



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 2Y6E / pdb_00002y6e
Title : Structure of the D1D2 domain of USP4, the conserved catalytic domain
Authors : Luna-Vargas, M.P.A.; Faesen, A.C.; van Dijk, W.J.; Rape, M.; Fish, A.; Sixma, T.K.
Deposited on : 2011-01-20
Resolution : 2.40 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

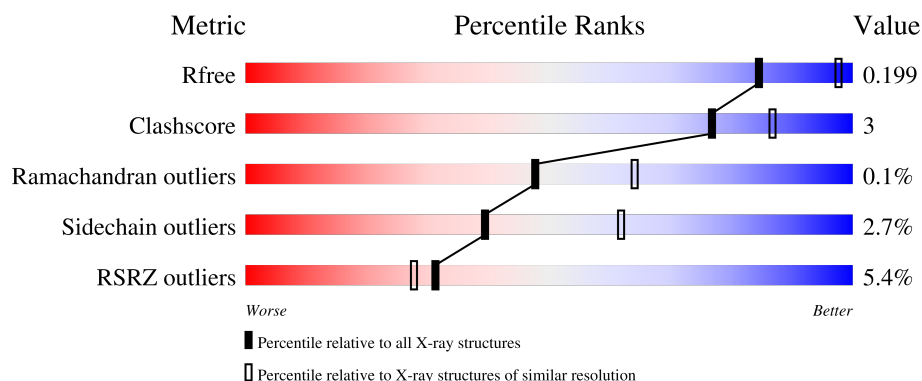
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	367	4% 84% 6% • 8%
1	B	367	4% 85% 7% • 8%
1	C	367	5% 84% 5% • 10%
1	D	367	7% 79% 9% • 11%
1	E	367	4% 80% 6% • 13%

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Mol	Chain	Length	Quality of chain
1	F	367	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CME	D	311	-	-	X	-
1	CME	E	311	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17209 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 UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2734	1750	464	502	18			
1	B	339	Total	C	N	O	S	0	0	0
			2738	1752	465	504	17			
1	C	331	Total	C	N	O	S	0	0	0
			2666	1709	453	487	17			
1	D	328	Total	C	N	O	S	0	0	0
			2646	1697	446	485	18			
1	E	319	Total	C	N	O	S	0	0	0
			2569	1649	432	473	15			
1	F	323	Total	C	N	O	S	0	0	0
			2591	1659	438	479	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLY	-	expression tag	UNP Q13107
A	295	MET	-	expression tag	UNP Q13107
A	491	GLY	-	linker	UNP Q13107
A	492	PRO	-	linker	UNP Q13107
B	294	GLY	-	expression tag	UNP Q13107
B	295	MET	-	expression tag	UNP Q13107
B	491	GLY	-	linker	UNP Q13107
B	492	PRO	-	linker	UNP Q13107
C	294	GLY	-	expression tag	UNP Q13107
C	295	MET	-	expression tag	UNP Q13107
C	491	GLY	-	linker	UNP Q13107
C	492	PRO	-	linker	UNP Q13107
D	294	GLY	-	expression tag	UNP Q13107
D	295	MET	-	expression tag	UNP Q13107
D	491	GLY	-	linker	UNP Q13107
D	492	PRO	-	linker	UNP Q13107
E	294	GLY	-	expression tag	UNP Q13107

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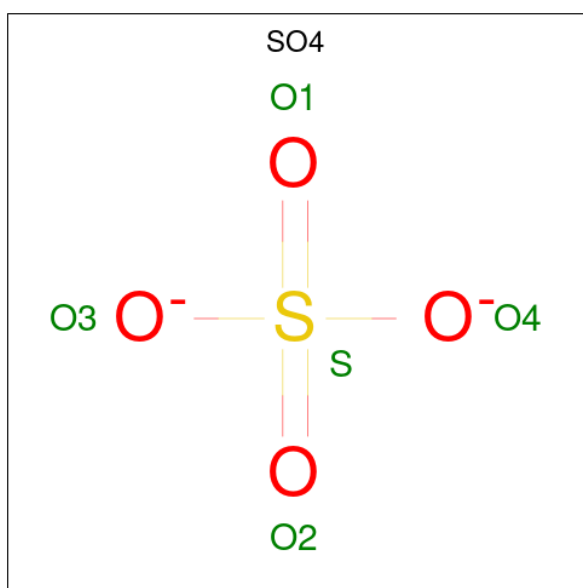
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Chain	Residue	Modelled	Actual	Comment	Reference
E	295	MET	-	expression tag	UNP Q13107
E	491	GLY	-	linker	UNP Q13107
E	492	PRO	-	linker	UNP Q13107
F	294	GLY	-	expression tag	UNP Q13107
F	295	MET	-	expression tag	UNP Q13107
F	491	GLY	-	linker	UNP Q13107
F	492	PRO	-	linker	UNP Q13107

