



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:00 AM UTC

PDB ID : 6SQR / pdb_00006sqr
Title : Crystal structure of Cat MDM2-S429E RING domain bound to UbcH5B-Ub
Authors : Magnussen, H.M.; Ahmed, S.F.; Huang, D.T.
Deposited on : 2019-09-04
Resolution : 2.18 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

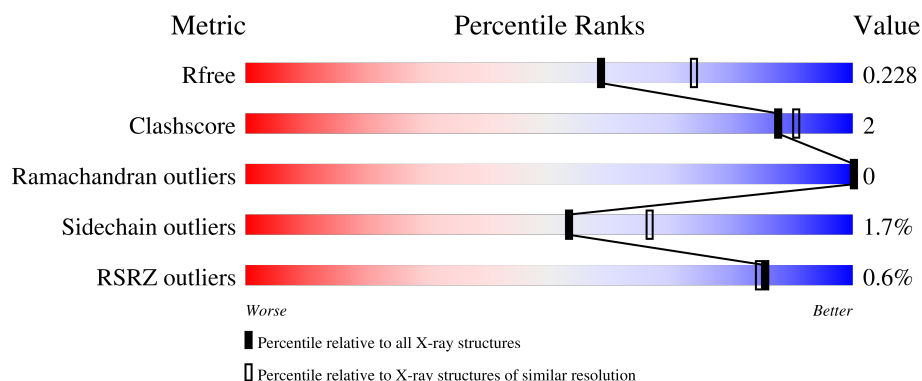
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

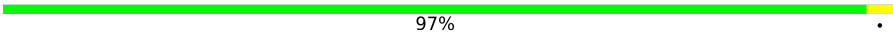
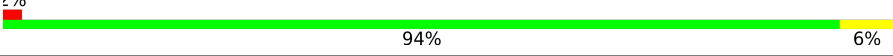
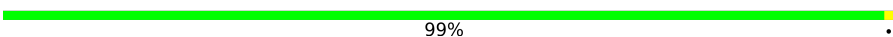
The reported resolution of this entry is 2.18 Å.

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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	69	 93% 7%
2	B	146	 97% .
2	E	146	 2% 94% 6%
2	H	146	 91% 9%
2	K	146	 99% .

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Mol	Chain	Length	Quality of chain
3	C	77	92% 8%
3	F	77	3% 84% 14%
3	L	77	97%
4	D	64	2% 91% 8%
4	J	64	2% 86% 12%
5	G	63	92% 8%
6	I	76	100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9560 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 E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			544	347	97	91	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	429	GLU	SER	engineered mutation	UNP Q7YRZ8
A	443	THR	GLY	engineered mutation	UNP Q7YRZ8

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1164	748	201	209	6			
2	E	146	Total	C	N	O	S	0	0	0
			1146	738	196	206	6			
2	H	146	Total	C	N	O	S	0	0	0
			1162	748	199	209	6			
2	K	146	Total	C	N	O	S	0	1	0
			1180	756	205	213	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ARG	SER	engineered mutation	UNP P62837
B	85	LYS	CYS	engineered mutation	UNP P62837
E	22	ARG	SER	engineered mutation	UNP P62837
E	85	LYS	CYS	engineered mutation	UNP P62837
H	22	ARG	SER	engineered mutation	UNP P62837
H	85	LYS	CYS	engineered mutation	UNP P62837
K	22	ARG	SER	engineered mutation	UNP P62837
K	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 3 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	77	Total	C	N	O	S	0	0	0
			586	370	100	115	1			
3	F	77	Total	C	N	O	S	0	1	0
			595	375	101	118	1			
3	L	77	Total	C	N	O	S	0	0	0
			603	378	105	119	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP J3QTR3
F	0	SER	-	expression tag	UNP J3QTR3
L	0	SER	-	expression tag	UNP J3QTR3

