



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:17 PM UTC

PDB ID : 6IP4 / pdb_00006ip4
Title : Crystal structure of Arabidopsis thaliana JM13 catalytic domain in complex with NOG and an H3K27me3 peptide
Authors : Hu, H.; Du, J.
Deposited on : 2018-11-02
Resolution : 2.60 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

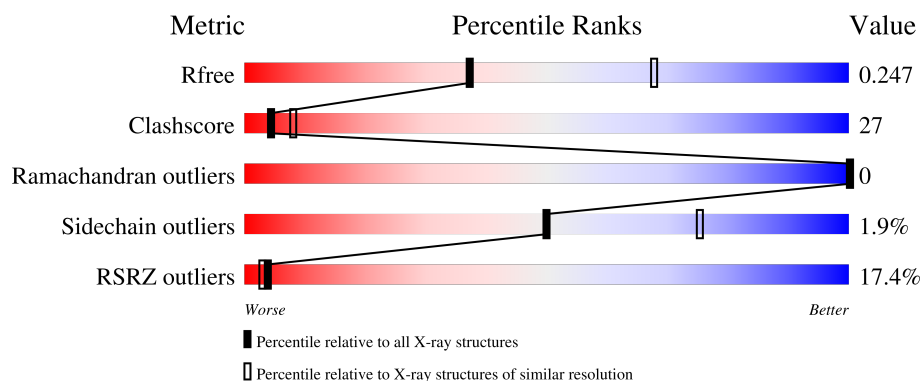
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	490	
2	B	12	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3892 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 Arabidopsis JM13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3731	2396	617	689	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	SER	-	expression tag	UNP F4KIX0

- Molecule 2 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			56	35	12	9			

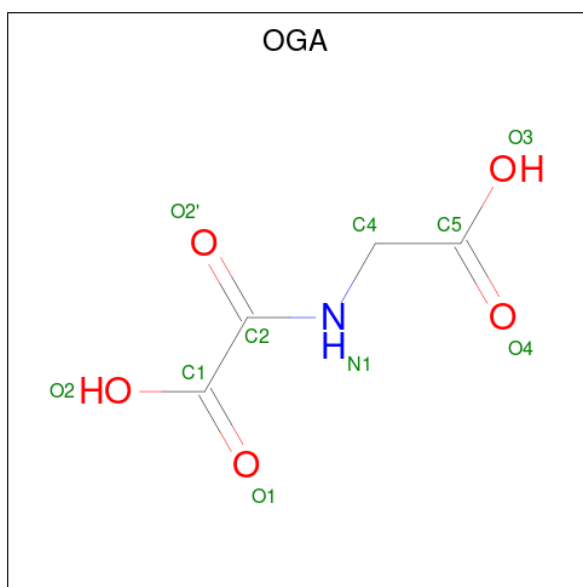
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

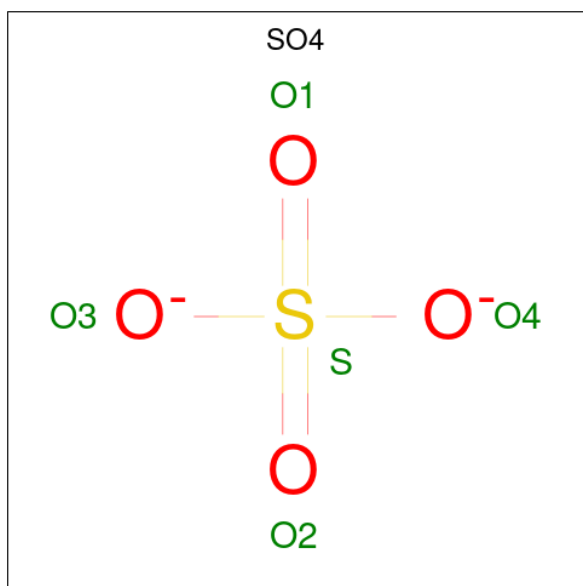
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C₄H₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

