



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:43 PM UTC

PDB ID : 1QDN / pdb_00001qdn
Title : AMINO TERMINAL DOMAIN OF THE N-ETHYLMALEIMIDE SENSITIVE FUSION PROTEIN (NSF)
Authors : May, A.P.; Misura, K.M.S.; Whiteheart, S.W.; Weis, W.I.
Deposited on : 1999-05-21
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

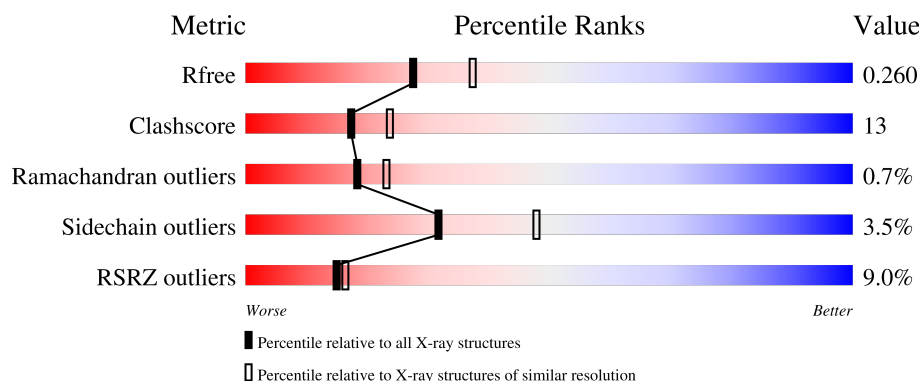
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	204	6% 70% 22% • 7%
1	B	204	8% 69% 22% • 7%
1	C	204	11% 66% 25% • 7%

2 Entry composition [i](#)

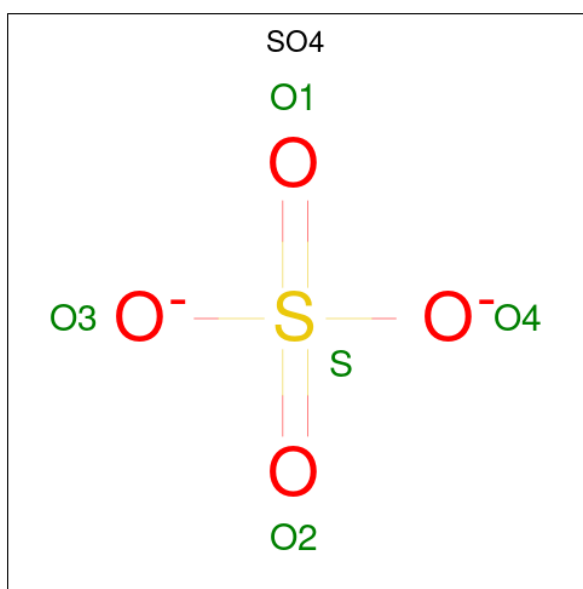
There are 4 unique types of molecules in this entry. The entry contains 4742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (N-ETHYLMALEIMIDE SENSITIVE FUSION PROTEIN (NSF)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	1	0
			1472	931	249	284	8			
1	B	189	Total	C	N	O	S	0	2	0
			1476	933	251	284	8			
1	C	190	Total	C	N	O	S	0	3	0
			1488	940	252	288	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



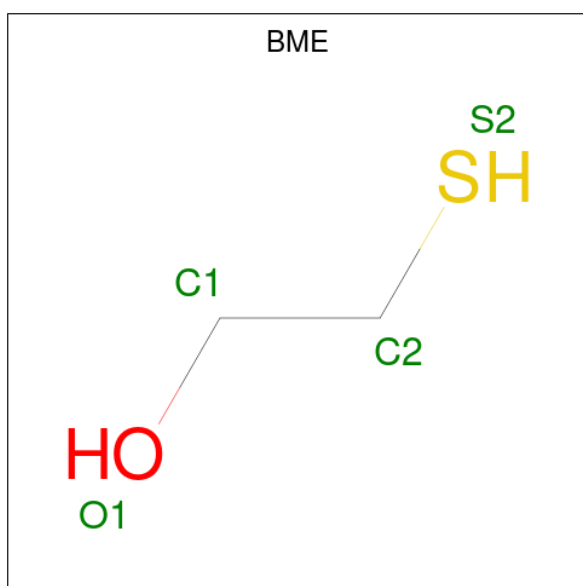
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is water.