- Molecule 4 is a protein called E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	64	Total	C	N	O	S	0	0	0
			498	319	92	78	9			
4	J	64	Total	C	N	O	S	0	0	0
			498	319	92	78	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	429	GLU	SER	engineered mutation	UNP Q7YRZ8
D	443	THR	GLY	engineered mutation	UNP Q7YRZ8
J	429	GLU	SER	engineered mutation	UNP Q7YRZ8
J	443	THR	GLY	engineered mutation	UNP Q7YRZ8

- Molecule 5 is a protein called E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	63	Total	C	N	O	S	0	0	0
			495	316	91	79	9			

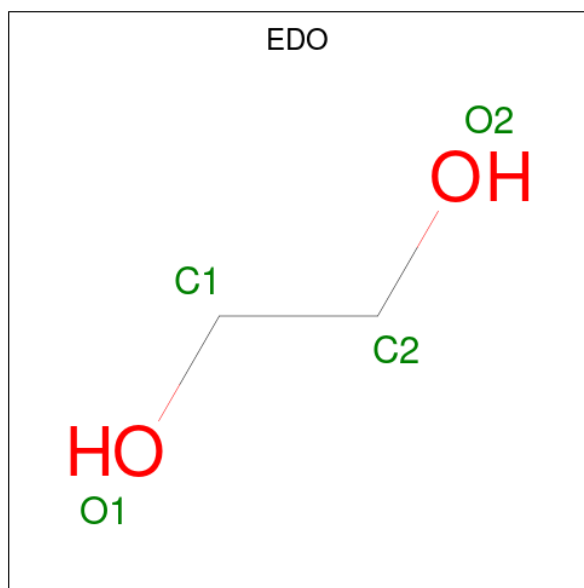
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	429	GLU	SER	engineered mutation	UNP Q7YRZ8
G	443	THR	GLY	engineered mutation	UNP Q7YRZ8

- Molecule 6 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		
7	K	1	Total	C	O	0	0
			4	2	2		

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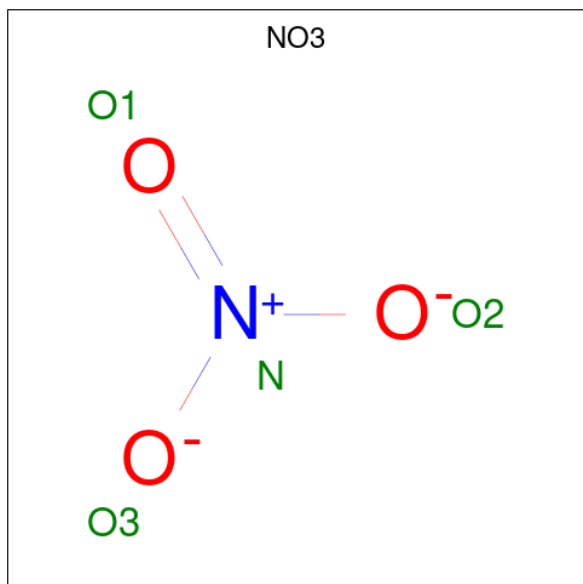
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	K	1	Total	C	O	0	0
			4	2	2		
7	K	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		
8	G	2	Total	Zn	0	0
			2	2		
8	J	2	Total	Zn	0	0
			2	2		

- Molecule 9 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	N	O	0	0
			4	1	3		
9	H	1	Total	N	O	0	0
			4	1	3		
9	I	1	Total	N	O	0	0
			4	1	3		

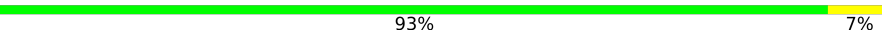
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	43	Total O 43 43	0	0
10	B	61	Total O 61 61	0	0
10	C	24	Total O 24 24	0	0
10	D	28	Total O 28 28	0	0
10	E	23	Total O 23 23	0	0
10	F	17	Total O 17 17	0	0
10	G	27	Total O 27 27	0	0
10	H	31	Total O 31 31	0	0
10	I	45	Total O 45 45	0	0
10	J	32	Total O 32 32	0	0
10	K	65	Total O 65 65	0	0
10	L	24	Total O 24 24	0	0

