



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 AM UTC

PDB ID : 5KNL / pdb_00005knl
Title : Crystal structure of *S. pombe* ubiquitin E1 (Uba1) in complex with Ubc15 and ubiquitin
Authors : Olsen, S.K.; Lv, Z.; Yuan, L.; Williams, K.
Deposited on : 2016-06-28
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
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

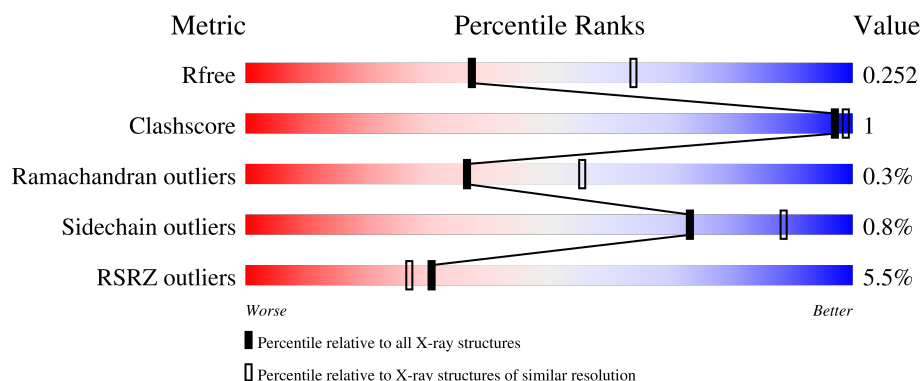
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	1001	5% 95% ..
1	D	1001	6% 95% ..
2	B	96	2% 73% 5% . 21%
2	E	96	4% 77% . 21%
3	C	175	5% 91% 6% ..

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Mol	Chain	Length	Quality of chain
3	F	175	7% 89% • • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38561 atoms, of which 19138 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-activating enzyme E1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	981	Total	C	H	N	O	S	0	0	0
			15342	4926	7637	1259	1481	39			
1	D	977	Total	C	H	N	O	S	0	0	0
			15280	4907	7607	1254	1473	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	expression tag	UNP O94609
D	12	SER	-	expression tag	UNP O94609

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	76	Total	C	H	N	O	S	0	0	0
			1236	375	623	119	118	1			
2	E	76	Total	C	H	N	O	S	0	0	0
			1236	375	623	119	118	1			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP A0A081CFF0
B	-18	GLY	-	expression tag	UNP A0A081CFF0
B	-17	SER	-	expression tag	UNP A0A081CFF0
B	-16	SER	-	expression tag	UNP A0A081CFF0
B	-15	HIS	-	expression tag	UNP A0A081CFF0
B	-14	HIS	-	expression tag	UNP A0A081CFF0
B	-13	HIS	-	expression tag	UNP A0A081CFF0
B	-12	HIS	-	expression tag	UNP A0A081CFF0
B	-11	HIS	-	expression tag	UNP A0A081CFF0
B	-10	HIS	-	expression tag	UNP A0A081CFF0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	expression tag	UNP A0A081CFF0
B	-8	SER	-	expression tag	UNP A0A081CFF0
B	-7	GLY	-	expression tag	UNP A0A081CFF0
B	-6	LEU	-	expression tag	UNP A0A081CFF0
B	-5	VAL	-	expression tag	UNP A0A081CFF0
B	-4	PRO	-	expression tag	UNP A0A081CFF0
B	-3	ARG	-	expression tag	UNP A0A081CFF0
B	-2	GLY	-	expression tag	UNP A0A081CFF0
B	-1	SER	-	expression tag	UNP A0A081CFF0
B	0	HIS	-	expression tag	UNP A0A081CFF0
B	6	ARG	LYS	engineered mutation	UNP A0A081CFF0
B	11	ARG	LYS	engineered mutation	UNP A0A081CFF0
B	27	ARG	LYS	engineered mutation	UNP A0A081CFF0
B	29	ARG	LYS	engineered mutation	UNP A0A081CFF0
B	33	ARG	LYS	engineered mutation	UNP A0A081CFF0
B	48	ARG	LYS	engineered mutation	UNP A0A081CFF0
B	57	ALA	SER	engineered mutation	UNP A0A081CFF0
B	63	ARG	LYS	engineered mutation	UNP A0A081CFF0
E	-19	MET	-	initiating methionine	UNP A0A081CFF0
E	-18	GLY	-	expression tag	UNP A0A081CFF0
E	-17	SER	-	expression tag	UNP A0A081CFF0
E	-16	SER	-	expression tag	UNP A0A081CFF0
E	-15	HIS	-	expression tag	UNP A0A081CFF0
E	-14	HIS	-	expression tag	UNP A0A081CFF0
E	-13	HIS	-	expression tag	UNP A0A081CFF0
E	-12	HIS	-	expression tag	UNP A0A081CFF0
E	-11	HIS	-	expression tag	UNP A0A081CFF0
E	-10	HIS	-	expression tag	UNP A0A081CFF0
E	-9	SER	-	expression tag	UNP A0A081CFF0
E	-8	SER	-	expression tag	UNP A0A081CFF0
E	-7	GLY	-	expression tag	UNP A0A081CFF0
E	-6	LEU	-	expression tag	UNP A0A081CFF0
E	-5	VAL	-	expression tag	UNP A0A081CFF0
E	-4	PRO	-	expression tag	UNP A0A081CFF0
E	-3	ARG	-	expression tag	UNP A0A081CFF0
E	-2	GLY	-	expression tag	UNP A0A081CFF0
E	-1	SER	-	expression tag	UNP A0A081CFF0
E	0	HIS	-	expression tag	UNP A0A081CFF0
E	6	ARG	LYS	engineered mutation	UNP A0A081CFF0
E	11	ARG	LYS	engineered mutation	UNP A0A081CFF0
E	27	ARG	LYS	engineered mutation	UNP A0A081CFF0
E	29	ARG	LYS	engineered mutation	UNP A0A081CFF0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	33	ARG	LYS	engineered mutation	UNP A0A081CFF0
E	48	ARG	LYS	engineered mutation	UNP A0A081CFF0
E	57	ALA	SER	engineered mutation	UNP A0A081CFF0
E	63	ARG	LYS	engineered mutation	UNP A0A081CFF0