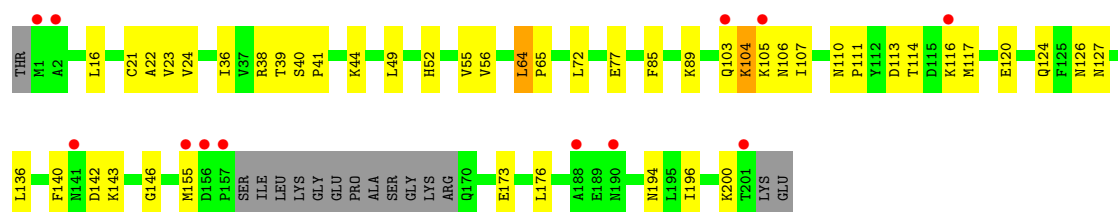
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total 93	O 93	0	0
4	B	79	Total 79	O 79	0	0
4	C	70	Total 70	O 70	0	0

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.

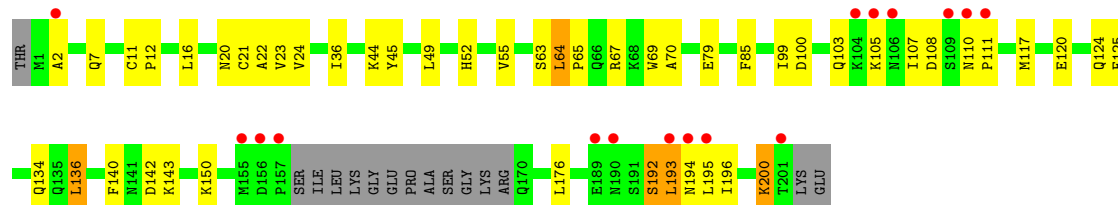
• Molecule 1: PROTEIN (N-ETHYLMALEIMIDE SENSITIVE FUSION PROTEIN (NSF))

Chain A: 



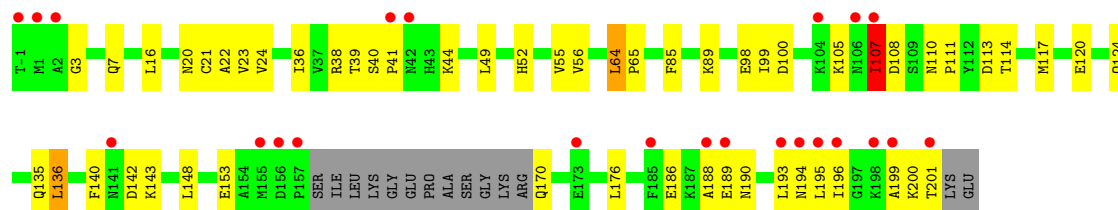
• Molecule 1: PROTEIN (N-ETHYLMALEIMIDE SENSITIVE FUSION PROTEIN (NSF))

Chain B: 



• Molecule 1: PROTEIN (N-ETHYLMALEIMIDE SENSITIVE FUSION PROTEIN (NSF))

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.90Å 101.90Å 126.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-2.30) 94.0 (30.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.31Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.220 , 0.260 0.221 , 0.260	Depositor DCC
R_{free} test set	1675 reflections (5.87%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4742	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: BME, SO4

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	0.40	0/1501	0.89	3/2024 (0.1%)
1	B	0.37	0/1509	0.87	4/2035 (0.2%)
1	C	0.37	0/1525	0.89	3/2057 (0.1%)
All	All	0.38	0/4535	0.89	10/6116 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ALA	N-CA-C	-7.87	97.24	109.76
1	B	22	ALA	N-CA-C	-7.42	97.97	109.76
1	C	22	ALA	N-CA-C	-7.04	97.77	109.46
1	A	24	VAL	N-CA-C	5.84	115.65	108.53
1	B	24	VAL	N-CA-C	5.70	115.48	108.53
1	C	24	VAL	N-CA-C	5.55	115.31	108.53
1	B	49	LEU	N-CA-C	5.49	118.64	110.52
1	C	49	LEU	N-CA-C	5.14	118.49	110.32
1	B	192	SER	N-CA-C	-5.09	107.57	112.97
1	A	49	LEU	N-CA-C	5.07	118.03	110.52

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	1472	0	1465	35	0
1	B	1476	0	1469	39	0
1	C	1488	0	1478	46	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
3	A	8	0	10	2	0
3	B	8	0	10	2	0
3	C	8	0	10	2	0
4	A	93	0	0	2	1
4	B	79	0	0	1	0
4	C	70	0	0	2	1
All	All	4742	0	4442	112	2

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 13.