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

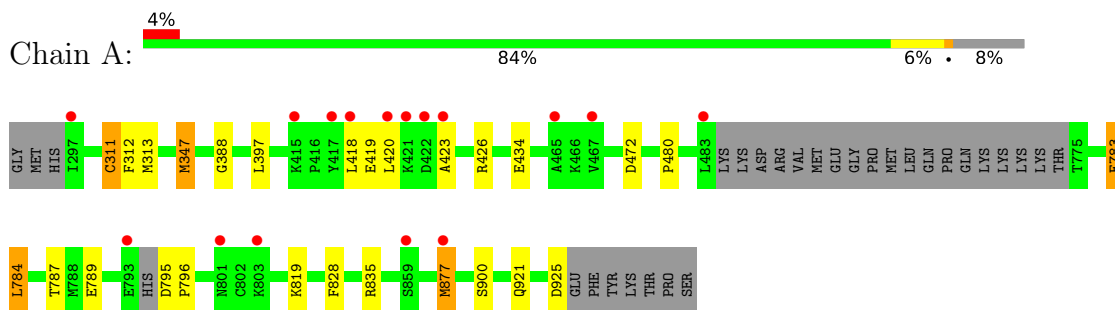
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	250	Total	O	0	0
			250	250		
4	B	232	Total	O	0	0
			232	232		
4	C	204	Total	O	0	0
			204	204		
4	D	214	Total	O	0	0
			214	214		
4	E	166	Total	O	0	0
			166	166		
4	F	183	Total	O	0	0
			183	183		

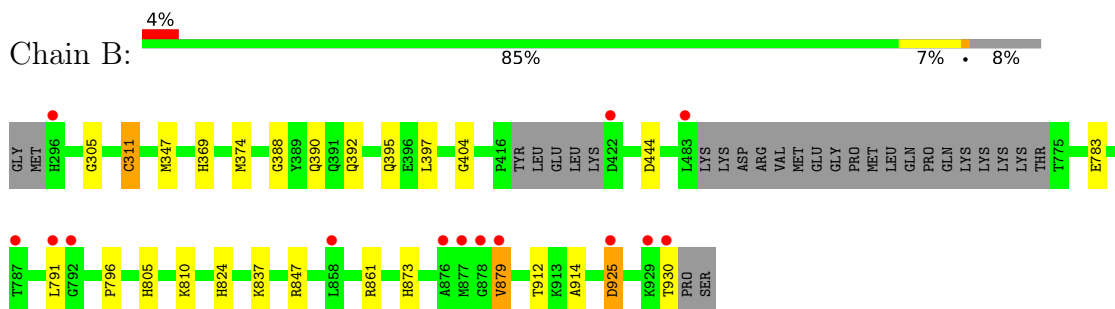
3 Residue-property plots [i](#)

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.

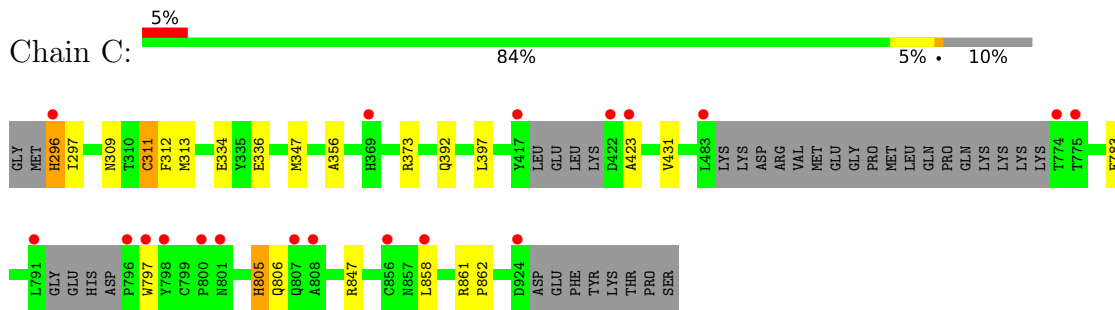
• Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4



