



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:28 AM UTC

PDB ID : 2O6V / pdb_00002o6v
Title : Crystal structure and solution NMR studies of Lys48-linked tetraubiquitin at neutral pH
Authors : Eddins, M.J.; Wolberger, C.
Deposited on : 2006-12-08
Resolution : 2.20 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

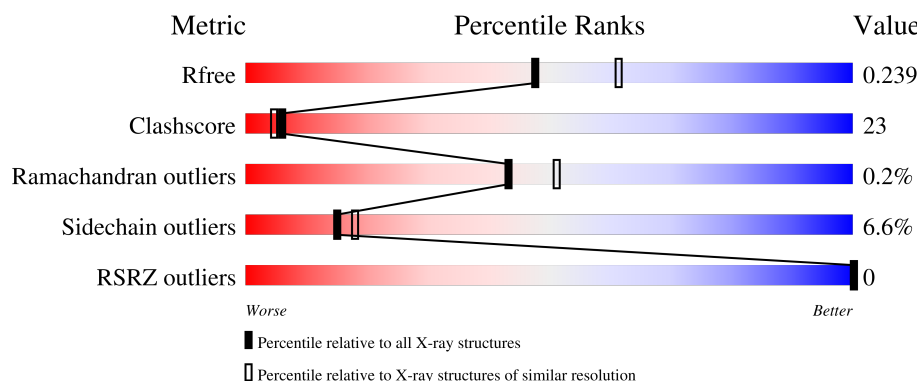
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

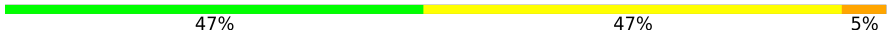
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	76	 78% 17% . .
1	C	76	 47% 47% 5%
1	E	76	 66% 32% ..
1	G	76	 62% 34% .
2	B	76	 64% 33% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	76	 72%24%.
3	D	76	 67%29%.
3	H	76	 49%43%5%..

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
4	SO4	A	801	-	-	X	-
4	SO4	E	804	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4976 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	75	Total	C	N	O	S	0	0	0
			592	375	104	112	1			
1	C	76	Total	C	N	O	S	0	0	0
			598	377	104	116	1			
1	E	75	Total	C	N	O	S	0	0	0
			595	376	104	114	1			
1	G	76	Total	C	N	O	S	0	0	0
			601	378	105	117	1			

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			600	376	107	115	2			
2	F	76	Total	C	N	O	S	0	0	0
			600	376	107	115	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	148	SLZ	LYS	engineered mutation	UNP P62988
B	163	ARG	LYS	engineered mutation	UNP P62988
F	548	SLZ	LYS	engineered mutation	UNP P62988
F	563	ARG	LYS	engineered mutation	UNP P62988

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	76	Total	C	N	O	S	0	0	0
			601	376	109	115	1			
3	H	75	Total	C	N	O	S	0	0	0
			596	373	108	115				

There are 4 discrepancies between the modelled and reference sequences:

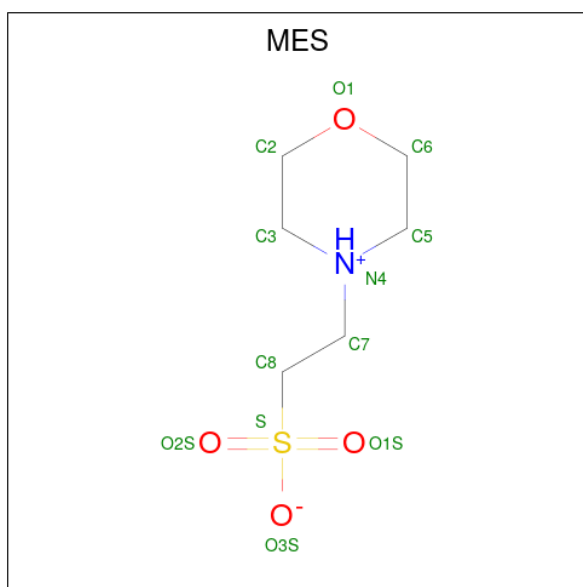
Chain	Residue	Modelled	Actual	Comment	Reference
D	348	ARG	LYS	engineered mutation	UNP P62988
D	363	ARG	LYS	engineered mutation	UNP P62988
H	748	ARG	LYS	engineered mutation	UNP P62988
H	763	ARG	LYS	engineered mutation	UNP P62988

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



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is water.