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 15.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	171	Total	C	H	N	O	S	0	0	0
			2718	877	1346	230	258	7			
3	F	162	Total	C	H	N	O	S	0	1	0
			2610	840	1302	222	239	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	168	LEU	-	expression tag	UNP Q9Y818
C	169	GLU	-	expression tag	UNP Q9Y818
C	170	HIS	-	expression tag	UNP Q9Y818
C	171	HIS	-	expression tag	UNP Q9Y818
C	172	HIS	-	expression tag	UNP Q9Y818
C	173	HIS	-	expression tag	UNP Q9Y818
C	174	HIS	-	expression tag	UNP Q9Y818
C	175	HIS	-	expression tag	UNP Q9Y818
F	168	LEU	-	expression tag	UNP Q9Y818
F	169	GLU	-	expression tag	UNP Q9Y818
F	170	HIS	-	expression tag	UNP Q9Y818
F	171	HIS	-	expression tag	UNP Q9Y818
F	172	HIS	-	expression tag	UNP Q9Y818
F	173	HIS	-	expression tag	UNP Q9Y818
F	174	HIS	-	expression tag	UNP Q9Y818
F	175	HIS	-	expression tag	UNP Q9Y818

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	7	Total	O	0	0
			7	7		
5	C	6	Total	O	0	0
			6	6		

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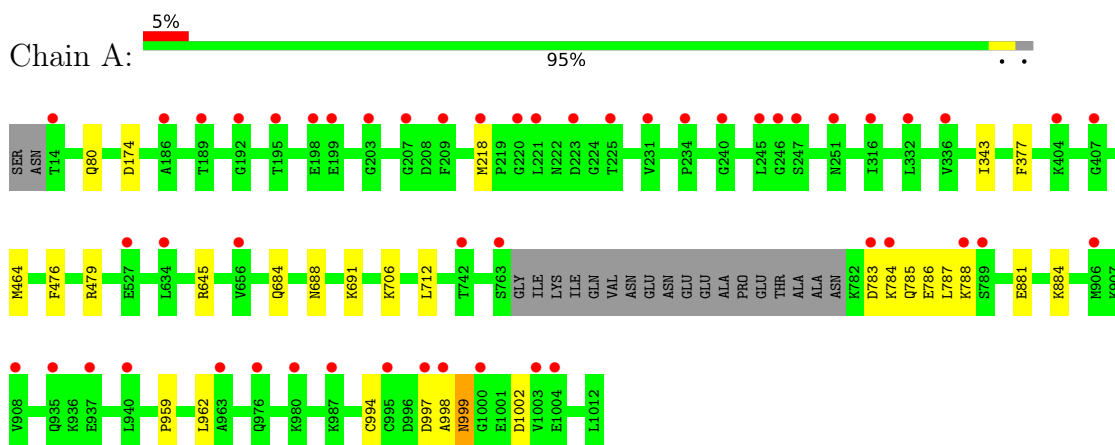
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	46	Total 46	O 46	0	0
5	E	2	Total 2	O 2	0	0
5	F	1	Total 1	O 1	0	0

