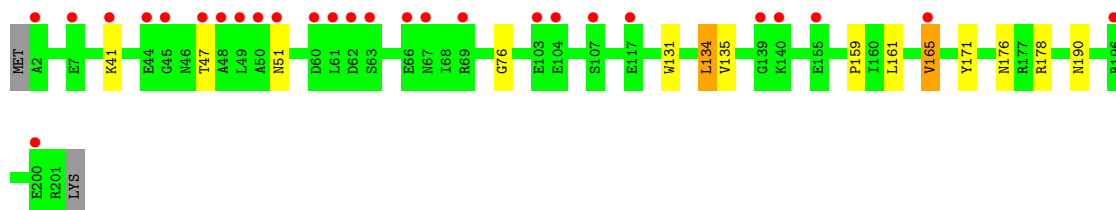
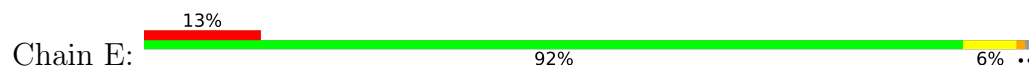


- Molecule 1: Superoxide dismutase [Mn]

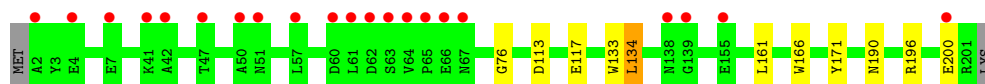
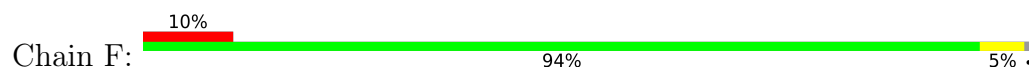




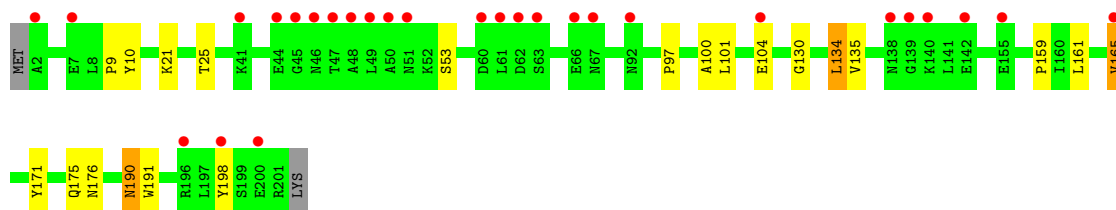
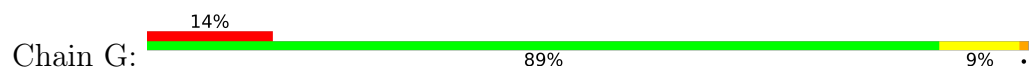
- Molecule 1: Superoxide dismutase [Mn]



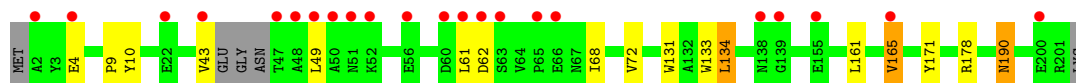
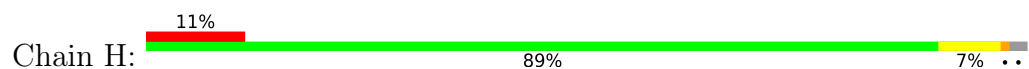
- Molecule 1: Superoxide dismutase [Mn]



- Molecule 1: Superoxide dismutase [Mn]