3 Residue-property plots [i](#)

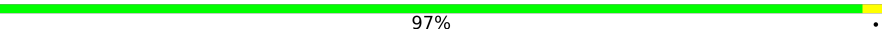
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: E3 ubiquitin-protein ligase Mdm2

Chain A:  93% 7%

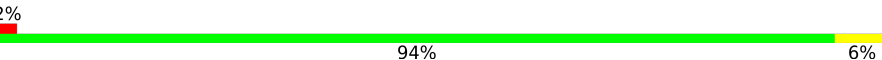


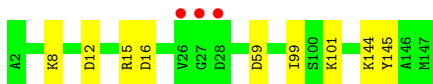
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain B:  97% .



- Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain E:  94% 6% 2%

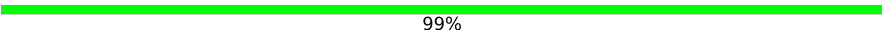


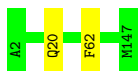
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain H:  91% 9%



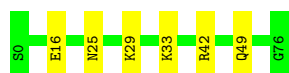
- Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain K:  99% .

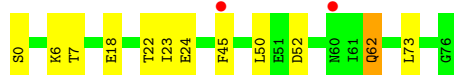
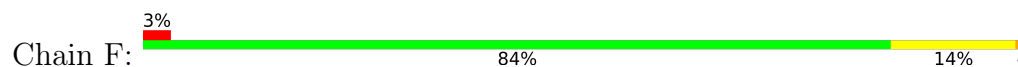


- Molecule 3: Ubiquitin-40S ribosomal protein S27a

Chain C:  92% 8%



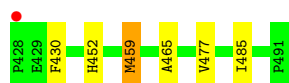
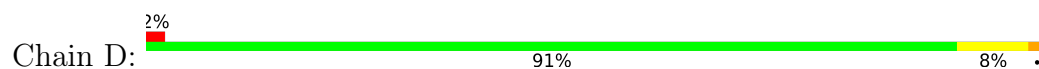
- Molecule 3: Ubiquitin-40S ribosomal protein S27a



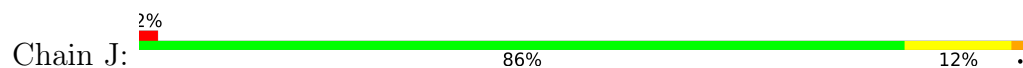
- Molecule 3: Ubiquitin-40S ribosomal protein S27a



- Molecule 4: E3 ubiquitin-protein ligase Mdm2



- Molecule 4: E3 ubiquitin-protein ligase Mdm2



- Molecule 5: E3 ubiquitin-protein ligase Mdm2



- Molecule 6: Polyubiquitin-C



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.51Å 163.88Å 70.60Å 90.00° 96.03° 90.00°	Depositor
Resolution (Å)	70.00 – 2.18 70.00 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.8 (70.00-2.18) 98.7 (70.00-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.166 , 0.227 0.168 , 0.228	Depositor DCC
R_{free} test set	3176 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9560	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: EDO, NO3, 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	0.35	0/558	0.54	0/753
2	B	0.35	0/1200	0.51	0/1637
2	E	0.25	0/1182	0.45	0/1616
2	H	0.29	0/1198	0.48	0/1634
2	K	0.32	0/1216	0.49	0/1657
3	C	0.33	0/592	0.47	0/799
3	F	0.24	0/604	0.44	0/815
3	L	0.29	0/609	0.47	0/820
4	D	0.48	1/512 (0.2%)	0.54	0/690
4	J	0.36	0/512	0.53	0/690
5	G	0.38	0/508	0.55	0/684
6	I	0.36	0/607	0.55	0/816
All	All	0.33	1/9298 (0.0%)	0.50	0/12611

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	430	PHE	C-N	8.10	1.52	1.33

There are no bond angle outliers.