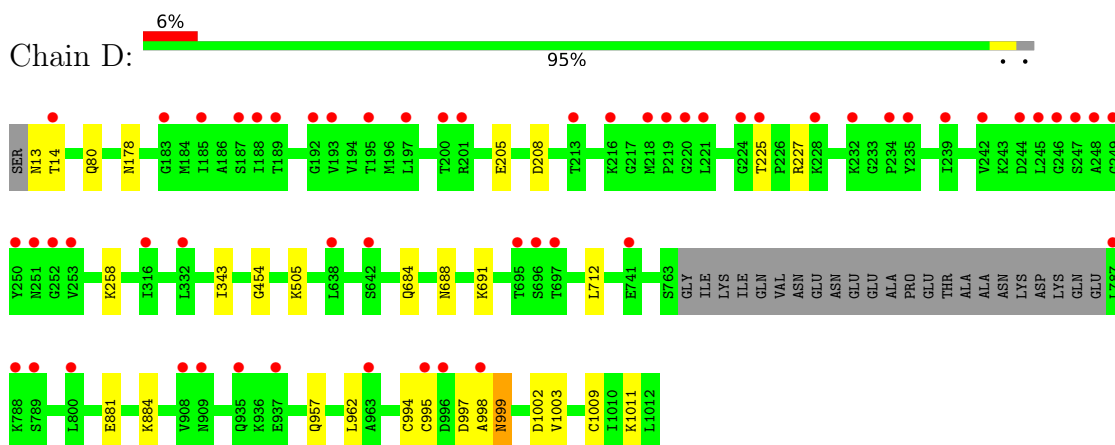
3 Residue-property plots [i](#)

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.

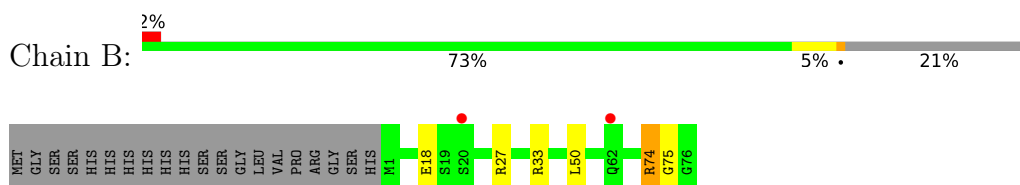
- Molecule 1: Ubiquitin-activating enzyme E1 1



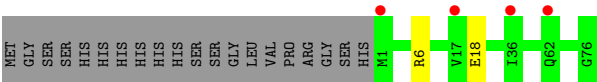
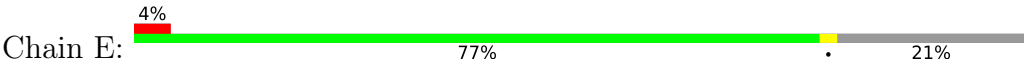
- Molecule 1: Ubiquitin-activating enzyme E1 1



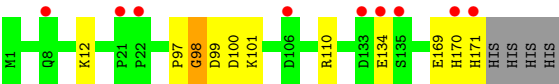
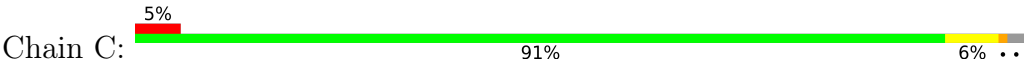
- Molecule 2: Ubiquitin



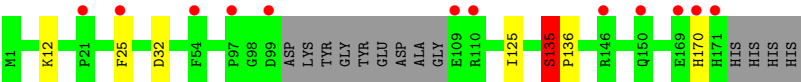
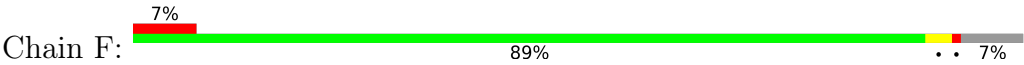
- Molecule 2: Ubiquitin