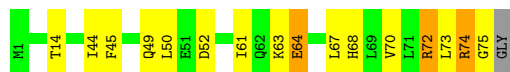
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	11	Total	O	0	0
			11	11		
6	C	16	Total	O	0	0
			16	16		
6	D	21	Total	O	0	0
			21	21		
6	E	24	Total	O	0	0
			24	24		
6	F	21	Total	O	0	0
			21	21		
6	G	14	Total	O	0	0
			14	14		
6	H	14	Total	O	0	0
			14	14		

3 Residue-property plots

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.

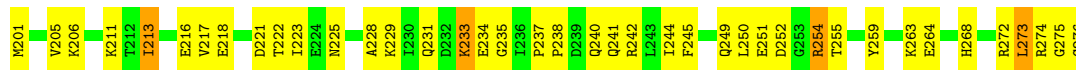
- Molecule 1: Ubiquitin

Chain A: 



- Molecule 1: Ubiquitin

Chain C: 



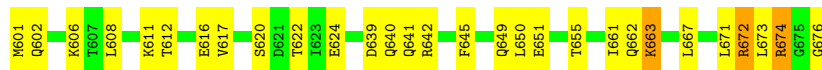
- Molecule 1: Ubiquitin

Chain E: 



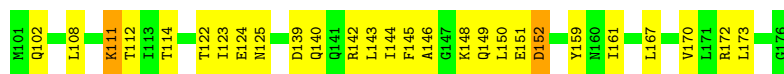
- Molecule 1: Ubiquitin

Chain G: 



- Molecule 2: Ubiquitin

Chain B: 

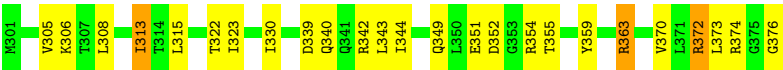


- Molecule 2: Ubiquitin

Chain F: 



● Molecule 3: Ubiquitin



● Molecule 3: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	59.10Å 77.08Å 139.36Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	38.00 – 2.20 38.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.4 (38.00-2.20) 91.1 (38.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.262 0.223 , 0.239	Depositor DCC
R_{free} test set	1463 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.114 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4976	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SLZ, MES, 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	0.54	0/598	0.96	1/804 (0.1%)
1	C	0.44	0/604	1.03	2/812 (0.2%)
1	E	0.46	0/601	0.97	1/808 (0.1%)
1	G	0.45	0/607	0.92	1/816 (0.1%)
2	B	0.42	0/596	0.89	1/801 (0.1%)
2	F	0.45	0/596	0.89	1/801 (0.1%)
3	D	0.47	0/607	0.96	0/816
3	H	0.41	0/602	0.98	2/811 (0.2%)
All	All	0.46	0/4811	0.95	9/6469 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	718	GLU	CA-C-N	7.32	127.33	119.28
3	H	718	GLU	C-N-CA	7.32	127.33	119.28
1	A	52	ASP	N-CA-C	6.95	119.45	111.11
2	B	152	ASP	N-CA-C	6.91	120.59	111.75
2	F	552	ASP	N-CA-C	6.70	122.35	111.37
1	C	273	LEU	N-CA-C	6.62	118.57	111.36
1	C	241	GLN	N-CA-C	5.50	119.03	110.17
1	E	407	THR	N-CA-C	-5.25	102.97	110.59
1	G	641	GLN	N-CA-C	5.17	118.37	110.20

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	592	0	621	22	0
1	C	598	0	619	50	0
1	E	595	0	620	32	0
1	G	601	0	623	29	0
2	B	600	0	618	32	0
2	F	600	0	619	25	0
3	D	601	0	619	28	0
3	H	596	0	614	45	0
4	A	5	0	0	2	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	5	0
5	B	12	0	13	0	0
5	D	12	0	13	0	0
6	A	28	0	0	1	0
6	B	11	0	0	2	0
6	C	16	0	0	5	0
6	D	21	0	0	2	0
6	E	24	0	0	2	0
6	F	21	0	0	1	0
6	G	14	0	0	1	0
6	H	14	0	0	3	0
All	All	4976	0	4979	223	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 23.