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	544	0	557	2	0
2	B	1164	0	1141	3	0
2	E	1146	0	1109	8	0
2	H	1162	0	1141	7	0
2	K	1180	0	1160	1	0
3	C	586	0	598	2	0
3	F	595	0	608	8	0
3	L	603	0	623	0	0
4	D	498	0	516	3	0
4	J	498	0	516	6	0
5	G	495	0	512	3	0
6	I	601	0	629	0	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
7	D	8	0	12	0	0
7	G	8	0	12	0	0
7	I	4	0	6	0	0
7	J	8	0	12	0	0
7	K	12	0	18	0	0
8	A	2	0	0	0	0
8	D	2	0	0	0	0
8	G	2	0	0	0	0
8	J	2	0	0	0	0
9	D	4	0	0	0	0
9	H	4	0	0	0	0
9	I	4	0	0	0	0
10	A	43	0	0	0	0
10	B	61	0	0	0	0
10	C	24	0	0	0	0
10	D	28	0	0	0	0
10	E	23	0	0	1	0
10	F	17	0	0	0	0
10	G	27	0	0	0	0
10	H	31	0	0	0	0
10	I	45	0	0	0	0
10	J	32	0	0	0	0
10	K	65	0	0	0	0
10	L	24	0	0	0	0
All	All	9560	0	9182	37	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 2.

All (37) 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)
4:J:465:ALA:HB1	4:J:485:ILE:HD12	1.78	0.66
3:C:16:GLU:O	3:C:29:LYS:NZ	2.27	0.65
2:E:16:ASP:OD2	3:F:6:LYS:NZ	2.31	0.59
3:F:45:PHE:HB3	3:F:50:LEU:HD21	1.85	0.58
5:G:459:MET:HB3	4:J:491:PRO:HG2	1.87	0.57
3:F:23:ILE:HB	3:F:52:ASP:HA	1.88	0.55
4:D:459:MET:HE3	4:D:477:VAL:HG13	1.88	0.54
2:E:8:LYS:NZ	2:E:12:ASP:OD2	2.34	0.54
2:E:59:ASP:OD1	2:E:59:ASP:N	2.32	0.54
2:H:115:PRO:HB2	2:H:128:LYS:HD2	1.89	0.53
1:A:491:PRO:HD2	4:D:459:MET:HG3	1.92	0.51
3:F:24:GLU:HB2	3:F:52:ASP:HB3	1.92	0.50
2:H:59:ASP:OD1	2:H:59:ASP:N	2.42	0.49
3:F:0:SER:HB2	3:F:18:GLU:HG2	1.95	0.49
4:D:465:ALA:HB1	4:D:485:ILE:HD12	1.95	0.49
2:E:144:LYS:HD2	2:E:145:TYR:CE2	2.48	0.48
3:C:42:ARG:NH2	3:C:49:GLN:HG2	2.30	0.47
5:G:465:ALA:HB1	5:G:485:ILE:HD12	1.97	0.46
4:J:459:MET:HE3	4:J:477:VAL:HG13	1.98	0.46
2:H:17:PRO:HA	2:H:18:PRO:HD3	1.90	0.45
4:J:467:LYS:HE2	2:K:62:PHE:CE2	2.52	0.44
2:B:59:ASP:OD1	2:B:59:ASP:N	2.46	0.43
2:E:101:LYS:NZ	3:F:7:THR:O	2.48	0.43
2:E:144:LYS:NZ	10:E:201:HOH:O	2.50	0.43
2:H:75:HIS:CE1	2:H:113:PRO:HB3	2.54	0.42
2:B:75:HIS:HA	2:B:76:PRO:HD3	1.92	0.42
2:E:12:ASP:OD1	2:E:15:ARG:NH2	2.50	0.42
3:F:62:GLN:H	3:F:62:GLN:HG2	1.71	0.41
2:B:78:ILE:HA	2:B:83:SER:O	2.20	0.41
4:J:454:LYS:HE2	4:J:454:LYS:HB3	1.89	0.41
2:E:144:LYS:HD2	2:E:145:TYR:CZ	2.56	0.41
3:F:73:LEU:HD12	3:F:73:LEU:C	2.46	0.41
2:H:8:LYS:NZ	2:H:12:ASP:OD2	2.46	0.41
1:A:435:ILE:H	1:A:435:ILE:HG13	1.67	0.41
2:H:104:LEU:HD12	2:H:104:LEU:HA	1.93	0.41
2:H:133:LYS:NZ	2:H:137:ILE:HD11	2.36	0.40
5:G:491:PRO:HG3	4:J:457:HIS:CD2	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	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	E	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	H	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	K	145/146 (99%)	140 (97%)	5 (3%)	0	100	100
3	C	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
3	F	76/77 (99%)	75 (99%)	1 (1%)	0	100	100
3	L	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
4	D	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
4	J	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
5	G	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	I	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
All	All	1129/1151 (98%)	1094 (97%)	35 (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	63/63 (100%)	60 (95%)	3 (5%)	23	27
2	B	127/130 (98%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	123/130 (95%)	122 (99%)	1 (1%)	73	83
2	H	127/130 (98%)	126 (99%)	1 (1%)	73	83
2	K	130/130 (100%)	129 (99%)	1 (1%)	73	83
3	C	64/69 (93%)	62 (97%)	2 (3%)	35	45
3	F	66/69 (96%)	64 (97%)	2 (3%)	36	46
3	L	68/69 (99%)	66 (97%)	2 (3%)	37	47
4	D	57/58 (98%)	55 (96%)	2 (4%)	32	40
4	J	57/58 (98%)	55 (96%)	2 (4%)	32	40
5	G	57/57 (100%)	56 (98%)	1 (2%)	51	65
6	I	68/68 (100%)	68 (100%)	0	100	100
All	All	1007/1031 (98%)	990 (98%)	17 (2%)	53	66