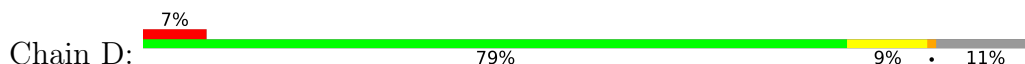
• Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4

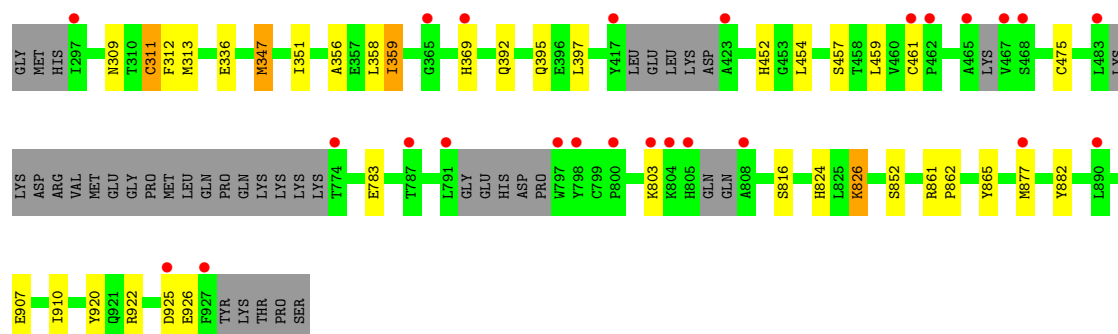


• Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4

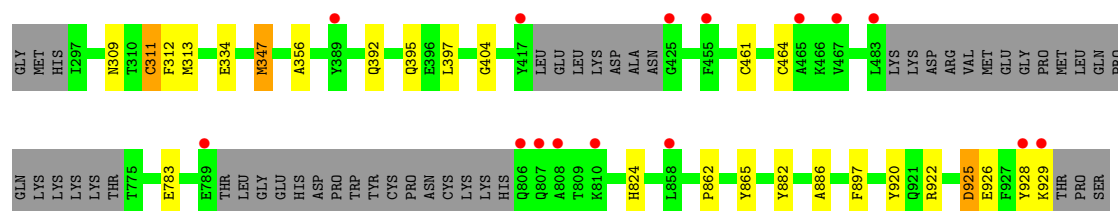
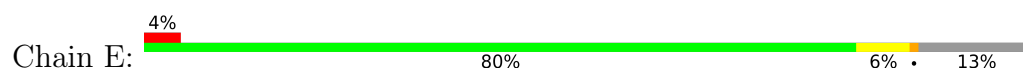


• Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4

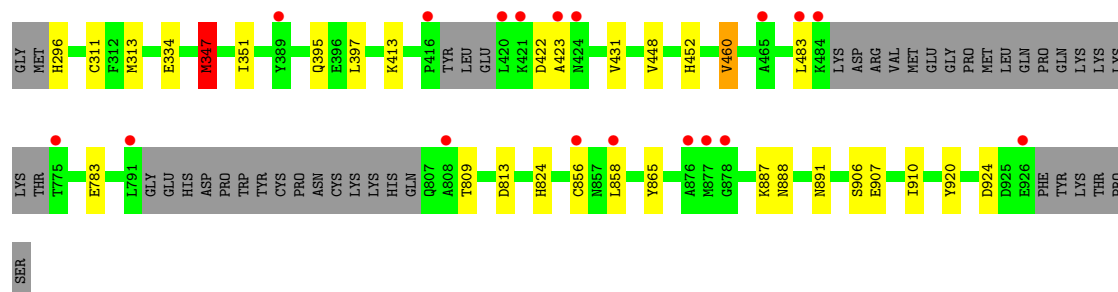
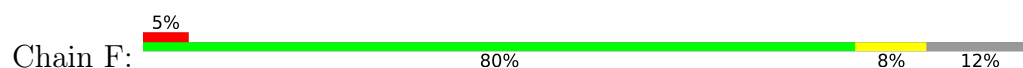




- Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4



- Molecule 1: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.50Å 151.03Å 178.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.59 – 2.40 44.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.59-2.40) 94.8 (44.59-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.178 , 0.210 (Not available) , 0.199	Depositor DCC
R_{free} test set	5583 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.5	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	0.95	EDS
Total number of atoms	17209	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: CME, SO4, ZN