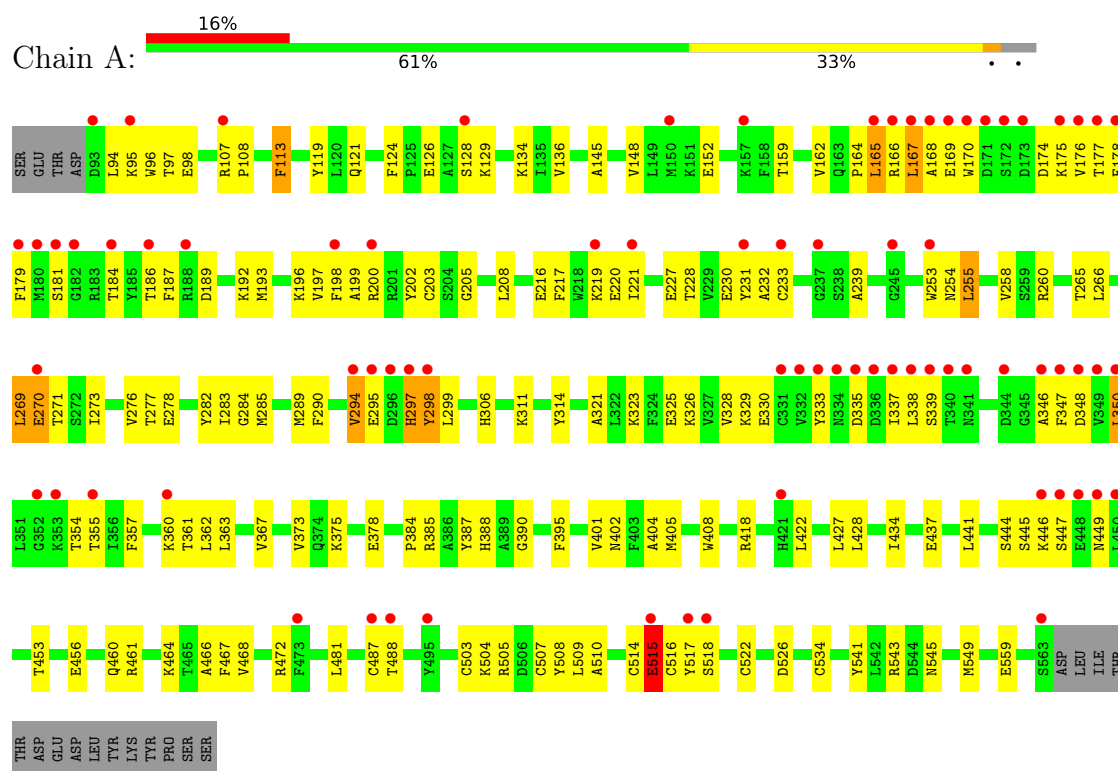
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	57	Total	O	0	0
			57	57		

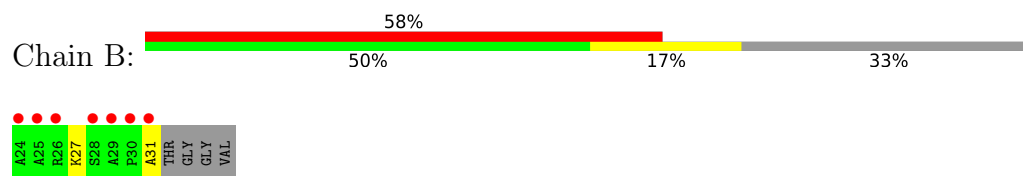
3 Residue-property plots [i](#)

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: Arabidopsis JMJ13



• Molecule 2: Histone H3.2



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.79Å 128.79Å 230.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 – 2.60 49.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.37-2.60) 93.3 (49.37-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.213 , 0.246 0.217 , 0.247	Depositor DCC
R_{free} test set	1681 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3892	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: OGA, M3L, NI, 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	0.57	0/3832	0.81	11/5194 (0.2%)
2	B	0.98	0/44	1.75	0/59
All	All	0.57	0/3876	0.83	11/5253 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	TYR	N-CA-C	-10.74	100.12	113.23
1	A	447	SER	N-CA-C	-8.55	102.40	113.17
1	A	515	GLU	N-CA-C	6.40	118.05	111.14
1	A	270	GLU	N-CA-C	6.34	117.99	111.14
1	A	254	ASN	N-CA-C	-6.24	100.59	109.96
1	A	269	LEU	CA-C-N	5.76	128.27	120.44
1	A	269	LEU	C-N-CA	5.76	128.27	120.44
1	A	488	THR	N-CA-C	5.69	117.56	111.36
1	A	165	LEU	N-CA-C	5.68	117.15	111.07
1	A	348	ASP	N-CA-CB	5.36	118.59	110.28
1	A	445	SER	N-CA-C	-5.22	105.59	111.28

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	3731	0	3663	200	0
2	B	56	0	62	6	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	10	0	3	0	0
6	A	35	0	0	1	0
7	A	57	0	0	11	0
All	All	3892	0	3728	202	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 27.