- Molecule 1: Superoxide dismutase [Mn]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.37Å 84.03Å 91.95Å 99.13° 105.98° 105.58°	Depositor
Resolution (Å)	45.90 – 1.60 45.90 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.9 (45.90-1.60) 90.0 (45.90-1.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.230 0.212 , 0.208	Depositor DCC
R_{free} test set	10942 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13464	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/1621	0.81	5/2214 (0.2%)
1	B	0.36	0/1599	0.80	4/2183 (0.2%)
1	C	0.36	0/1621	0.76	5/2214 (0.2%)
1	D	0.36	0/1600	0.79	5/2183 (0.2%)
1	E	0.36	0/1621	0.79	3/2214 (0.1%)
1	F	0.38	0/1621	0.82	5/2214 (0.2%)
1	G	0.39	0/1621	0.80	4/2214 (0.2%)
1	H	0.39	0/1599	0.79	3/2183 (0.1%)
All	All	0.37	0/12903	0.79	34/17619 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	TRP	N-CA-C	-7.49	99.94	110.50
1	B	134	LEU	N-CA-C	-7.19	96.56	108.34
1	D	166	TRP	N-CA-C	-7.00	99.93	110.28
1	A	134	LEU	N-CA-C	-6.97	97.04	108.41
1	E	134	LEU	N-CA-C	-6.64	97.59	108.41
1	D	134	LEU	N-CA-C	-6.63	97.61	108.41
1	B	171	TYR	N-CA-C	6.57	118.52	111.36
1	H	134	LEU	N-CA-C	-6.44	97.92	108.41
1	F	134	LEU	N-CA-C	-6.42	97.94	108.41
1	G	134	LEU	N-CA-C	-6.25	98.21	108.41
1	H	171	TYR	N-CA-C	6.22	118.06	111.28
1	A	171	TYR	N-CA-C	6.04	117.86	111.28
1	G	171	TYR	N-CA-C	5.99	117.81	111.28
1	C	76	GLY	N-CA-C	-5.90	105.35	112.49
1	E	171	TYR	N-CA-C	5.89	117.70	111.28
1	D	133	TRP	N-CA-C	5.80	118.67	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	TYR	N-CA-C	5.75	118.33	111.71
1	F	133	TRP	N-CA-C	5.69	118.05	109.23
1	A	166	TRP	N-CA-C	-5.66	101.90	110.28
1	C	134	LEU	N-CA-C	-5.61	98.04	108.02
1	H	133	TRP	N-CA-C	5.56	117.85	109.23
1	B	166	TRP	N-CA-C	-5.54	102.08	110.28
1	E	76	GLY	N-CA-C	-5.42	105.83	112.77
1	A	133	TRP	N-CA-C	5.41	118.04	109.50
1	C	171	TYR	N-CA-C	5.37	117.13	111.28
1	C	133	TRP	N-CA-C	5.32	117.77	109.52
1	D	171	TYR	N-CA-C	5.32	117.16	111.36
1	F	76	GLY	N-CA-C	-5.32	105.97	112.77
1	B	133	TRP	N-CA-C	5.25	117.17	109.24
1	A	175	GLN	CB-CA-C	-5.14	110.63	116.54
1	C	53	SER	N-CA-C	-5.05	103.86	110.53
1	G	53	SER	N-CA-C	-5.03	103.89	110.53
1	D	76	GLY	N-CA-C	-5.03	106.33	112.77
1	G	175	GLN	CB-CA-C	-5.02	110.77	116.54

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	1576	0	1481	9	0
1	B	1555	0	1465	11	0
1	C	1576	0	1481	12	0
1	D	1556	0	1457	15	0
1	E	1576	0	1481	10	0
1	F	1576	0	1481	4	0
1	G	1576	0	1481	18	0
1	H	1555	0	1465	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	115	0	0	0	0
3	B	114	0	0	1	0
3	C	98	0	0	0	0
3	D	103	0	0	0	0
3	E	123	0	0	1	0
3	F	117	0	0	0	0
3	G	111	0	0	0	0
3	H	129	0	0	1	0
All	All	13464	0	11792	88	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 4.