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	0.83	2/2791 (0.1%)	1.17	1/3780 (0.0%)
1	B	0.83	0/2798	1.19	3/3793 (0.1%)
1	C	0.81	1/2723 (0.0%)	1.19	6/3691 (0.2%)
1	D	0.82	0/2700	1.20	4/3656 (0.1%)
1	E	0.80	0/2620	1.18	5/3547 (0.1%)
1	F	0.80	1/2641 (0.0%)	1.21	4/3577 (0.1%)
All	All	0.82	4/16273 (0.0%)	1.19	23/22044 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	MET	SD-CE	-8.01	1.59	1.79
1	C	347	MET	SD-CE	-7.36	1.61	1.79
1	A	877	MET	SD-CE	-5.50	1.65	1.79
1	F	347	MET	SD-CE	-5.12	1.66	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	HIS	CA-C-N	6.56	129.29	120.50
1	C	296	HIS	C-N-CA	6.56	129.29	120.50
1	D	852	SER	CA-C-N	6.37	129.46	120.28
1	D	852	SER	C-N-CA	6.37	129.46	120.28
1	B	925	ASP	CA-CB-CG	6.20	118.80	112.60
1	E	925	ASP	CA-CB-CG	6.09	118.69	112.60
1	F	334	GLU	CA-C-N	5.27	129.04	120.60
1	F	334	GLU	C-N-CA	5.27	129.04	120.60
1	E	356	ALA	CA-C-N	5.25	127.27	120.44
1	E	356	ALA	C-N-CA	5.25	127.27	120.44
1	A	388	GLY	N-CA-C	5.23	117.38	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	GLU	CA-C-N	5.20	128.91	120.60
1	C	334	GLU	C-N-CA	5.20	128.91	120.60
1	E	334	GLU	CA-C-N	5.17	128.87	120.60
1	E	334	GLU	C-N-CA	5.17	128.87	120.60
1	B	444	ASP	CA-CB-CG	5.12	117.72	112.60
1	F	924	ASP	CA-C-N	5.10	127.12	120.28
1	F	924	ASP	C-N-CA	5.10	127.12	120.28
1	B	879	VAL	N-CA-CB	5.05	116.35	110.65
1	C	356	ALA	CA-C-N	5.02	126.96	120.44
1	C	356	ALA	C-N-CA	5.02	126.96	120.44
1	D	356	ALA	CA-C-N	5.00	126.94	120.44
1	D	356	ALA	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2734	0	2668	13	0
1	B	2738	0	2646	15	0
1	C	2666	0	2588	13	0
1	D	2646	0	2565	21	0
1	E	2569	0	2501	18	0
1	F	2591	0	2525	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	250	0	0	0	0
4	B	232	0	0	1	0
4	C	204	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	214	0	0	1	0
4	E	166	0	0	1	0
4	F	183	0	0	2	0
All	All	17209	0	15493	90	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 3.