All (202) 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:A:481:LEU:HG	1:A:487:CYS:SG	1.75	1.26
1:A:166:ARG:HG2	1:A:221:ILE:O	1.30	1.24
1:A:166:ARG:CD	1:A:355:THR:HG21	1.67	1.23
1:A:167:LEU:CD1	1:A:227:GLU:HG2	1.72	1.20
1:A:231:TYR:HD2	1:A:233:CYS:SG	1.64	1.19
1:A:167:LEU:HD11	1:A:227:GLU:HG2	1.31	1.12
1:A:231:TYR:OH	1:A:282:TYR:HB3	1.47	1.12
1:A:294:VAL:HG22	1:A:387:TYR:CE1	1.87	1.08
1:A:231:TYR:CD2	1:A:233:CYS:SG	2.43	1.07
1:A:166:ARG:HD3	1:A:355:THR:CG2	1.84	1.06
1:A:346:ALA:HB1	1:A:422:LEU:HD21	1.36	1.04
1:A:294:VAL:CG2	1:A:387:TYR:CZ	2.42	1.01
1:A:294:VAL:CG2	1:A:387:TYR:CE1	2.44	0.99
1:A:481:LEU:CG	1:A:487:CYS:SG	2.52	0.98
1:A:231:TYR:HH	1:A:282:TYR:HD2	1.04	0.97
1:A:166:ARG:HD3	1:A:355:THR:HG21	0.97	0.96
1:A:516:CYS:O	1:A:517:TYR:HB2	1.65	0.94
1:A:217:PHE:CE2	1:A:221:ILE:HD11	2.04	0.93
1:A:427:LEU:HD12	1:A:428:LEU:HG	1.49	0.92
1:A:217:PHE:CZ	1:A:221:ILE:HD11	2.05	0.92
1:A:198:PHE:CD2	1:A:205:GLY:HA2	2.07	0.90
1:A:294:VAL:HG22	1:A:387:TYR:CZ	2.04	0.89
1:A:346:ALA:CB	1:A:422:LEU:HD21	2.05	0.86
1:A:166:ARG:CG	1:A:221:ILE:O	2.22	0.86
1:A:165:LEU:HD12	1:A:289:MET:SD	2.17	0.84
1:A:503:CYS:SG	1:A:505:ARG:HG3	2.18	0.84
1:A:294:VAL:HG21	1:A:387:TYR:CZ	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:CD1	1:A:428:LEU:HG	2.07	0.83
1:A:196:LYS:O	1:A:200:ARG:HG3	1.79	0.82
1:A:94:LEU:HD11	1:A:219:LYS:HG3	1.61	0.82
1:A:198:PHE:HD2	1:A:205:GLY:HA2	1.41	0.81
1:A:350:LEU:HD12	1:A:350:LEU:O	1.79	0.80
1:A:270:GLU:HG2	1:A:271:THR:N	1.95	0.80
1:A:96:TRP:CD1	1:A:360:LYS:HD2	2.17	0.80
1:A:94:LEU:HD12	1:A:219:LYS:HE3	1.64	0.80
1:A:481:LEU:CD1	1:A:487:CYS:SG	2.71	0.79
1:A:231:TYR:OH	1:A:282:TYR:CB	2.30	0.78
1:A:277:THR:HG22	1:A:278:GLU:HG3	1.64	0.77
1:A:167:LEU:O	1:A:168:ALA:C	2.28	0.77
1:A:165:LEU:CD1	1:A:289:MET:SD	2.73	0.76
1:A:166:ARG:CD	1:A:355:THR:CG2	2.55	0.76
1:A:113:PHE:CE2	1:A:253:TRP:CD1	2.74	0.76
1:A:167:LEU:HD11	1:A:227:GLU:CG	2.14	0.75
1:A:339:SER:HB3	1:A:354:THR:HG22	1.72	0.71
1:A:516:CYS:SG	1:A:518:SER:OG	2.47	0.71
1:A:294:VAL:HG22	1:A:387:TYR:CD1	2.26	0.70
7:A:705:HOH:O	2:B:27:M3L:CM2	2.37	0.70
1:A:282:TYR:OH	2:B:27:M3L:HM32	1.92	0.70