All (112) 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:85:PHE:HB3	3:C:401:BME:H12	1.47	0.96
1:A:85:PHE:HB3	3:A:401:BME:H12	1.44	0.95
1:B:85:PHE:HB3	3:B:401:BME:H12	1.46	0.94
1:C:38:ARG:HH21	1:C:44:LYS:HE2	1.38	0.86
1:A:21:CYS:O	3:A:400:BME:H12	1.79	0.82
1:B:20[B]:ASN:OD1	1:B:136:LEU:HD22	1.81	0.81
1:B:21:CYS:O	3:B:400:BME:H12	1.81	0.79
1:C:21:CYS:O	3:C:400:BME:H12	1.83	0.78
1:C:135:GLN:NE2	1:C:148:LEU:HB2	1.98	0.78
1:A:89:LYS:HG3	4:A:525:HOH:O	1.89	0.73
1:B:2:ALA:HB1	1:B:79:GLU:OE2	1.89	0.73
1:C:107:ILE:HG12	1:C:107:ILE:O	1.89	0.72
1:C:135:GLN:HE21	1:C:148:LEU:HD13	1.58	0.69
1:C:38:ARG:HH21	1:C:44:LYS:CE	2.05	0.69
1:C:135:GLN:HE22	1:C:148:LEU:HB2	1.58	0.68
1:C:23:VAL:HG12	1:C:55:VAL:HG21	1.76	0.67
1:B:23:VAL:HG12	1:B:55:VAL:HG21	1.75	0.66
1:A:38:ARG:NH2	1:A:44:LYS:HE3	2.14	0.63
1:C:113:ASP:HA	1:C:196:ILE:HG13	1.80	0.63
1:A:23:VAL:HG12	1:A:55:VAL:HG21	1.81	0.62
1:C:41:PRO:HA	4:C:547:HOH:O	1.99	0.62
1:B:111:PRO:HB3	1:B:194:ASN:ND2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HH21	1:A:44:LYS:HE3	1.65	0.61
1:C:111:PRO:CA	1:C:194:ASN:HD22	2.14	0.60
1:A:105:LYS:O	1:A:105:LYS:HD3	2.02	0.60
1:C:111:PRO:HB2	1:C:196:ILE:HD13	1.85	0.58
1:C:111:PRO:HA	1:C:194:ASN:HD22	1.67	0.58
1:A:113:ASP:O	1:A:117:MET:HG3	2.04	0.58
1:A:56:VAL:CG1	1:B:124:GLN:HB3	2.36	0.56
1:B:111:PRO:HB3	1:B:194:ASN:HD22	1.71	0.56
1:A:120:GLU:O	1:A:124:GLN:HG2	2.06	0.56
1:C:38:ARG:NH2	1:C:44:LYS:HE2	2.15	0.55
1:A:114:THR:HG21	1:A:200:LYS:HG2	1.89	0.55
1:C:100:ASP:OD2	1:C:188:ALA:HB3	2.05	0.55
1:C:20[B]:ASN:ND2	1:C:136:LEU:HD22	2.22	0.54
1:A:104:LYS:O	1:A:107:ILE:HG13	2.07	0.54
1:A:103:GLN:HB2	1:A:106:ASN:ND2	2.22	0.54
1:C:120:GLU:O	1:C:124:GLN:HG2	2.08	0.54
1:A:56:VAL:HG13	1:B:124:GLN:HB3	1.90	0.53
1:C:110:ASN:O	1:C:194:ASN:HB3	2.09	0.53
1:B:36:ILE:HD11	1:B:44:LYS:HD3	1.90	0.53
1:C:186:GLU:HB3	1:C:201:THR:OG1	2.09	0.53
1:B:107:ILE:HG21	1:B:192:SER:HB2	1.91	0.52
1:B:120:GLU:O	1:B:124:GLN:HG2	2.10	0.51
1:B:111:PRO:HB2	1:B:196:ILE:HD13	1.92	0.51
1:A:36:ILE:HD11	1:A:44:LYS:HB3	1.92	0.50
1:C:99:ILE:HG12	1:C:100:ASP:N	2.26	0.50
1:C:89:LYS:HG3	4:C:533:HOH:O	2.12	0.50
1:B:69:TRP:CE3	1:B:134:GLN:HG3	2.47	0.50
1:B:193:LEU:HD22	1:B:195:LEU:CD1	2.41	0.50
1:B:99:ILE:HG12	1:B:100:ASP:N	2.27	0.49
1:A:111:PRO:HB2	1:A:196:ILE:HD13	1.95	0.49
1:A:146:GLY:HA3	4:A:577:HOH:O	2.11	0.49
1:A:56:VAL:HG13	1:B:124:GLN:CB	2.42	0.49
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.95	0.49
1:C:114:THR:OG1	1:C:199:ALA:HB3	2.13	0.49