All (223) 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)
3:H:716:GLU:O	3:H:717:VAL:HG22	1.38	1.22
1:G:663:LYS:H	1:G:663:LYS:HD2	1.06	1.19
1:E:449:GLN:HE22	2:F:572:ARG:NH1	1.52	1.07
3:H:702:GLN:HE21	3:H:714:THR:HG23	1.22	1.01
1:C:273:LEU:HD11	3:D:351:GLU:HG2	1.45	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLY:HA2	3:D:359:TYR:CE2	2.01	0.96
1:C:242:ARG:HE	1:C:272:ARG:HH11	1.14	0.94
1:A:72:ARG:HD2	4:A:801:SO4:O3	1.68	0.92
3:H:717:VAL:HG21	3:H:729:LYS:HE3	1.54	0.90
3:H:722:THR:HA	3:H:755:THR:HA	1.52	0.89
3:H:723:ILE:HG12	3:H:752:ASP:HA	1.53	0.89
1:E:444:ILE:HD13	2:F:570:VAL:HG11	1.55	0.87
3:H:716:GLU:C	3:H:717:VAL:HG22	2.01	0.86
1:C:237:PRO:HG2	1:C:240:GLN:HB2	1.57	0.85
2:B:142:ARG:HH21	2:B:172:ARG:HH11	1.20	0.85
2:B:123:ILE:HD13	2:B:150:LEU:HB3	1.58	0.84
1:G:663:LYS:H	1:G:663:LYS:CD	1.87	0.84
3:H:717:VAL:HG21	3:H:729:LYS:CE	2.08	0.81
1:G:663:LYS:HD2	1:G:663:LYS:N	1.91	0.81
1:G:639:ASP:OD2	1:G:676:GLY:HA2	1.81	0.79
3:H:719:PRO:HG3	3:H:763:ARG:NH2	1.99	0.78
3:H:716:GLU:O	3:H:717:VAL:CG2	2.27	0.78
1:E:449:GLN:NE2	2:F:572:ARG:NH1	2.31	0.77
2:B:102:GLN:HG3	2:B:114:THR:HG23	1.67	0.76
3:D:342:ARG:HB2	3:D:370:VAL:HG22	1.66	0.75
2:B:161:ILE:HD13	2:B:167:LEU:HD11	1.69	0.74
1:G:622:THR:OG1	1:G:624:GLU:HG3	1.88	0.74
3:D:340:GLN:HA	3:D:372:ARG:HB2	1.69	0.73
1:A:61:ILE:HD13	1:A:67:LEU:HD21	1.71	0.72
2:B:123:ILE:HD12	2:B:151:GLU:O	1.88	0.72
3:H:705:VAL:HG13	6:H:99:HOH:O	1.89	0.72
1:C:242:ARG:NE	1:C:272:ARG:HD2	2.04	0.72
3:H:702:GLN:NE2	3:H:714:THR:HG23	2.03	0.71
3:H:703:ILE:C	3:H:704:PHE:HD2	1.97	0.71
1:A:72:ARG:NH1	1:A:74:ARG:HD3	2.05	0.71
2:B:123:ILE:CD1	2:B:150:LEU:HB3	2.20	0.71
1:E:423:ILE:HB	1:E:452:ASP:HA	1.73	0.71
2:B:124:GLU:CG	2:B:152:ASP:HB3	2.21	0.71
1:C:240:GLN:HG3	1:C:276:GLY:HA3	1.73	0.70
3:H:743:LEU:HD22	6:H:99:HOH:O	1.90	0.70
3:D:315:LEU:HD11	3:D:330:ILE:HD11	1.73	0.70
3:H:723:ILE:CG1	3:H:752:ASP:HA	2.21	0.70
1:A:49:GLN:NE2	2:B:172:ARG:HE	1.89	0.69
1:G:662:GLN:HB2	1:G:663:LYS:HD2	1.74	0.69
2:B:142:ARG:HB2	2:B:170:VAL:HG23	1.73	0.69
1:G:601:MET:HB3	1:G:617:VAL:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:742:ARG:NH2	3:H:772:ARG:HD2	2.06	0.69
1:C:233:LYS:NZ	6:C:68:HOH:O	2.25	0.69
1:C:273:LEU:HD11	3:D:351:GLU:CG	2.20	0.69
1:A:70:VAL:HG21	2:B:144:ILE:HD13	1.75	0.69
2:B:111:LYS:HE3	2:B:111:LYS:HA	1.75	0.68
1:E:454:ARG:HG3	1:E:459:TYR:OH	1.93	0.68
1:E:474:ARG:HH12	3:H:758:ASP:HB3	1.59	0.67
2:B:142:ARG:NH2	2:B:172:ARG:HH11	1.91	0.66
1:E:474:ARG:C	1:E:474:ARG:HD3	2.21	0.66
1:A:72:ARG:HG3	2:B:149:GLN:CD	2.21	0.66
1:G:672:ARG:HH12	3:H:742:ARG:CZ	2.09	0.65