1:A:335:ASP:CG	1:A:338:LEU:HD22	2.17	0.69
1:A:402:ASN:OD1	2:B:27:M3L:HE3	1.93	0.69
1:A:113:PHE:CE1	1:A:253:TRP:CE2	2.81	0.68
1:A:298:TYR:HA	7:A:704:HOH:O	1.94	0.68
1:A:231:TYR:OH	1:A:282:TYR:CD2	2.41	0.67
1:A:509:LEU:HD21	1:A:549:MET:HE1	1.77	0.67
1:A:273:ILE:H	1:A:277:THR:HB	1.60	0.66
1:A:124:PHE:O	1:A:128:SER:HB3	1.97	0.65
1:A:350:LEU:HD12	1:A:350:LEU:C	2.19	0.65
1:A:323:LYS:HG2	1:A:367:VAL:HG12	1.80	0.64
1:A:193:MET:HE2	1:A:197:VAL:HG11	1.79	0.64
1:A:231:TYR:CE2	1:A:233:CYS:SG	2.87	0.63
1:A:360:LYS:HA	1:A:363:LEU:HD12	1.80	0.63
1:A:196:LYS:O	1:A:200:ARG:CG	2.47	0.63
1:A:298:TYR:C	7:A:704:HOH:O	2.42	0.63
1:A:337:ILE:HD13	1:A:357:PHE:HB2	1.81	0.62
1:A:94:LEU:CD1	1:A:219:LYS:HG3	2.30	0.62
1:A:217:PHE:CE2	1:A:221:ILE:CD1	2.82	0.62
1:A:255:LEU:O	1:A:258:VAL:HG12	2.01	0.61
1:A:510:ALA:HA	1:A:541:TYR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:HIS:CE1	1:A:428:LEU:H	2.18	0.61
7:A:705:HOH:O	2:B:27:M3L:HM22	1.98	0.61
1:A:328:VAL:HB	1:A:347:PHE:HZ	1.65	0.61
1:A:297:HIS:ND1	1:A:427:LEU:HB3	2.16	0.60
1:A:113:PHE:CZ	1:A:253:TRP:CE2	2.88	0.60
1:A:298:TYR:O	1:A:384:PRO:HA	2.01	0.60
1:A:298:TYR:CA	7:A:704:HOH:O	2.47	0.60
1:A:337:ILE:HG21	1:A:357:PHE:HB3	1.84	0.60
1:A:481:LEU:HD11	1:A:487:CYS:SG	2.41	0.60
1:A:170:TRP:CE3	1:A:178:PHE:HE2	2.19	0.60
1:A:515:GLU:HB2	1:A:534:CYS:HB2	1.84	0.59
1:A:167:LEU:HD12	1:A:227:GLU:HG2	1.79	0.59
1:A:509:LEU:CD2	1:A:549:MET:HE1	2.32	0.59
1:A:148:VAL:HG11	1:A:239:ALA:O	2.02	0.59
1:A:385:ARG:NH2	1:A:418:ARG:NH1	2.51	0.59
1:A:508:TYR:O	1:A:543:ARG:NH1	2.33	0.58
1:A:337:ILE:CD1	1:A:361:THR:HG21	2.33	0.58
1:A:113:PHE:CE1	1:A:253:TRP:CZ2	2.91	0.58
1:A:270:GLU:HG2	1:A:271:THR:H	1.68	0.58
1:A:362:LEU:HB3	1:A:367:VAL:HG22	1.84	0.58
1:A:107:ARG:NH1	1:A:136:VAL:HG11	2.19	0.57
1:A:526:ASP:N	6:A:610:SO4:O1	2.32	0.57
1:A:346:ALA:CB	1:A:422:LEU:CD2	2.82	0.56
1:A:113:PHE:CD2	1:A:253:TRP:CD1	2.93	0.56
1:A:338:LEU:HG	1:A:339:SER:O	2.06	0.56
1:A:175:LYS:HG3	1:A:179:PHE:HE1	1.70	0.56
1:A:297:HIS:HE1	1:A:428:LEU:H	1.53	0.56
1:A:186:THR:HB	1:A:189:ASP:OD1	2.05	0.56
1:A:329:LYS:HG2	1:A:347:PHE:HE1	1.71	0.56