All (90) 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:D:311:CME:SD	1:D:311:CME:SG	2.32	1.28
1:B:311:CME:SD	1:B:311:CME:SG	2.42	1.16
1:A:877:MET:HE2	1:B:369:HIS:HB2	1.28	1.14
1:C:311:CME:HZ3	1:C:392:GLN:HB2	1.30	1.11
1:C:309:ASN:OD1	1:C:311:CME:HE2	1.75	0.85
1:C:311:CME:CZ	1:C:392:GLN:HB2	2.09	0.82
1:D:347:MET:HE2	1:D:351:ILE:HG13	1.64	0.79
1:B:912:THR:HG22	1:B:914:ALA:H	1.49	0.76
1:B:347:MET:HE1	1:B:404:GLY:HA2	1.68	0.75
1:C:311:CME:HZ3	1:C:392:GLN:CB	2.15	0.73
1:E:347:MET:HE1	1:E:404:GLY:HA2	1.70	0.72
1:E:309:ASN:OD1	1:E:311:CME:HE2	1.91	0.70
1:C:313:MET:HA	1:C:397:LEU:HD22	1.73	0.70
1:E:313:MET:HA	1:E:397:LEU:HD22	1.74	0.69
1:F:313:MET:HA	1:F:397:LEU:HD22	1.74	0.68
1:A:819:LYS:HE3	1:A:921:GLN:HE21	1.60	0.65
1:D:313:MET:HA	1:D:397:LEU:HD22	1.79	0.64
1:B:311:CME:HE2	1:B:392:GLN:HB2	1.79	0.64
1:F:813:ASP:HB3	1:F:856:CYS:SG	2.39	0.63
1:E:862:PRO:HD2	1:E:928:TYR:CD1	2.33	0.63
1:A:313:MET:HA	1:A:397:LEU:HD22	1.82	0.62
1:A:311:CME:HE2	1:A:312:PHE:HB3	1.81	0.61
1:E:395:GLN:HG3	1:E:824:HIS:CD2	2.37	0.59
1:C:313:MET:HA	1:C:397:LEU:CD2	2.32	0.59
1:B:912:THR:HG21	4:B:2209:HOH:O	2.02	0.59
1:F:888:ASN:HD22	1:F:891:ASN:H	1.53	0.56
1:D:395:GLN:HG3	1:D:824:HIS:CD2	2.40	0.56
1:B:374:MET:HE1	1:C:373:ARG:HB2	1.89	0.55
1:F:423:ALA:CB	1:F:431:VAL:HG22	2.37	0.55
1:D:347:MET:HG3	1:D:351:ILE:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:907:GLU:HA	1:D:910:ILE:HD12	1.90	0.54
1:E:395:GLN:HG3	1:E:824:HIS:CG	2.42	0.54
1:E:392:GLN:HG3	4:E:2048:HOH:O	2.07	0.54
1:D:311:CME:HZ3	1:D:392:GLN:HB2	1.91	0.53
1:B:837:LYS:NZ	1:B:873:HIS:HD2	2.07	0.53
1:F:448:VAL:HA	1:F:452:HIS:ND1	2.24	0.53
1:F:347:MET:HG3	1:F:351:ILE:CG1	2.39	0.53
1:E:311:CME:HZ3	1:E:392:GLN:CB	2.39	0.52
1:D:395:GLN:HG3	1:D:824:HIS:CG	2.44	0.51
1:A:877:MET:CE	1:B:369:HIS:HB2	2.21	0.51
1:F:887:LYS:NZ	4:F:2144:HOH:O	2.44	0.50
1:C:805:HIS:H	1:C:805:HIS:CD2	2.29	0.49
1:E:886:ALA:HB3	1:E:897:PHE:CE1	2.48	0.49
1:A:828:PHE:CD1	1:A:835[B]:ARG:HD3	2.47	0.49
1:A:795:ASP:N	1:A:796:PRO:HD3	2.28	0.49
1:C:423:ALA:HB2	1:C:431:VAL:HG11	1.96	0.48
1:B:861:ARG:HB3	1:B:930:THR:HG22	1.96	0.48
1:E:461:CYS:SG	1:E:464:CYS:HB3	2.52	0.48
1:C:336:GLU:HB2	4:C:2020:HOH:O	2.13	0.48
1:A:423:ALA:HA	1:A:426:ARG:HH11	1.79	0.47
1:B:388:GLY:HA3	1:B:390:GLN:OE1	2.14	0.47
1:B:395:GLN:HG2	1:B:824:HIS:CE1	2.50	0.47
1:E:311:CME:HZ2	1:E:882:TYR:CE1	2.49	0.47
1:D:309:ASN:OD1	1:D:311:CME:HE2	2.15	0.47
1:A:783:GLU:O	1:A:787:THR:HG23	2.15	0.46
1:C:296:HIS:CD2	1:C:297:ILE:HD12	2.51	0.46
1:A:877:MET:HE1	1:B:305:GLY:N	2.31	0.46
1:F:907:GLU:HA	1:F:910:ILE:HD12	1.96	0.46
1:D:311:CME:SD	1:D:312:PHE:N	2.85	0.45
1:F:413:LYS:NZ	4:F:2064:HOH:O	2.48	0.45
1:D:311:CME:HZ2	1:D:882:TYR:HE1	1.81	0.45
1:F:460:VAL:HG13	1:F:809:THR:OG1	2.16	0.45
1:D:865:TYR:HB3	1:D:920:TYR:HB3	1.99	0.44
1:F:865:TYR:HB3	1:F:920:TYR:HB3	1.98	0.44
1:A:426:ARG:HH22	1:A:434:GLU:CD	2.26	0.44
1:F:347:MET:HG3	1:F:351:ILE:HG12	1.99	0.43
1:D:454:LEU:HB2	1:D:816:SER:OG	2.17	0.43
1:E:311:CME:HZ2	1:E:882:TYR:HE1	1.82	0.43
1:E:865:TYR:CE2	1:E:922:ARG:HB2	2.54	0.43
1:E:865:TYR:HB3	1:E:920:TYR:HB3	2.00	0.43
1:B:791:LEU:HD21	1:B:810:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:CME:SD	1:C:312:PHE:N	2.89	0.42
1:D:336:GLU:HB2	4:D:2018:HOH:O	2.19	0.42
1:C:861:ARG:NH1	1:C:862:PRO:O	2.53	0.42
1:F:395:GLN:HG2	1:F:824:HIS:CE1	2.54	0.42
1:A:423:ALA:HA	1:A:426:ARG:HD3	2.02	0.42
1:D:347:MET:HG3	1:D:351:ILE:HG12	2.01	0.42
1:D:861:ARG:NH1	1:D:862:PRO:O	2.53	0.42
1:E:311:CME:HZ3	1:E:392:GLN:HB2	2.02	0.42
1:A:480:PRO:HG2	1:A:784:LEU:HD13	2.02	0.41
1:D:311:CME:HZ3	1:D:392:GLN:H	1.84	0.41
1:E:311:CME:HZ3	1:E:392:GLN:HB3	2.02	0.41
1:E:312:PHE:CD2	1:E:392:GLN:HG2	2.55	0.41
1:D:452:HIS:CD2	1:D:475:CYS:HB3	2.56	0.41
1:D:359:ILE:HA	1:D:359:ILE:HD13	1.80	0.41
1:D:311:CME:HZ2	1:D:882:TYR:CE1	2.57	0.40
1:D:861:ARG:NH1	1:D:922:ARG:HD2	2.37	0.40
1:F:423:ALA:CB	1:F:431:VAL:CG2	3.00	0.40
1:B:796:PRO:HG2	1:B:805:HIS:HB3	2.03	0.40
1:E:312:PHE:CG	1:E:392:GLN:HG2	2.57	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	331/367 (90%)	324 (98%)	7 (2%)	0	100	100
1	B	332/367 (90%)	322 (97%)	10 (3%)	0	100	100
1	C	322/367 (88%)	316 (98%)	6 (2%)	0	100	100
1	D	315/367 (86%)	307 (98%)	7 (2%)	1 (0%)	36	50
1	E	310/367 (84%)	303 (98%)	6 (2%)	1 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	314/367 (86%)	309 (98%)	5 (2%)	0	100	100
All	All	1924/2202 (87%)	1881 (98%)	41 (2%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	925	ASP
1	D	826	LYS