All (88) 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:B:6:PRO:HG3	1:B:83:LYS:HD2	1.74	0.69
1:G:101:LEU:HA	1:G:104:GLU:OE1	1.94	0.67
1:C:134:LEU:HB3	1:C:161:LEU:HB3	1.77	0.66
1:B:96:GLU:HG3	1:B:112:PHE:CD2	2.31	0.65
1:E:134:LEU:HB3	1:E:161:LEU:HB3	1.79	0.65
1:F:113:ASP:O	1:F:117:GLU:HG3	1.99	0.63
1:G:190:ASN:C	1:G:190:ASN:HD22	2.06	0.63
1:B:113:ASP:O	1:B:117:GLU:HG3	1.99	0.63
1:C:131:TRP:HA	1:C:165:VAL:HG23	1.81	0.62
1:A:134:LEU:HB3	1:A:161:LEU:HB3	1.80	0.62
1:D:61:LEU:HD12	1:D:69:ARG:HG3	1.81	0.61
1:G:97:PRO:HG3	1:G:191:TRP:CE3	2.37	0.60
1:H:131:TRP:HA	1:H:165:VAL:HG23	1.84	0.60
1:G:135:VAL:HG12	1:G:159:PRO:HA	1.84	0.59
1:G:100:ALA:O	1:G:104:GLU:CD	2.45	0.59
1:D:190:ASN:HD22	1:D:190:ASN:C	2.10	0.58
1:G:130:GLY:O	1:G:165:VAL:HG22	2.04	0.57
1:E:131:TRP:HA	1:E:165:VAL:HG23	1.87	0.56
1:B:190:ASN:C	1:B:190:ASN:HD22	2.13	0.56
1:G:134:LEU:HB3	1:G:161:LEU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:HD22	1:A:190:ASN:C	2.14	0.55
1:H:4:GLU:HG3	3:H:286:HOH:O	2.07	0.54
1:B:68:ILE:O	1:B:72:VAL:HG23	2.08	0.53
1:D:134:LEU:HB3	1:D:161:LEU:HB3	1.90	0.53
1:H:190:ASN:HD22	1:H:190:ASN:C	2.15	0.53
1:C:114:LYS:O	1:C:117:GLU:HG2	2.09	0.53
1:G:9:PRO:HG2	1:G:10:TYR:CD2	2.44	0.53
1:G:104:GLU:CD	1:G:198:TYR:CZ	2.87	0.52
1:F:190:ASN:C	1:F:190:ASN:HD22	2.15	0.52
1:E:190:ASN:C	1:E:190:ASN:HD22	2.17	0.52
1:C:97:PRO:HG3	1:C:191:TRP:CE3	2.45	0.52
1:E:41:LYS:HG3	3:E:248:HOH:O	2.10	0.51
1:A:47:THR:HG22	1:A:51:ASN:HD21	1.76	0.51
1:G:130:GLY:C	1:G:165:VAL:HG22	2.35	0.51
1:G:9:PRO:HG2	1:G:10:TYR:CE2	2.47	0.51
1:G:100:ALA:O	1:G:104:GLU:OE2	2.28	0.50
1:C:190:ASN:C	1:C:190:ASN:HD22	2.19	0.50
1:D:96:GLU:HG3	1:D:112:PHE:CD2	2.45	0.50
1:G:97:PRO:HG3	1:G:191:TRP:CD2	2.46	0.50
1:C:97:PRO:HG3	1:C:191:TRP:CD2	2.46	0.49
1:A:97:PRO:HG3	1:A:191:TRP:CE3	2.48	0.49
1:A:176:ASN:HD22	1:A:176:ASN:H	1.60	0.49
1:D:43:VAL:HG12	1:D:43:VAL:O	2.13	0.49
1:H:134:LEU:HB3	1:H:161:LEU:HB3	1.95	0.48
1:E:47:THR:HG22	1:E:51:ASN:ND2	2.28	0.48
1:G:21:LYS:O	1:G:25:THR:HG23	2.13	0.48
1:H:68:ILE:O	1:H:72:VAL:HG23	2.12	0.48
1:F:134:LEU:HB3	1:F:161:LEU:HB3	1.95	0.48
1:G:104:GLU:CD	1:G:198:TYR:OH	2.56	0.48
1:G:176:ASN:H	1:G:176:ASN:HD22	1.62	0.48
1:B:6:PRO:HG3	1:B:83:LYS:CD	2.44	0.47
1:D:97:PRO:HG3	1:D:191:TRP:CE3	2.49	0.47
1:A:190:ASN:HD21	1:A:192:ASP:HB2	1.80	0.47
1:C:53:SER:OG	1:C:56:GLU:HG3	2.14	0.47