• Molecule 3: Ubiquitin-conjugating enzyme E2 15



• Molecule 3: Ubiquitin-conjugating enzyme E2 15



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.11Å 82.24Å 135.38Å 102.10° 95.78° 90.86°	Depositor
Resolution (Å)	28.31 – 2.50 28.31 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (28.31-2.50) 96.8 (28.31-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.216 , 0.251 0.219 , 0.252	Depositor DCC
R_{free} test set	10829 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	38561	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: 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	0.30	0/7876	0.62	0/10660
1	D	0.29	0/7844	0.61	0/10618
2	B	0.29	0/618	0.61	0/831
2	E	0.30	0/618	0.59	0/831
3	C	0.30	0/1411	0.66	0/1915
3	F	0.31	0/1348	0.73	3/1829 (0.2%)
All	All	0.29	0/19715	0.63	3/26684 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	135	SER	CA-C-N	5.87	141.09	127.00
3	F	135	SER	C-N-CA	5.87	141.09	127.00
3	F	135	SER	C-N-CD	-5.85	107.73	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	135	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7705	7637	7634	12	0
1	D	7673	7607	7607	13	0
2	B	613	623	625	3	0
2	E	613	623	625	1	0
3	C	1372	1346	1341	6	0
3	F	1308	1302	1298	4	0
4	A	20	0	0	0	0
4	B	5	0	0	1	0
4	D	15	0	0	0	0
4	F	5	0	0	0	0
5	A	32	0	0	0	0
5	B	7	0	0	0	0
5	C	6	0	0	0	0
5	D	46	0	0	0	0
5	E	2	0	0	1	0
5	F	1	0	0	0	0
All	All	19423	19138	19130	35	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 1.