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	294/321 (92%)	284 (97%)	10 (3%)	32	54
1	B	293/321 (91%)	288 (98%)	5 (2%)	53	74
1	C	285/321 (89%)	279 (98%)	6 (2%)	47	69
1	D	283/321 (88%)	270 (95%)	13 (5%)	24	41
1	E	274/321 (85%)	270 (98%)	4 (2%)	57	77
1	F	277/321 (86%)	269 (97%)	8 (3%)	37	60
All	All	1706/1926 (89%)	1660 (97%)	46 (3%)	39	62

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	MET
1	A	418	LEU
1	A	419	GLU
1	A	420	LEU
1	A	472	ASP
1	A	783	GLU
1	A	784	LEU
1	A	789	GLU
1	A	900	SER

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Mol	Chain	Res	Type
1	A	925	ASP
1	B	397	LEU
1	B	783	GLU
1	B	847	ARG
1	B	879	VAL
1	B	925	ASP
1	C	783	GLU
1	C	797	TRP
1	C	805	HIS
1	C	806	GLN
1	C	847	ARG
1	C	858	LEU
1	D	347	MET
1	D	358	LEU
1	D	359	ILE
1	D	369	HIS
1	D	457	SER
1	D	459	LEU
1	D	461	CYS
1	D	783	GLU
1	D	803	LYS
1	D	826	LYS
1	D	877	MET
1	D	925	ASP
1	D	926	GLU
1	E	347	MET
1	E	783	GLU
1	E	926	GLU
1	E	929	LYS
1	F	296	HIS
1	F	347	MET
1	F	422	ASP
1	F	460	VAL
1	F	483	LEU
1	F	783	GLU
1	F	858	LEU
1	F	906	SER

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	361	GLN

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	921	GLN
1	B	361	GLN
1	B	857	ASN
1	B	873	HIS
1	B	901	ASN
1	C	296	HIS
1	C	361	GLN
1	C	805	HIS
1	C	872	ASN
1	D	322	ASN
1	D	361	GLN
1	D	391	GLN
1	D	901	ASN
1	E	361	GLN
1	E	857	ASN
1	F	296	HIS
1	F	361	GLN
1	F	391	GLN
1	F	807	GLN
1	F	872	ASN
1	F	888	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	B	311	1	8,9,10	2.03	1 (12%)	6,9,11	3.78	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	D	311	1	8,9,10	1.59	1 (12%)	6,9,11	2.16	2 (33%)
1	CME	C	311	1	8,9,10	1.32	1 (12%)	6,9,11	2.36	3 (50%)
1	CME	E	311	1	8,9,10	1.27	1 (12%)	6,9,11	2.03	1 (16%)
1	CME	F	311	1	8,9,10	0.91	0	6,9,11	1.95	2 (33%)
1	CME	A	311	1	8,9,10	1.33	1 (12%)	6,9,11	2.78	3 (50%)