1:G:190:ASN:C	1:G:190:ASN:ND2	2.72	0.47
1:H:165:VAL:HG12	1:H:178:ARG:CZ	2.45	0.47
1:E:165:VAL:HG12	1:E:178:ARG:CZ	2.44	0.46
1:C:176:ASN:H	1:C:176:ASN:HD22	1.64	0.46
1:B:97:PRO:HG3	1:B:191:TRP:CD2	2.50	0.46
1:F:196:ARG:NH2	1:F:200:GLU:OE2	2.50	0.45
1:A:47:THR:HG22	1:A:51:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:VAL:CG1	1:H:49:LEU:HB2	2.46	0.44
1:D:65:PRO:HD2	1:D:68:ILE:HD11	2.00	0.44
1:D:113:ASP:O	1:D:117:GLU:HG3	2.17	0.44
1:H:43:VAL:HG13	1:H:49:LEU:HB2	2.00	0.43
1:D:54:VAL:O	1:D:58:VAL:HG23	2.19	0.43
1:C:167:GLU:HB2	1:D:167:GLU:HB2	2.01	0.43
1:H:9:PRO:HG2	1:H:10:TYR:CD2	2.54	0.43
1:E:47:THR:HG22	1:E:51:ASN:HD21	1.84	0.43
1:C:104:GLU:O	1:C:108:VAL:HG23	2.19	0.43
1:G:165:VAL:O	1:G:165:VAL:HG23	2.18	0.43
1:B:97:PRO:HG3	1:B:191:TRP:CE3	2.53	0.42
1:H:9:PRO:HG2	1:H:10:TYR:CE2	2.55	0.42
1:A:190:ASN:C	1:A:190:ASN:ND2	2.78	0.42
1:E:176:ASN:HD22	1:E:176:ASN:H	1.68	0.42
1:B:6:PRO:HB3	1:B:83:LYS:HE2	2.02	0.42
1:D:190:ASN:C	1:D:190:ASN:ND2	2.78	0.42
1:C:165:VAL:HG12	1:C:178:ARG:CZ	2.49	0.41
1:D:37:THR:HG22	1:D:41:LYS:HE3	2.02	0.41
1:B:134:LEU:HB3	1:B:161:LEU:HB3	2.01	0.41
1:C:8:LEU:HA	1:C:9:PRO:HD3	1.85	0.41
1:D:97:PRO:HG3	1:D:191:TRP:CD2	2.55	0.41
1:E:135:VAL:HG12	1:E:159:PRO:HA	2.02	0.41
1:B:96:GLU:HG2	3:B:266:HOH:O	2.20	0.41
1:D:67:ASN:ND2	1:D:68:ILE:HG23	2.36	0.41
1:A:97:PRO:HG3	1:A:191:TRP:CD2	2.56	0.40
1:E:190:ASN:C	1:E:190:ASN:ND2	2.80	0.40
1:D:193:GLU:OE2	1:D:196:ARG:NH1	2.54	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	198/202 (98%)	193 (98%)	5 (2%)	0	100	100
1	B	193/202 (96%)	186 (96%)	7 (4%)	0	100	100
1	C	198/202 (98%)	193 (98%)	5 (2%)	0	100	100
1	D	193/202 (96%)	187 (97%)	6 (3%)	0	100	100
1	E	198/202 (98%)	193 (98%)	5 (2%)	0	100	100
1	F	198/202 (98%)	192 (97%)	6 (3%)	0	100	100
1	G	198/202 (98%)	191 (96%)	7 (4%)	0	100	100
1	H	193/202 (96%)	187 (97%)	6 (3%)	0	100	100
All	All	1569/1616 (97%)	1522 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	164/167 (98%)	163 (99%)	1 (1%)	78	66
1	B	162/167 (97%)	162 (100%)	0	100	100
1	C	164/167 (98%)	162 (99%)	2 (1%)	63	43
1	D	162/167 (97%)	160 (99%)	2 (1%)	63	43
1	E	164/167 (98%)	163 (99%)	1 (1%)	78	66
1	F	164/167 (98%)	164 (100%)	0	100	100
1	G	164/167 (98%)	162 (99%)	2 (1%)	63	43
1	H	162/167 (97%)	158 (98%)	4 (2%)	42	18
All	All	1306/1336 (98%)	1294 (99%)	12 (1%)	70	55