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

Mol	Chain	Res	Type
1	A	427	GLU
1	A	452	HIS
1	A	459	MET
3	C	25	ASN
3	C	33	LYS
4	D	452	HIS
4	D	459	MET
2	E	99	ILE
3	F	22	THR
3	F	62	GLN
5	G	452	HIS
2	H	140	GLU
4	J	452	HIS
4	J	467	LYS
2	K	20	GLN
3	L	49	GLN
3	L	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	55	HIS

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Mol	Chain	Res	Type
2	E	32	HIS
2	E	55	HIS
5	G	442	GLN
4	J	483	GLN

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 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	$\# Z > 2$
9	NO3	H	201	-	1,3,3	0.60	0	0,3,3	-	-
7	EDO	K	201	-	3,3,3	0.42	0	2,2,2	0.38	0
7	EDO	K	202	-	3,3,3	0.42	0	2,2,2	0.31	0
9	NO3	I	102	-	1,3,3	0.46	0	0,3,3	-	-
9	NO3	D	503	-	1,3,3	0.66	0	0,3,3	-	-
7	EDO	D	502	-	3,3,3	0.51	0	2,2,2	0.34	0
7	EDO	I	101	-	3,3,3	0.56	0	2,2,2	0.09	0
7	EDO	G	502	-	3,3,3	0.46	0	2,2,2	0.29	0
7	EDO	K	203	-	3,3,3	0.41	0	2,2,2	0.54	0
7	EDO	A	501	-	3,3,3	0.46	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	J	502	-	3,3,3	0.48	0	2,2,2	0.36	0
7	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.34	0
7	EDO	J	501	-	3,3,3	0.48	0	2,2,2	0.41	0
7	EDO	B	201	-	3,3,3	0.55	0	2,2,2	0.34	0
7	EDO	G	501	-	3,3,3	0.45	0	2,2,2	0.34	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
7	EDO	K	201	-	-	1/1/1/1	-
7	EDO	K	202	-	-	0/1/1/1	-
7	EDO	D	502	-	-	1/1/1/1	-
7	EDO	I	101	-	-	0/1/1/1	-
7	EDO	G	502	-	-	1/1/1/1	-
7	EDO	K	203	-	-	0/1/1/1	-
7	EDO	A	501	-	-	0/1/1/1	-
7	EDO	J	502	-	-	0/1/1/1	-
7	EDO	D	501	-	-	0/1/1/1	-
7	EDO	J	501	-	-	1/1/1/1	-
7	EDO	B	201	-	-	0/1/1/1	-
7	EDO	G	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	502	EDO	O1-C1-C2-O2
7	J	501	EDO	O1-C1-C2-O2
7	K	201	EDO	O1-C1-C2-O2
7	G	502	EDO	O1-C1-C2-O2