1:G:661:ILE:HD13	1:G:667:LEU:HD21	1.78	0.65
3:D:342:ARG:HB2	3:D:370:VAL:CG2	2.26	0.65
3:D:342:ARG:NH2	3:D:372:ARG:HG2	2.10	0.65
1:E:444:ILE:CD1	2:F:570:VAL:HG11	2.26	0.65
1:G:642:ARG:HD2	1:G:649:GLN:NE2	2.11	0.65
1:E:454:ARG:HD2	6:E:8:HOH:O	1.96	0.64
1:G:606:LYS:HG2	1:G:612:THR:OG1	1.97	0.64
1:C:231:GLN:OE1	1:C:238:PRO:HD3	1.97	0.64
3:H:754:ARG:HD2	3:H:759:TYR:OH	1.97	0.64
1:C:218:GLU:N	1:C:221:ASP:OD2	2.31	0.63
2:F:511:LYS:HG2	6:F:61:HOH:O	1.98	0.63
2:B:123:ILE:HB	2:B:152:ASP:HA	1.81	0.63
2:B:142:ARG:HE	2:B:172:ARG:HD2	1.63	0.63
3:D:363:ARG:HD2	6:D:76:HOH:O	1.98	0.63
3:D:373:LEU:HB2	3:D:376:GLY:O	1.98	0.63
4:E:804:SO4:S	2:F:572:ARG:NH1	2.72	0.62
1:G:672:ARG:NE	1:G:674:ARG:HD2	2.14	0.62
3:H:716:GLU:C	3:H:717:VAL:CG2	2.71	0.62
1:C:217:VAL:HA	1:C:229:LYS:NZ	2.14	0.62
3:D:315:LEU:HD21	3:D:330:ILE:HD13	1.82	0.62
2:F:526:VAL:HG21	2:F:556:LEU:HD21	1.82	0.62
1:G:672:ARG:HE	1:G:674:ARG:HD2	1.65	0.61
1:C:222:THR:HA	1:C:255:THR:HA	1.81	0.61
2:F:548:SLZ:HB2	1:G:673:LEU:HD23	1.83	0.61
3:H:704:PHE:HD2	3:H:704:PHE:N	1.99	0.60
3:D:315:LEU:HD11	3:D:330:ILE:CD1	2.31	0.60
3:H:704:PHE:N	3:H:704:PHE:CD2	2.69	0.60
1:A:68:HIS:HD2	6:A:807:HOH:O	1.84	0.60
4:E:804:SO4:O4	2:F:572:ARG:NH1	2.32	0.60
2:B:142:ARG:HB2	2:B:170:VAL:CG2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HG21	3:D:308:LEU:HD22	1.84	0.60
3:H:754:ARG:HD2	3:H:759:TYR:CZ	2.38	0.59
3:H:719:PRO:HG3	3:H:763:ARG:HH22	1.66	0.59
6:B:907:HOH:O	1:C:275:GLY:HA3	2.02	0.59
1:A:63:LYS:O	1:A:64:GLU:HB2	2.03	0.59
1:G:672:ARG:HH12	3:H:742:ARG:NH2	2.00	0.59
4:A:801:SO4:O2	2:B:172:ARG:NH2	2.36	0.58
1:E:422:THR:HA	1:E:455:THR:HA	1.85	0.58
3:D:323:ILE:HB	3:D:352:ASP:HA	1.84	0.58
1:E:470:VAL:HG21	2:F:544:ILE:HD13	1.86	0.57
2:B:123:ILE:HG23	2:B:143:LEU:HD12	1.85	0.57
1:A:73:LEU:HD12	1:A:73:LEU:N	2.19	0.57
1:C:237:PRO:HG2	1:C:240:GLN:CB	2.30	0.57
4:E:804:SO4:O3	2:F:572:ARG:CZ	2.53	0.57
1:E:454:ARG:NH1	1:E:458:ASP:OD2	2.38	0.57
1:E:473:LEU:HD22	1:G:673:LEU:HB2	1.87	0.57
1:C:240:GLN:HA	6:C:86:HOH:O	2.05	0.56
2:B:111:LYS:HE3	2:B:112:THR:H	1.70	0.56
1:A:72:ARG:NH1	1:A:74:ARG:CD	2.66	0.56
2:F:540:GLN:HG2	2:F:573:LEU:HG	1.87	0.56
1:G:645:PHE:HB3	1:G:650:LEU:HD21	1.89	0.55
1:C:273:LEU:HA	1:C:276:GLY:O	2.05	0.55
1:C:228:ALA:HB1	3:H:704:PHE:CE1	2.41	0.55
3:D:306:LYS:HE2	6:D:67:HOH:O	2.06	0.55
3:D:373:LEU:CG	3:D:373:LEU:O	2.53	0.55
1:E:440:GLN:OE1	1:E:473:LEU:HG	2.07	0.55
2:B:123:ILE:HD13	2:B:150:LEU:CB	2.33	0.54
2:B:140:GLN:HG2	2:B:173:LEU:HG	1.90	0.54
1:E:451:GLU:OE2	2:F:574:ARG:HD3	2.08	0.54
1:C:205:VAL:HB	1:C:213:ILE:HG23	1.89	0.54