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	C	66	GLU

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Mol	Chain	Res	Type
1	C	165	VAL
1	D	61	LEU
1	D	190	ASN
1	E	165	VAL
1	G	165	VAL
1	G	190	ASN
1	H	61	LEU
1	H	62	ASP
1	H	165	VAL
1	H	190	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	137	ASN
1	A	173	ASN
1	A	176	ASN
1	A	190	ASN
1	B	173	ASN
1	B	175	GLN
1	B	190	ASN
1	C	137	ASN
1	C	148	ASN
1	C	176	ASN
1	C	190	ASN
1	D	67	ASN
1	D	118	GLN
1	D	173	ASN
1	D	175	GLN
1	D	190	ASN
1	E	51	ASN
1	E	92	ASN
1	E	137	ASN
1	E	173	ASN
1	E	176	ASN
1	E	190	ASN
1	F	67	ASN
1	F	173	ASN
1	F	175	GLN
1	F	190	ASN
1	G	176	ASN

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Mol	Chain	Res	Type
1	G	190	ASN
1	H	173	ASN
1	H	175	GLN
1	H	190	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/202 (99%)	0.56	24 (12%) 9 8	8, 16, 34, 45	0
1	B	197/202 (97%)	0.74	32 (16%) 4 4	8, 16, 41, 49	0
1	C	200/202 (99%)	0.80	32 (16%) 5 4	9, 19, 36, 44	0
1	D	197/202 (97%)	0.75	33 (16%) 4 3	9, 18, 41, 48	0
1	E	200/202 (99%)	0.62	27 (13%) 7 6	8, 16, 35, 46	0
1	F	200/202 (99%)	0.47	21 (10%) 11 11	8, 15, 34, 43	0
1	G	200/202 (99%)	0.59	28 (14%) 6 6	8, 17, 35, 44	0
1	H	197/202 (97%)	0.59	22 (11%) 10 10	8, 16, 35, 44	0
All	All	1591/1616 (98%)	0.64	219 (13%) 6 6	8, 17, 36, 49	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	50	ALA	11.3
1	B	47	THR	7.8
1	D	50	ALA	7.4
1	D	61	LEU	6.7
1	G	47	THR	6.5
1	B	48	ALA	6.3
1	H	51	ASN	6.2
1	A	47	THR	6.0
1	G	104	GLU	5.9
1	H	49	LEU	5.6
1	H	48	ALA	5.4
1	B	49	LEU	5.1
1	H	2	ALA	5.1
1	A	48	ALA	5.0
1	F	2	ALA	4.8
1	C	2	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	51	ASN	4.7
1	E	2	ALA	4.6
1	H	47	THR	4.6
1	C	165	VAL	4.5
1	B	60	ASP	4.5
1	B	50	ALA	4.5
1	D	63	SER	4.4
1	C	47	THR	4.4
1	B	43	VAL	4.3
1	A	61	LEU	4.3
1	B	61	LEU	4.3
1	A	2	ALA	4.3
1	C	50	ALA	4.2
1	B	56	GLU	4.2
1	A	60	ASP	4.1
1	H	52	LYS	4.1
1	A	62	ASP	4.1
1	D	60	ASP	4.1
1	B	51	ASN	4.0
1	B	64	VAL	4.0
1	H	165	VAL	4.0
1	E	50	ALA	4.0
1	E	165	VAL	4.0
1	B	62	ASP	3.8
1	C	48	ALA	3.8
1	C	66	GLU	3.7
1	E	47	THR	3.7
1	D	43	VAL	3.7
1	B	138	ASN	3.7
1	E	48	ALA	3.7
1	G	155	GLU	3.6
1	H	138	ASN	3.6
1	D	62	ASP	3.6
1	F	62	ASP	3.6
1	D	2	ALA	3.4
1	H	60	ASP	3.4
1	F	61	LEU	3.4
1	G	62	ASP	3.3
1	H	62	ASP	3.3
1	E	49	LEU	3.3
1	D	136	VAL	3.3
1	B	136	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	51	ASN	3.3
1	A	155	GLU	3.3
1	D	45	GLY	3.2
1	B	66	GLU	3.2
1	D	155	GLU	3.2
1	C	103	GLU	3.2
1	F	41	LYS	3.2
1	G	50	ALA	3.2
1	C	95	GLY	3.2
1	G	165	VAL	3.2
1	D	103	GLU	3.1
1	E	44	GLU	3.1
1	H	43	VAL	3.1
1	F	155	GLU	3.1
1	A	49	LEU	3.1
1	A	67	ASN	3.1
1	G	2	ALA	3.1
1	C	67	ASN	3.0
1	G	67	ASN	3.0
1	D	57	LEU	3.0
1	A	66	GLU	3.0
1	G	61	LEU	3.0
1	B	52	LYS	3.0
1	A	103	GLU	3.0
1	C	156	GLY	3.0
1	D	52	LYS	2.9
1	B	155	GLU	2.9