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
1	CME	B	311	1	-	3/5/8/10	-
1	CME	D	311	1	-	3/5/8/10	-
1	CME	C	311	1	-	4/5/8/10	-
1	CME	E	311	1	-	3/5/8/10	-
1	CME	F	311	1	-	4/5/8/10	-
1	CME	A	311	1	-	2/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	CME	SD-SG	5.48	2.42	2.03
1	D	311	CME	SD-SG	4.06	2.32	2.03
1	A	311	CME	SD-SG	3.32	2.27	2.03
1	C	311	CME	SD-SG	3.20	2.26	2.03
1	E	311	CME	SD-SG	3.10	2.25	2.03

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	CME	CE-SD-SG	7.29	135.46	103.46
1	A	311	CME	CE-SD-SG	5.11	125.91	103.46
1	B	311	CME	CB-SG-SD	4.81	116.30	103.86
1	E	311	CME	CB-SG-SD	4.63	115.85	103.86
1	C	311	CME	CB-CA-C	3.92	121.45	110.80
1	D	311	CME	CB-SG-SD	3.92	114.00	103.86
1	F	311	CME	CB-SG-SD	3.58	113.12	103.86
1	A	311	CME	CB-CA-C	3.34	119.86	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	311	CME	CB-CA-C	2.99	118.91	110.80
1	C	311	CME	CB-SG-SD	2.70	110.84	103.86
1	C	311	CME	OH-CZ-CE	2.68	121.29	110.82
1	B	311	CME	OH-CZ-CE	-2.49	101.10	110.82
1	A	311	CME	CB-SG-SD	2.32	109.86	103.86
1	D	311	CME	CE-SD-SG	2.10	112.68	103.46

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	311	CME	CE-SD-SG-CB
1	B	311	CME	CZ-CE-SD-SG
1	D	311	CME	CA-CB-SG-SD
1	E	311	CME	CA-CB-SG-SD
1	B	311	CME	CE-SD-SG-CB
1	C	311	CME	CE-SD-SG-CB
1	D	311	CME	CE-SD-SG-CB
1	F	311	CME	CE-SD-SG-CB
1	B	311	CME	CA-CB-SG-SD
1	C	311	CME	CA-CB-SG-SD
1	F	311	CME	CA-CB-SG-SD
1	A	311	CME	CA-CB-SG-SD
1	E	311	CME	CE-SD-SG-CB
1	C	311	CME	SD-CE-CZ-OH
1	F	311	CME	SD-CE-CZ-OH
1	C	311	CME	CZ-CE-SD-SG
1	E	311	CME	CZ-CE-SD-SG
1	D	311	CME	CZ-CE-SD-SG
1	F	311	CME	CZ-CE-SD-SG

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	311	CME	2	0
1	D	311	CME	7	0
1	C	311	CME	5	0
1	E	311	CME	6	0
1	A	311	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	SO4	A	1926	-	4,4,4	0.50	0	6,6,6	0.22	0
3	SO4	C	1925	-	4,4,4	0.47	0	6,6,6	0.17	0