3:D:340:GLN:HA	3:D:372:ARG:CB	2.37	0.54
1:G:622:THR:HA	1:G:655:THR:HA	1.89	0.53
1:A:49:GLN:HE22	2:B:172:ARG:NE	2.06	0.53
1:G:640:GLN:OE1	1:G:673:LEU:HG	2.08	0.53
1:C:201:MET:HE1	6:C:80:HOH:O	2.08	0.53
1:E:449:GLN:HE22	2:F:572:ARG:HH12	1.49	0.53
1:C:242:ARG:NE	1:C:272:ARG:HH11	1.96	0.52
1:C:272:ARG:HG3	3:D:349:GLN:HE22	1.74	0.52
4:E:804:SO4:O3	2:F:572:ARG:NH2	2.42	0.52
2:B:123:ILE:HD11	2:B:159:TYR:CE1	2.44	0.52
1:C:223:ILE:HG13	1:C:251:GLU:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:340:GLN:CA	3:D:372:ARG:HB2	2.39	0.52
3:H:742:ARG:HB2	3:H:770:VAL:HG22	1.90	0.52
1:C:205:VAL:O	1:C:213:ILE:HG23	2.10	0.51
1:C:242:ARG:HE	1:C:272:ARG:HD2	1.75	0.51
1:E:422:THR:O	1:E:426:VAL:HG23	2.10	0.51
1:C:225:ASN:ND2	3:H:702:GLN:OE1	2.43	0.51
1:C:201:MET:CE	1:C:263:LYS:N	2.74	0.51
3:D:305:VAL:HB	3:D:313:ILE:HG23	1.91	0.51
1:A:49:GLN:HE22	2:B:172:ARG:HE	1.57	0.51
3:D:351:GLU:HB2	3:D:354:ARG:CG	2.41	0.51
1:C:245:PHE:HB3	1:C:250:LEU:HD21	1.92	0.51
1:E:468:HIS:HD2	6:E:5:HOH:O	1.93	0.51
1:C:242:ARG:NH2	1:C:272:ARG:HD3	2.26	0.50
1:A:49:GLN:NE2	2:B:172:ARG:NE	2.59	0.50
1:G:608:LEU:HD12	3:H:744:ILE:HG21	1.93	0.49
1:C:231:GLN:O	1:C:235:GLY:N	2.38	0.49
1:C:240:GLN:HG3	1:C:276:GLY:CA	2.42	0.49
3:H:707:THR:OG1	3:H:711:LYS:HB3	2.12	0.49
1:A:72:ARG:O	1:A:74:ARG:N	2.45	0.49
3:D:351:GLU:HB2	3:D:354:ARG:HG2	1.94	0.49
3:H:702:GLN:NE2	3:H:704:PHE:CE2	2.79	0.48
1:E:463:LYS:HE2	1:E:464:GLU:OE2	2.14	0.48
1:E:474:ARG:CZ	3:H:754:ARG:HD3	2.43	0.48
1:G:671:LEU:HB3	1:G:673:LEU:CD1	2.43	0.48
1:G:651:GLU:OE2	3:H:774:ARG:HA	2.14	0.48
1:C:272:ARG:HE	1:C:274:ARG:NH1	2.12	0.48
3:H:717:VAL:HB	3:H:721:ASP:OD1	2.14	0.48
1:C:276:GLY:HA3	6:C:86:HOH:O	2.14	0.47
1:C:201:MET:N	1:C:217:VAL:O	2.48	0.47
1:C:244:ILE:HD13	3:D:370:VAL:HG11	1.97	0.47
1:E:444:ILE:HD13	2:F:570:VAL:CG1	2.35	0.47
1:C:201:MET:O	1:C:217:VAL:N	2.47	0.47
3:D:343:LEU:C	3:D:344:ILE:HG13	2.40	0.47
1:E:449:GLN:NE2	2:F:572:ARG:CZ	2.78	0.47
1:A:73:LEU:HD13	6:B:904:HOH:O	2.15	0.47
3:H:713:ILE:HG13	3:H:713:ILE:O	2.14	0.47
1:C:201:MET:CE	6:C:80:HOH:O	2.63	0.46
1:C:223:ILE:HG12	1:C:254:ARG:O	2.16	0.46
2:F:542:ARG:CZ	2:F:572:ARG:HD2	2.45	0.46
1:C:201:MET:O	1:C:216:GLU:HA	2.16	0.46
1:C:272:ARG:HG3	3:D:349:GLN:NE2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:548:SLZ:CD	1:G:673:LEU:O	2.63	0.46
3:H:716:GLU:HB3	6:H:132:HOH:O	2.15	0.46
2:B:142:ARG:NE	2:B:172:ARG:HD2	2.31	0.46
1:A:73:LEU:N	1:A:73:LEU:CD1	2.79	0.45
3:D:372:ARG:HD2	3:D:372:ARG:C	2.41	0.45
2:B:111:LYS:CE	2:B:112:THR:H	2.29	0.45
1:A:44:ILE:HD13	2:B:170:VAL:HG11	1.97	0.45
1:G:674:ARG:H	1:G:674:ARG:HG3	1.52	0.45