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	69/69 (100%)	-0.58	0 100 100	20, 26, 53, 81	0
2	B	146/146 (100%)	-0.35	0 100 100	20, 31, 49, 57	0
2	E	146/146 (100%)	0.41	3 (2%) 63 63	26, 53, 80, 99	0
2	H	146/146 (100%)	-0.17	0 100 100	23, 38, 60, 78	0
2	K	146/146 (100%)	-0.46	0 100 100	13, 30, 49, 64	1 (0%)
3	C	77/77 (100%)	-0.15	0 100 100	23, 40, 62, 73	0
3	F	77/77 (100%)	0.36	2 (2%) 57 56	24, 52, 86, 94	1 (1%)
3	L	77/77 (100%)	-0.17	0 100 100	21, 40, 60, 67	0
4	D	64/64 (100%)	-0.51	1 (1%) 70 70	21, 28, 47, 72	0
4	J	64/64 (100%)	-0.51	1 (1%) 70 70	20, 26, 45, 73	0
5	G	63/63 (100%)	-0.56	0 100 100	20, 28, 44, 74	0
6	I	76/76 (100%)	-0.56	0 100 100	18, 27, 40, 51	0
All	All	1151/1151 (100%)	-0.23	7 (0%) 85 84	13, 34, 70, 99	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	428	PRO	3.0
2	E	26	VAL	2.6
3	F	60	ASN	2.5
4	J	428	PRO	2.4
2	E	28	ASP	2.2
2	E	27	GLY	2.1
3	F	45	PHE	2.1

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
9	NO3	D	503	4/4	0.76	0.15	71,73,75,76	0
7	EDO	D	502	4/4	0.77	0.17	58,60,63,63	0
7	EDO	D	501	4/4	0.79	0.20	46,57,62,65	0
9	NO3	I	102	4/4	0.82	0.20	73,73,74,74	0
7	EDO	J	501	4/4	0.90	0.11	37,39,46,50	0
7	EDO	B	201	4/4	0.93	0.09	34,37,37,41	0
9	NO3	H	201	4/4	0.93	0.13	43,57,58,58	0
7	EDO	K	201	4/4	0.93	0.10	48,49,50,52	0
7	EDO	K	202	4/4	0.94	0.12	34,35,39,43	0
7	EDO	K	203	4/4	0.95	0.09	32,33,35,37	0
7	EDO	G	501	4/4	0.95	0.08	35,43,45,47	0
7	EDO	I	101	4/4	0.96	0.06	31,32,33,34	0
7	EDO	A	501	4/4	0.96	0.06	28,33,35,35	0
7	EDO	G	502	4/4	0.97	0.09	36,36,37,37	0
7	EDO	J	502	4/4	0.97	0.06	32,34,36,37	0
8	ZN	D	505	1/1	1.00	0.01	26,26,26,26	0
8	ZN	G	503	1/1	1.00	0.02	30,30,30,30	0
8	ZN	G	504	1/1	1.00	0.01	22,22,22,22	0
8	ZN	J	503	1/1	1.00	0.01	25,25,25,25	0
8	ZN	J	504	1/1	1.00	0.02	24,24,24,24	0
8	ZN	A	502	1/1	1.00	0.01	26,26,26,26	0
8	ZN	A	503	1/1	1.00	0.01	24,24,24,24	0
8	ZN	D	504	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.