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	336/367 (91%)	-0.21	16 (4%)	35	32	14, 39, 116, 140	1 (0%)
1	B	338/367 (92%)	-0.19	14 (4%)	41	37	23, 40, 103, 125	0
1	C	330/367 (89%)	-0.04	19 (5%)	29	25	24, 45, 103, 152	0
1	D	327/367 (89%)	0.07	25 (7%)	20	16	26, 45, 119, 265	0
1	E	318/367 (86%)	-0.03	15 (4%)	36	32	29, 46, 96, 139	0
1	F	322/367 (87%)	0.09	18 (5%)	30	26	26, 49, 94, 145	0
All	All	1971/2202 (89%)	-0.05	107 (5%)	31	28	14, 45, 103, 265	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	928	TYR	6.8
1	B	878	GLY	5.8
1	D	791	LEU	5.5
1	F	420	LEU	5.5
1	C	483	LEU	5.2
1	B	877	MET	4.9
1	D	423	ALA	4.7
1	F	877	MET	4.6
1	D	797	TRP	4.6
1	A	418	LEU	4.3
1	D	462	PRO	4.2
1	D	467	VAL	4.2
1	F	926	GLU	4.1
1	A	420	LEU	4.0
1	D	417	TYR	4.0
1	D	877	MET	4.0
1	C	791	LEU	3.7
1	E	806	GLN	3.7
1	C	924	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	796	PRO	3.6
1	B	929	LYS	3.5
1	E	483	LEU	3.5
1	C	797	TRP	3.5
1	D	927	PHE	3.4
1	C	423	ALA	3.4
1	E	417	TYR	3.4
1	B	930	THR	3.3
1	B	296	HIS	3.3
1	F	423	ALA	3.3
1	A	483	LEU	3.2
1	D	803	LYS	3.2
1	D	465	ALA	3.2
1	D	483	LEU	3.2
1	F	878	GLY	3.1
1	A	859	SER	3.1
1	D	805	HIS	3.1
1	C	774	THR	3.0
1	C	417	TYR	3.0
1	E	455	PHE	3.0
1	A	417	TYR	2.9
1	E	789	GLU	2.9
1	F	858	LEU	2.9
1	E	807	GLN	2.9
1	F	484	LYS	2.9
1	D	925	ASP	2.9
1	E	929	LYS	2.9
1	F	416	PRO	2.9
1	B	483	LEU	2.9
1	B	876	ALA	2.8
1	F	465	ALA	2.8
1	A	423	ALA	2.8
1	D	461	CYS	2.8
1	D	468	SER	2.7
1	E	467	VAL	2.7
1	E	858	LEU	2.7
1	C	775	THR	2.7
1	B	422	ASP	2.7
1	C	798	TYR	2.7
1	D	774	THR	2.7
1	C	807	GLN	2.7
1	F	483	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	791	LEU	2.6
1	D	804	LYS	2.6
1	A	465	ALA	2.6
1	E	465	ALA	2.6
1	D	798	TYR	2.6
1	F	876	ALA	2.6
1	F	389	TYR	2.5
1	C	296	HIS	2.5
1	C	808	ALA	2.5
1	E	425	GLY	2.5
1	F	424	ASN	2.4
1	E	808	ALA	2.4
1	F	808	ALA	2.4
1	D	787	THR	2.4
1	A	415	LYS	2.3
1	C	856	CYS	2.3
1	D	808	ALA	2.3
1	D	369	HIS	2.3
1	A	297	ILE	2.3
1	A	801	ASN	2.2
1	F	775	THR	2.2
1	C	858	LEU	2.2
1	F	421	LYS	2.2
1	A	793	GLU	2.2
1	F	856	CYS	2.2
1	A	421	LYS	2.2
1	A	422	ASP	2.2
1	A	877	MET	2.2
1	C	800	PRO	2.2
1	C	369	HIS	2.2
1	B	858	LEU	2.2
1	E	389	TYR	2.2
1	E	810	LYS	2.1
1	D	890	LEU	2.1
1	A	467	VAL	2.1
1	B	879	VAL	2.1
1	B	792	GLY	2.1
1	D	365	GLY	2.1
1	B	787	THR	2.1
1	A	803	LYS	2.1
1	C	801	ASN	2.0
1	B	925	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	422	ASP	2.0
1	D	800	PRO	2.0
1	B	791	LEU	2.0
1	D	297	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	D	311	10/11	0.86	0.16	31,37,53,53	0
1	CME	A	311	10/11	0.88	0.16	27,32,45,47	0
1	CME	C	311	10/11	0.89	0.15	38,41,58,59	0
1	CME	B	311	10/11	0.90	0.13	23,28,44,44	0
1	CME	F	311	10/11	0.90	0.15	35,43,66,68	0
1	CME	E	311	10/11	0.91	0.15	32,37,56,58	0

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
3	SO4	C	1925	5/5	0.83	0.23	118,121,122,125	0
2	ZN	E	1000	1/1	0.85	0.14	123,123,123,123	0
2	ZN	F	1000	1/1	0.86	0.10	99,99,99,99	0
2	ZN	D	1000	1/1	0.87	0.08	162,162,162,162	0
3	SO4	A	1926	5/5	0.89	0.14	100,104,105,105	0
2	ZN	A	1000	1/1	0.96	0.07	159,159,159,159	0
2	ZN	C	1000	1/1	0.97	0.05	103,103,103,103	0
2	ZN	B	1000	1/1	0.99	0.04	88,88,88,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.