3:D:339:ASP:OD1	3:D:340:GLN:HG3	2.16	0.45
1:E:434:GLU:OE1	1:G:611:LYS:HE2	2.17	0.45
1:E:440:GLN:OE1	1:E:473:LEU:CD1	2.65	0.45
1:E:474:ARG:C	1:E:474:ARG:CD	2.88	0.45
2:F:531:GLN:O	2:F:535:GLY:N	2.46	0.45
2:B:111:LYS:HE3	2:B:111:LYS:CA	2.46	0.44
1:C:201:MET:HE2	1:C:263:LYS:HB2	1.98	0.44
1:G:639:ASP:OD2	1:G:676:GLY:CA	2.61	0.44
2:F:548:SLZ:HD2	1:G:673:LEU:O	2.16	0.44
3:H:708:LEU:HD23	3:H:770:VAL:HG12	1.99	0.44
1:E:442:ARG:NH2	4:E:804:SO4:O2	2.29	0.43
1:G:606:LYS:NZ	6:G:130:HOH:O	2.47	0.43
1:C:222:THR:HG22	1:C:225:ASN:CG	2.43	0.43
1:C:272:ARG:HE	1:C:274:ARG:CZ	2.31	0.43
1:E:474:ARG:NH2	3:H:754:ARG:HG2	2.33	0.43
1:E:444:ILE:HA	1:E:448:LYS:O	2.19	0.43
1:E:454:ARG:HB2	1:E:459:TYR:CE1	2.54	0.43
2:F:523:ILE:HG23	2:F:543:LEU:HD12	2.01	0.43
1:C:201:MET:HE2	1:C:263:LYS:N	2.33	0.43
2:F:531:GLN:HB2	2:F:536:ILE:O	2.18	0.43
1:E:440:GLN:HE21	3:H:748:ARG:NH2	2.17	0.42
1:C:225:ASN:N	1:C:225:ASN:HD22	2.16	0.42
1:C:263:LYS:O	1:C:264:GLU:HB2	2.19	0.42
3:H:719:PRO:HA	3:H:756:LEU:HB2	2.00	0.42
1:A:72:ARG:HG3	2:B:149:GLN:OE1	2.20	0.42
1:A:63:LYS:O	1:A:63:LYS:HG3	2.18	0.42
1:C:206:LYS:O	1:C:268:HIS:HA	2.19	0.42
1:C:228:ALA:HB1	3:H:704:PHE:HE1	1.82	0.42
3:D:322:THR:HA	3:D:355:THR:HA	2.02	0.42
3:H:717:VAL:HG21	3:H:729:LYS:CD	2.50	0.42
2:B:145:PHE:O	2:B:146:ALA:HB3	2.20	0.42
2:F:542:ARG:HB2	2:F:570:VAL:HG23	2.02	0.41
1:A:73:LEU:O	1:A:74:ARG:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:722:THR:OG1	3:H:724:GLU:HG2	2.20	0.41
1:C:242:ARG:HH21	1:C:272:ARG:HD3	1.85	0.41
1:E:413:ILE:O	1:E:413:ILE:HG13	2.20	0.41
2:B:122:THR:H	2:B:125:ASN:HD22	1.69	0.41
1:G:601:MET:O	1:G:616:GLU:HA	2.21	0.41
3:H:723:ILE:HG13	3:H:724:GLU:N	2.34	0.41
1:C:250:LEU:HD22	1:C:259:TYR:CE1	2.55	0.41
3:H:731:GLN:O	3:H:735:GLY:N	2.54	0.41
1:A:45:PHE:HB3	1:A:50:LEU:HD21	2.02	0.40
3:H:708:LEU:HD13	3:H:708:LEU:HA	1.77	0.40
2:F:522:THR:H	2:F:525:ASN:HD22	1.69	0.40
1:C:211:LYS:HE2	1:C:234:GLU:OE1	2.22	0.40
1:E:437:PRO:HA	1:E:438:PRO:HD3	1.92	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	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	C	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
1	E	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	G	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	B	73/76 (96%)	73 (100%)	0	0	100	100
2	F	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
3	D	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
3	H	73/76 (96%)	69 (94%)	3 (4%)	1 (1%)	9	7
All	All	587/608 (96%)	569 (97%)	17 (3%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	717	VAL