All (35) 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:684:GLN:O	1:D:688:ASN:ND2	2.32	0.61
2:B:33:ARG:NH1	4:B:101:SO4:O3	2.36	0.59
1:D:1009:CYS:SG	1:D:1011:LYS:NZ	2.68	0.57
1:D:13:ASN:OD1	1:D:14:THR:N	2.37	0.57
1:A:997:ASP:O	1:A:999:ASN:N	2.40	0.55
1:D:997:ASP:O	1:D:999:ASN:N	2.40	0.54
1:D:225:THR:O	1:D:227:ARG:NH1	2.41	0.54
1:A:684:GLN:O	1:A:688:ASN:ND2	2.41	0.51
3:F:135:SER:HB3	3:F:136:PRO:HA	1.94	0.49
1:D:178:ASN:O	1:D:258:LYS:NZ	2.43	0.49
1:D:994:CYS:SG	3:F:12:LYS:NZ	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:GLN:O	1:A:787:LEU:N	2.45	0.48
3:C:98:GLY:O	3:C:110:ARG:NH1	2.47	0.48
1:A:783:ASP:OD1	1:A:783:ASP:N	2.47	0.47
1:D:957:GLN:NE2	3:F:32:ASP:OD2	2.48	0.47
3:F:25:PHE:HZ	3:F:125:ILE:HG12	1.81	0.46
2:B:27:ARG:NH2	2:B:50:LEU:O	2.48	0.45
1:A:994:CYS:SG	3:C:12:LYS:NZ	2.81	0.45
1:D:881:GLU:O	1:D:884:LYS:NZ	2.50	0.44
2:E:6:ARG:NH1	5:E:101:HOH:O	2.46	0.44
3:C:169:GLU:O	3:C:171:HIS:N	2.50	0.44
1:A:645:ARG:HG3	1:A:788:LYS:CE	2.48	0.44
1:A:706:LYS:NZ	3:C:134:GLU:O	2.33	0.43
1:A:783:ASP:HA	1:A:784:LYS:C	2.43	0.43
1:D:995:CYS:O	1:D:1003:VAL:N	2.47	0.43
1:A:476:PHE:O	1:A:479:ARG:NH1	2.49	0.42
2:B:74:ARG:HD3	2:B:75:GLY:N	2.34	0.41
3:C:100:ASP:HB3	3:C:101:LYS:HA	2.02	0.41
1:D:454:GLY:O	1:D:505:LYS:NZ	2.49	0.41
1:A:959:PRO:HA	1:A:962:LEU:HB2	2.02	0.41
3:C:97:PRO:HA	3:C:98:GLY:HA2	1.87	0.41
1:A:174:ASP:O	1:A:377:PHE:N	2.42	0.40
1:D:957:GLN:HB2	1:D:962:LEU:HD11	2.03	0.40
1:A:881:GLU:O	1:A:884:LYS:NZ	2.55	0.40
1:D:205:GLU:N	1:D:208:ASP:OD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	977/1001 (98%)	923 (94%)	52 (5%)	2 (0%)	43 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	973/1001 (97%)	923 (95%)	49 (5%)	1 (0%)	48	68
2	B	74/96 (77%)	71 (96%)	3 (4%)	0	100	100
2	E	74/96 (77%)	71 (96%)	3 (4%)	0	100	100
3	C	169/175 (97%)	160 (95%)	6 (4%)	3 (2%)	6	12
3	F	159/175 (91%)	152 (96%)	5 (3%)	2 (1%)	9	18
All	All	2426/2544 (95%)	2300 (95%)	118 (5%)	8 (0%)	36	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	170	HIS
1	A	786	GLU
1	A	998	ALA
3	C	170	HIS
1	D	998	ALA
3	F	135	SER
3	C	99	ASP
3	C	98	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	860/877 (98%)	852 (99%)	8 (1%)	70	87
1	D	857/877 (98%)	851 (99%)	6 (1%)	76	89
2	B	67/84 (80%)	65 (97%)	2 (3%)	36	64
2	E	67/84 (80%)	66 (98%)	1 (2%)	57	80
3	C	154/160 (96%)	154 (100%)	0	100	100
3	F	149/160 (93%)	149 (100%)	0	100	100
All	All	2154/2242 (96%)	2137 (99%)	17 (1%)	73	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	218	MET
1	A	343	ILE
1	A	464	MET
1	A	691	LYS
1	A	712	LEU
1	A	999	ASN
1	A	1002	ASP
2	B	18	GLU
2	B	74	ARG
1	D	80	GLN
1	D	343	ILE
1	D	691	LYS
1	D	712	LEU
1	D	999	ASN
1	D	1002	ASP
2	E	18	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	735	ASN
1	A	999	ASN
1	D	122	ASN
1	D	684	GLN
1	D	735	ASN
2	E	68	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 [i](#)