1:A:40:SER:HB2	1:A:41:PRO:HD2	1.95	0.48
1:A:39:THR:HG22	1:A:72:LEU:HD21	1.94	0.48
1:B:103:GLN:C	1:B:105:LYS:N	2.70	0.48
1:B:103:GLN:C	1:B:105:LYS:H	2.21	0.48
1:A:120:GLU:OE1	1:C:7:GLN:NE2	2.47	0.48
1:B:117:MET:HE3	1:B:140:PHE:CD2	2.48	0.48
1:B:195:LEU:HD12	1:B:195:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASP:OD2	1:B:110:ASN:HB2	2.14	0.47
1:C:195:LEU:C	1:C:200:LYS:HZ1	2.22	0.47
1:B:16:LEU:HD11	1:B:52:HIS:CD2	2.49	0.47
1:B:7[B]:GLN:HG2	4:B:560:HOH:O	2.15	0.47
1:B:7[A]:GLN:HE22	1:C:120:GLU:CD	2.23	0.47
1:A:36:ILE:CG1	1:A:44:LYS:HB3	2.44	0.46
1:A:103:GLN:HB2	1:A:106:ASN:HD22	1.80	0.46
1:B:142:ASP:C	1:B:143:LYS:HD2	2.40	0.46
1:B:36:ILE:HD11	1:B:44:LYS:HB3	1.97	0.46
1:B:195:LEU:O	1:B:200:LYS:HE3	2.15	0.46
1:B:20[A]:ASN:ND2	1:B:125:PHE:CZ	2.83	0.46
1:B:193:LEU:HD22	1:B:195:LEU:HD12	1.97	0.46
1:A:16:LEU:HD11	1:A:52:HIS:CD2	2.51	0.46
1:C:99:ILE:HG23	1:C:193:LEU:HD13	1.98	0.46
1:C:195:LEU:HB3	1:C:200:LYS:HE2	1.98	0.45
1:C:16:LEU:HD11	1:C:52:HIS:CD2	2.51	0.45
1:B:63:SER:O	1:B:67:ARG:HG3	2.16	0.45
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.98	0.45
1:A:124:GLN:HB3	1:C:56:VAL:HG13	1.98	0.45
1:B:69:TRP:CD2	1:B:134:GLN:HG3	2.51	0.45
1:C:20[B]:ASN:CG	1:C:136:LEU:HD22	2.42	0.45
1:C:99:ILE:CG1	1:C:100:ASP:N	2.80	0.44
1:C:186:GLU:O	1:C:186:GLU:HG3	2.17	0.44
1:C:117:MET:HE3	1:C:140:PHE:CD2	2.52	0.43
1:C:142:ASP:C	1:C:143:LYS:HD2	2.44	0.43
1:A:126:ASN:O	1:A:127:ASN:HB2	2.18	0.43
1:C:189:GLU:O	1:C:190:ASN:HB2	2.19	0.42
1:B:45:TYR:CZ	1:B:70:ALA:HA	2.55	0.42
1:A:110:ASN:O	1:A:194:ASN:HB3	2.20	0.42
1:A:113:ASP:OD1	1:A:116:LYS:HE3	2.19	0.42
1:C:64:LEU:HB3	1:C:65:PRO:HD3	2.01	0.42
1:C:110:ASN:HB3	1:C:111:PRO:HD2	2.01	0.42
1:C:98:GLU:HA	1:C:186:GLU:O	2.19	0.42
1:A:36:ILE:HD11	1:A:44:LYS:CB	2.50	0.42
1:B:99:ILE:CG1	1:B:100:ASP:N	2.83	0.41
1:C:111:PRO:HA	1:C:194:ASN:ND2	2.34	0.41
1:A:142:ASP:C	1:A:143:LYS:HD2	2.45	0.41
1:B:7[A]:GLN:NE2	1:C:120:GLU:OE1	2.52	0.41
1:B:200:LYS:HB2	1:B:200:LYS:NZ	2.36	0.41
1:C:64:LEU:CB	1:C:65:PRO:HD3	2.51	0.41
1:A:113:ASP:OD2	1:A:113:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:HG2	1:A:124:GLN:HE21	1.86	0.41
1:A:124:GLN:HB3	1:C:56:VAL:CG1	2.51	0.41
1:C:153:GLU:HA	1:C:170:GLN:O	2.21	0.41
1:A:117:MET:HE3	1:A:140:PHE:CD2	2.56	0.40
1:C:36:ILE:HD11	1:C:44:LYS:HD3	2.02	0.40
1:B:11:CYS:HA	1:B:12:PRO:HD3	1.97	0.40
1:C:39:THR:O	1:C:40:SER:HB3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:516:HOH:O	4:C:516:HOH:O[7_555]	1.04	1.16
4:A:553:HOH:O	4:A:553:HOH:O[7_555]	1.67	0.53