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	66/68 (97%)	62 (94%)	4 (6%)	17	20
1	C	67/68 (98%)	62 (92%)	5 (8%)	12	14
1	E	67/68 (98%)	66 (98%)	1 (2%)	57	73
1	G	68/68 (100%)	63 (93%)	5 (7%)	13	14
2	B	66/67 (98%)	63 (96%)	3 (4%)	24	33
2	F	66/67 (98%)	62 (94%)	4 (6%)	17	20
3	D	66/68 (97%)	62 (94%)	4 (6%)	17	20
3	H	66/68 (97%)	57 (86%)	9 (14%)	3	3
All	All	532/542 (98%)	497 (93%)	35 (7%)	15	18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	64	GLU
1	A	72	ARG
1	A	74	ARG
2	B	108	LEU
2	B	111	LYS
2	B	139	ASP
1	C	213	ILE
1	C	233	LYS
1	C	249	GLN
1	C	252	ASP
1	C	254	ARG
3	D	313	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	363	ARG
3	D	372	ARG
3	D	374	ARG
1	E	454	ARG
2	F	511	LYS
2	F	524	GLU
2	F	563	ARG
2	F	573	LEU
1	G	602	GLN
1	G	620	SER
1	G	663	LYS
1	G	672	ARG
1	G	674	ARG
3	H	704	PHE
3	H	708	LEU
3	H	717	VAL
3	H	718	GLU
3	H	740	GLN
3	H	751	GLU
3	H	764	GLU
3	H	770	VAL
3	H	773	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	2	GLN
1	A	49	GLN
1	A	68	HIS
2	B	125	ASN
2	B	131	GLN
1	C	225	ASN
1	C	260	ASN
1	C	262	GLN
3	D	302	GLN
3	D	349	GLN
1	E	449	GLN
1	E	460	ASN
1	E	462	GLN
1	E	468	HIS
2	F	502	GLN
2	F	525	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	549	GLN
2	F	568	HIS
1	G	602	GLN
1	G	649	GLN
3	H	725	ASN
3	H	731	GLN
3	H	740	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	SLZ	B	148	2,1	7,8,9	0.81	0	5,8,10	1.35	1 (20%)
2	SLZ	F	548	2,1	7,8,9	0.79	0	5,8,10	1.36	1 (20%)