9 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	$\# Z > 2$
4	SO4	D	1103	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	F	201	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	1103	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	B	101	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	1101	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	1101	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	D	1102	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	1102	-	4,4,4	0.24	0	6,6,6	0.05	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	101	SO4	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	981/1001 (98%)	0.15	51 (5%)	33 29	12, 48, 114, 175	0
1	D	977/1001 (97%)	0.15	56 (5%)	29 26	13, 48, 121, 203	0
2	B	76/96 (79%)	0.12	2 (2%)	57 52	24, 50, 95, 120	0
2	E	76/96 (79%)	0.30	4 (5%)	32 28	22, 66, 115, 154	0
3	C	171/175 (97%)	0.38	9 (5%)	32 28	25, 53, 107, 157	0
3	F	162/175 (92%)	0.56	12 (7%)	20 18	20, 63, 111, 162	2 (1%)
All	All	2443/2544 (96%)	0.20	134 (5%)	30 27	12, 50, 115, 203	2 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	LEU	7.2
1	D	250	TYR	5.8
1	D	193	VAL	5.8
3	F	99	ASP	5.1
1	A	14	THR	4.8
1	A	788	LYS	4.6
1	A	220	GLY	4.6
1	D	247	SER	4.5
3	C	170	HIS	4.5
3	F	25	PHE	4.3
3	C	21	PRO	4.3
1	D	219	PRO	4.2
1	D	249	GLY	4.2
1	D	185	ILE	4.1
1	A	247	SER	4.1
1	A	221	LEU	4.1
1	A	245	LEU	4.1
1	D	221	LEU	4.1
3	C	171	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	998	ALA	4.0
1	A	1003	VAL	3.9
3	C	135	SER	3.8
1	A	763	SER	3.8
1	A	656	VAL	3.7
1	A	209	PHE	3.7
3	F	21	PRO	3.7
1	D	935	GLN	3.5
1	D	234	PRO	3.5
1	D	14	THR	3.4
1	A	234	PRO	3.4
1	A	940	LEU	3.4
1	A	976	GLN	3.4
3	F	150	GLN	3.4
2	E	36	ILE	3.3
3	F	109	GLU	3.3
1	D	316	ILE	3.3
3	F	170	HIS	3.2
1	D	201	ARG	3.2
1	A	937	GLU	3.2
1	D	242	VAL	3.1
1	A	198	GLU	3.1
1	D	244	ASP	3.1
1	A	192	GLY	3.0
1	D	246	GLY	3.0
1	D	187	SER	3.0
2	E	62	GLN	3.0
1	D	200	THR	2.9
1	D	787	LEU	2.9
2	B	20	SER	2.9
1	D	789	SER	2.9
3	C	133	ASP	2.9
1	D	251	ASN	2.9
1	A	963	ALA	2.9
1	A	240	GLY	2.9
1	A	1000	GLY	2.9
1	D	248	ALA	2.8
1	A	1004	GLU	2.8
1	A	336	VAL	2.8
1	D	642	SER	2.7
1	A	997	ASP	2.7
1	D	252	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	188	ILE	2.7
1	A	404	LYS	2.7
1	D	908	VAL	2.7
1	D	224	GLY	2.6
1	D	239	ILE	2.6
3	F	97	PRO	2.6
1	A	908	VAL	2.6
1	A	783	ASP	2.6
2	B	62	GLN	2.6
1	A	527	GLU	2.6
1	D	253	VAL	2.6
1	D	696	SER	2.6
1	A	199	GLU	2.5
1	D	741	GLU	2.5
1	D	800	LEU	2.5
1	D	638	LEU	2.5
1	D	218	MET	2.5
1	A	203	GLY	2.5
1	A	998	ALA	2.5
1	D	195	THR	2.4
1	A	223	ASP	2.4
1	A	316	ILE	2.4
1	A	995	CYS	2.4
1	A	251	ASN	2.4
3	C	22	PRO	2.4
1	D	788	LYS	2.4
1	D	937	GLU	2.4
1	A	742	THR	2.3
1	A	784	LYS	2.3
1	A	332	LEU	2.3
3	C	134	GLU	2.3
1	D	695	THR	2.3
1	D	220	GLY	2.3
1	D	216	LYS	2.3
3	F	54	PHE	2.3
2	E	17	VAL	2.3
1	A	935	GLN	2.3
3	C	8	GLN	2.3
1	D	235	TYR	2.3
1	D	995	CYS	2.3
1	A	225	THR	2.2
3	C	106	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	189	THR	2.2
1	D	332	LEU	2.2
1	A	231	VAL	2.2
1	D	183	GLY	2.2
1	A	634	LEU	2.2
1	A	980	LYS	2.2
1	A	246	GLY	2.1
1	D	697	THR	2.1
1	D	996	ASP	2.1
1	A	186	ALA	2.1
1	D	909	ASN	2.1
1	A	195	THR	2.1
1	A	207	GLY	2.1
1	D	213	THR	2.1
3	F	146	ARG	2.1
1	A	987	LYS	2.1
1	A	218	MET	2.1
2	E	1	MET	2.1
1	D	963	ALA	2.1
1	D	225	THR	2.1
1	A	906	MET	2.1
3	F	171	HIS	2.1
1	A	407	GLY	2.1
1	A	189	THR	2.1
1	D	232	LYS	2.1
1	A	789	SER	2.1
1	D	228	LYS	2.0
3	F	110	ARG	2.0
1	D	197	LEU	2.0
3	F	169	GLU	2.0
1	D	192	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	F	201	5/5	0.69	0.17	129,129,130,131	0
4	SO4	B	101	5/5	0.76	0.09	99,100,101,101	0
4	SO4	D	1102	5/5	0.82	0.14	92,92,94,95	0
4	SO4	D	1101	5/5	0.90	0.11	55,56,60,61	0
4	SO4	A	1101	5/5	0.92	0.11	46,49,50,51	0
4	SO4	A	1103	5/5	0.95	0.09	49,51,51,53	0
4	SO4	A	1104	5/5	0.96	0.07	34,36,39,47	0
4	SO4	D	1103	5/5	0.97	0.06	37,39,44,44	0
4	SO4	A	1102	5/5	0.97	0.10	38,43,44,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.