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	186/204 (91%)	182 (98%)	4 (2%)	0	100	100
1	B	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
1	C	189/204 (93%)	178 (94%)	7 (4%)	4 (2%)	5	4
All	All	562/612 (92%)	538 (96%)	20 (4%)	4 (1%)	18	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	LYS
1	C	108	ASP
1	C	107	ILE
1	C	3	GLY

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	164/175 (94%)	156 (95%)	8 (5%)	22	34
1	B	165/175 (94%)	159 (96%)	6 (4%)	31	47
1	C	167/175 (95%)	163 (98%)	4 (2%)	43	62
All	All	496/525 (94%)	478 (96%)	18 (4%)	32	47

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	77	GLU
1	A	104	LYS
1	A	136	LEU
1	A	155	MET
1	A	173[A]	GLU
1	A	173[B]	GLU
1	A	176	LEU
1	B	64	LEU
1	B	136	LEU
1	B	150	LYS
1	B	176	LEU
1	B	193	LEU
1	B	200	LYS
1	C	64	LEU
1	C	107	ILE
1	C	136	LEU
1	C	176	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	106	ASN
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	126	ASN
1	A	127	ASN
1	A	182	GLN
1	A	194	ASN
1	B	103	GLN
1	B	110	ASN
1	B	123	GLN
1	B	124	GLN
1	B	126	ASN
1	B	128	GLN
1	B	135	GLN
1	B	194	ASN
1	C	7	GLN
1	C	123	GLN
1	C	124	GLN
1	C	126	ASN
1	C	128	GLN
1	C	135	GLN
1	C	194	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](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BME	B	400	1	3,3,3	0.56	0	2,2,2	1.57	0
2	SO4	C	508	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	A	505	-	4,4,4	0.38	0	6,6,6	0.10	0
2	SO4	C	504	-	4,4,4	0.40	0	6,6,6	0.07	0
3	BME	A	400	1	3,3,3	0.52	0	2,2,2	1.57	0
2	SO4	A	501	-	4,4,4	0.38	0	6,6,6	0.15	0
3	BME	B	401	1	3,3,3	0.50	0	2,2,2	0.97	0
2	SO4	B	503	-	4,4,4	0.37	0	6,6,6	0.08	0
3	BME	A	401	1	3,3,3	0.50	0	2,2,2	1.00	0
3	BME	C	400	1	3,3,3	0.63	0	2,2,2	1.64	0
3	BME	C	401	1	3,3,3	0.45	0	2,2,2	0.91	0
2	SO4	B	506	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	B	507	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	A	502	-	4,4,4	0.41	0	6,6,6	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	A	400	1	-	1/1/1/1	-
3	BME	B	401	1	-	1/1/1/1	-
3	BME	A	401	1	-	1/1/1/1	-
3	BME	C	400	1	-	1/1/1/1	-
3	BME	C	401	1	-	1/1/1/1	-
3	BME	B	400	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	BME	O1-C1-C2-S2
3	A	401	BME	O1-C1-C2-S2
3	B	400	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
3	B	401	BME	O1-C1-C2-S2
3	C	400	BME	O1-C1-C2-S2
3	C	401	BME	O1-C1-C2-S2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	BME	1	0
3	A	400	BME	1	0
3	B	401	BME	1	0
3	A	401	BME	1	0
3	C	400	BME	1	0
3	C	401	BME	1	0