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
2	SLZ	B	148	2,1	-	3/5/7/9	-
2	SLZ	F	548	2,1	-	0/5/7/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	548	SLZ	CB-SG-CD	2.76	110.46	102.26
2	B	148	SLZ	CB-SG-CD	2.49	109.64	102.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	148	SLZ	N-CA-CB-SG
2	B	148	SLZ	C-CA-CB-SG
2	B	148	SLZ	CE-CD-SG-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	548	SLZ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	A	801	-	4,4,4	1.14	0	6,6,6	1.30	1 (16%)
5	MES	D	902	-	12,12,12	1.15	1 (8%)	15,16,16	0.99	0
4	SO4	D	803	-	4,4,4	1.11	0	6,6,6	1.28	1 (16%)
5	MES	B	901	-	12,12,12	1.60	1 (8%)	15,16,16	0.86	0
4	SO4	B	802	-	4,4,4	1.19	0	6,6,6	1.36	1 (16%)
4	SO4	E	804	-	4,4,4	1.00	0	6,6,6	1.42	1 (16%)

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
5	MES	B	901	-	-	0/6/14/14	0/1/1/1
5	MES	D	902	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	MES	C8-S	4.26	1.83	1.77
5	D	902	MES	C8-S	2.65	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	804	SO4	O4-S-O3	3.15	125.89	108.54
4	B	802	SO4	O4-S-O3	3.00	125.05	108.54
4	A	801	SO4	O4-S-O3	2.87	124.34	108.54
4	D	803	SO4	O4-S-O3	2.83	124.16	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	SO4	2	0
4	E	804	SO4	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	75/76 (98%)	-1.26	0 100 100	27, 37, 54, 77	0
1	C	76/76 (100%)	-1.16	0 100 100	31, 53, 65, 83	0
1	E	75/76 (98%)	-1.26	0 100 100	29, 41, 54, 80	0
1	G	76/76 (100%)	-1.24	0 100 100	32, 46, 69, 80	0
2	B	75/76 (98%)	-1.18	0 100 100	34, 51, 64, 76	0
2	F	75/76 (98%)	-1.25	0 100 100	33, 45, 58, 62	0
3	D	76/76 (100%)	-1.22	0 100 100	29, 39, 67, 86	0
3	H	75/76 (98%)	-1.06	0 100 100	36, 62, 78, 89	0
All	All	603/608 (99%)	-1.20	0 100 100	27, 46, 70, 89	0

There are no RSRZ outliers to report.

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
2	SLZ	B	148	9/10	0.98	0.06	55,57,77,81	0
2	SLZ	F	548	9/10	0.99	0.04	42,45,72,75	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
5	MES	B	901	12/12	0.95	0.07	90,90,93,94	12
5	MES	D	902	12/12	0.97	0.08	85,87,92,93	12
4	SO4	D	803	5/5	0.98	0.05	83,83,85,85	0
4	SO4	A	801	5/5	0.98	0.05	73,74,74,75	5
4	SO4	B	802	5/5	0.98	0.05	82,82,82,84	5
4	SO4	E	804	5/5	0.99	0.04	79,79,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.