1	H	61	LEU	2.9
1	B	63	SER	2.9
1	G	48	ALA	2.9
1	E	67	ASN	2.9
1	G	92	ASN	2.9
1	A	50	ALA	2.9
1	D	59	ALA	2.9
1	C	49	LEU	2.9
1	A	52	LYS	2.9
1	G	200	GLU	2.8
1	D	7	GLU	2.8
1	D	44	GLU	2.8
1	H	155	GLU	2.8
1	A	41	LYS	2.8
1	B	59	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	95	GLY	2.8
1	C	138	ASN	2.8
1	G	138	ASN	2.8
1	D	66	GLU	2.8
1	E	60	ASP	2.8
1	B	65	PRO	2.8
1	F	138	ASN	2.8
1	H	56	GLU	2.8
1	B	139	GLY	2.8
1	G	44	GLU	2.7
1	E	62	ASP	2.7
1	A	7	GLU	2.7
1	H	200	GLU	2.7
1	C	4	GLU	2.7
1	E	63	SER	2.7
1	D	68	ILE	2.7
1	A	117	GLU	2.6
1	A	140	LYS	2.6
1	G	49	LEU	2.6
1	F	200	GLU	2.6
1	E	41	LYS	2.6
1	C	117	GLU	2.6
1	F	66	GLU	2.6
1	E	196	ARG	2.6
1	H	4	GLU	2.6
1	C	107	SER	2.6
1	C	51	ASN	2.6
1	A	46	ASN	2.5
1	A	51	ASN	2.5
1	E	51	ASN	2.5
1	E	66	GLU	2.5
1	A	44	GLU	2.5
1	C	142	GLU	2.5
1	C	134	LEU	2.5
1	D	58	VAL	2.5
1	C	44	GLU	2.5
1	E	200	GLU	2.5
1	G	66	GLU	2.5
1	C	60	ASP	2.4
1	G	60	ASP	2.4
1	E	140	LYS	2.4
1	F	64	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	51	ASN	2.4
1	D	200	GLU	2.4
1	E	7	GLU	2.4
1	B	67	ASN	2.4
1	B	137	ASN	2.4
1	G	63	SER	2.4
1	B	58	VAL	2.4
1	F	67	ASN	2.4
1	D	41	LYS	2.4
1	C	106	ASN	2.3
1	H	65	PRO	2.3
1	B	57	LEU	2.3
1	C	61	LEU	2.3
1	F	57	LEU	2.3
1	G	196	ARG	2.3
1	D	64	VAL	2.3
1	G	7	GLU	2.3
1	C	46	ASN	2.3
1	D	138	ASN	2.3
1	D	96	GLU	2.3
1	E	69	ARG	2.3
1	G	139	GLY	2.3
1	F	42	ALA	2.3
1	C	139	GLY	2.3
1	D	65	PRO	2.2
1	A	98	THR	2.2
1	F	47	THR	2.2
1	D	4	GLU	2.2
1	H	22	GLU	2.2
1	D	201	ARG	2.2
1	H	63	SER	2.2
1	A	113	ASP	2.2
1	F	60	ASP	2.2
1	G	45	GLY	2.2
1	A	56	GLU	2.2
1	E	104	GLU	2.2
1	F	50	ALA	2.2
1	H	139	GLY	2.2
1	E	103	GLU	2.2
1	D	46	ASN	2.2
1	C	136	VAL	2.2
1	C	62	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	96	GLU	2.2
1	B	200	GLU	2.2
1	F	7	GLU	2.2
1	G	142	GLU	2.2
1	F	139	GLY	2.2
1	C	140	LYS	2.2
1	C	155	GLU	2.1
1	A	45	GLY	2.1
1	E	45	GLY	2.1
1	G	41	LYS	2.1
1	C	63	SER	2.1
1	H	66	GLU	2.1
1	C	108	VAL	2.1
1	D	137	ASN	2.1
1	B	117	GLU	2.1
1	C	104	GLU	2.1
1	D	69	ARG	2.1
1	C	41	LYS	2.1
1	D	67	ASN	2.1
1	E	107	SER	2.1
1	F	63	SER	2.1
1	E	61	LEU	2.1
1	B	83	LYS	2.1
1	G	140	LYS	2.1
1	E	155	GLU	2.0
1	F	4	GLU	2.0
1	G	46	ASN	2.0
1	B	201	ARG	2.0
1	F	65	PRO	2.0
1	B	103	GLU	2.0
1	E	117	GLU	2.0
1	E	139	GLY	2.0
1	B	68	ILE	2.0
1	G	198	TYR	2.0
1	D	42	ALA	2.0

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

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

6.3 Carbohydrates [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(Å ²)	Q<0.9
2	MN	B	203	1/1	0.99	0.02	10,10,10,10	0
2	MN	C	203	1/1	0.99	0.03	10,10,10,10	0
2	MN	D	203	1/1	0.99	0.02	9,9,9,9	0
2	MN	F	203	1/1	0.99	0.03	9,9,9,9	0
2	MN	H	203	1/1	0.99	0.03	10,10,10,10	0
2	MN	A	203	1/1	1.00	0.02	9,9,9,9	0
2	MN	G	203	1/1	1.00	0.02	8,8,8,8	0
2	MN	E	203	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.