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	189/204 (92%)	0.41	12 (6%) 26 28	15, 28, 54, 63	1 (0%)
1	B	189/204 (92%)	0.42	16 (8%) 16 18	12, 28, 65, 82	2 (1%)
1	C	190/204 (93%)	0.62	23 (12%) 8 9	13, 32, 76, 87	3 (1%)
All	All	568/612 (92%)	0.48	51 (8%) 15 16	12, 30, 66, 87	6 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-1	THR	4.9
1	C	155	MET	4.2
1	A	157	PRO	3.9
1	A	155	MET	3.6
1	C	106	ASN	3.6
1	B	190	ASN	3.5
1	C	173	GLU	3.4
1	A	2	ALA	3.3
1	C	201	THR	3.3
1	B	155	MET	3.2
1	C	157	PRO	3.2
1	B	157	PRO	3.1
1	B	201	THR	2.9
1	A	141	ASN	2.8
1	A	103	GLN	2.7
1	B	194	ASN	2.7
1	C	195	LEU	2.7
1	C	42	ASN	2.7
1	C	107	ILE	2.7
1	B	104	LYS	2.7
1	C	193	LEU	2.6
1	C	188	ALA	2.6
1	B	193	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	104	LYS	2.5
1	B	195	LEU	2.5
1	B	105	LYS	2.5
1	A	201	THR	2.5
1	A	156	ASP	2.4
1	C	1	MET	2.4
1	C	156	ASP	2.4
1	B	2	ALA	2.4
1	A	105	LYS	2.4
1	C	196	ILE	2.3
1	B	106	ASN	2.3
1	C	199	ALA	2.3
1	A	116	LYS	2.3
1	A	190	ASN	2.3
1	C	2	ALA	2.3
1	C	194	ASN	2.2
1	C	185	PHE	2.2
1	B	156	ASP	2.2
1	A	188	ALA	2.2
1	B	110	ASN	2.1
1	C	141	ASN	2.1
1	C	189	GLU	2.1
1	A	1	MET	2.1
1	C	198	LYS	2.1
1	B	189	GLU	2.1
1	B	111	PRO	2.1
1	C	41	PRO	2.0
1	B	109	SER	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(Å ²)	Q<0.9
2	SO4	B	507	5/5	0.74	0.14	89,89,90,90	0
2	SO4	C	508	5/5	0.79	0.16	93,93,94,94	0
2	SO4	B	506	5/5	0.84	0.16	76,77,77,77	0
2	SO4	A	505	5/5	0.86	0.14	68,69,69,70	0
2	SO4	B	503	5/5	0.87	0.17	74,75,75,76	0
2	SO4	C	504	5/5	0.92	0.09	52,53,54,54	0
3	BME	C	400	4/4	0.93	0.11	25,25,26,30	0
2	SO4	A	501	5/5	0.94	0.10	41,41,42,43	0
3	BME	C	401	4/4	0.95	0.09	26,26,28,30	0
3	BME	B	400	4/4	0.96	0.10	24,25,27,29	0
3	BME	B	401	4/4	0.96	0.09	27,27,28,28	0
3	BME	A	400	4/4	0.97	0.10	20,23,26,30	0
3	BME	A	401	4/4	0.97	0.08	24,27,27,29	0
2	SO4	A	502	5/5	0.99	0.04	20,20,21,23	0

6.5 Other polymers

There are no such residues in this entry.