1:A:335:ASP:OD1	1:A:338:LEU:HD13	2.06	0.56
1:A:193:MET:O	1:A:197:VAL:HG13	2.06	0.55
1:A:290:PHE:CZ	1:A:390:GLY:HA3	2.41	0.55
1:A:231:TYR:OH	1:A:282:TYR:HD2	1.81	0.55
1:A:232:ALA:HB3	1:A:283:ILE:HB	1.88	0.55
1:A:166:ARG:HB2	1:A:221:ILE:HG23	1.88	0.55
1:A:265:THR:HB	7:A:735:HOH:O	2.07	0.54
1:A:427:LEU:HD12	1:A:428:LEU:CG	2.32	0.54
1:A:175:LYS:O	1:A:179:PHE:HD1	1.91	0.54
1:A:337:ILE:HG22	1:A:337:ILE:O	2.08	0.54
1:A:375:LYS:HD3	7:A:714:HOH:O	2.08	0.54
1:A:385:ARG:NH2	1:A:418:ARG:HH12	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:CG	1:A:271:THR:N	2.67	0.53
1:A:198:PHE:CE2	1:A:205:GLY:HA2	2.43	0.53
1:A:467:PHE:HZ	1:A:549:MET:HB3	1.73	0.53
1:A:145:ALA:O	1:A:148:VAL:HG12	2.09	0.52
1:A:178:PHE:HA	1:A:181:SER:OG	2.10	0.52
1:A:148:VAL:HG23	1:A:152:GLU:CD	2.33	0.52
1:A:167:LEU:CB	1:A:170:TRP:HE1	2.21	0.52
1:A:284:GLY:O	1:A:395:PHE:HA	2.09	0.52
1:A:94:LEU:HD11	1:A:219:LYS:CG	2.37	0.52
1:A:96:TRP:HD1	1:A:360:LYS:HD2	1.70	0.51
1:A:165:LEU:HD11	1:A:217:PHE:CE1	2.45	0.51
1:A:362:LEU:HB3	1:A:367:VAL:CG2	2.39	0.51
1:A:202:TYR:OH	1:A:216:GLU:OE1	2.28	0.51
1:A:121:GLN:HG2	1:A:453:THR:OG1	2.11	0.51
1:A:176:VAL:HG23	2:B:31:ALA:O	2.11	0.50
1:A:297:HIS:O	1:A:298:TYR:HB2	2.10	0.50
1:A:167:LEU:HB2	1:A:170:TRP:HE1	1.77	0.49
1:A:231:TYR:CE2	1:A:233:CYS:HA	2.47	0.49
1:A:507:CYS:SG	1:A:522:CYS:HB3	2.52	0.49
1:A:165:LEU:HD13	1:A:289:MET:SD	2.51	0.49
1:A:230:GLU:O	1:A:285:MET:HE3	2.12	0.49
1:A:294:VAL:HG21	1:A:387:TYR:OH	2.13	0.49
1:A:260:ARG:HG2	7:A:712:HOH:O	2.12	0.49
1:A:299:LEU:CD2	1:A:404:ALA:HB2	2.43	0.49
1:A:516:CYS:O	1:A:517:TYR:CB	2.45	0.49
1:A:107:ARG:HH11	1:A:136:VAL:HG11	1.78	0.48
1:A:449:ASN:OD1	1:A:460:GLN:NE2	2.41	0.48
1:A:159:THR:OG1	1:A:184:THR:HG22	2.14	0.48
1:A:337:ILE:HD12	1:A:361:THR:HG21	1.95	0.48
1:A:282:TYR:HB2	7:A:709:HOH:O	2.14	0.48
1:A:164:PRO:O	1:A:164:PRO:HG2	2.12	0.48
1:A:294:VAL:O	1:A:295:GLU:HB2	2.13	0.48
1:A:385:ARG:HH21	1:A:418:ARG:NH1	2.12	0.48
1:A:170:TRP:CZ3	1:A:178:PHE:HE2	2.31	0.47
1:A:273:ILE:HB	1:A:276:VAL:HB	1.97	0.47
1:A:314:TYR:O	1:A:388:HIS:HA	2.15	0.47
1:A:446:LYS:O	1:A:446:LYS:HD2	2.14	0.47
1:A:545:ASN:O	1:A:549:MET:HG3	2.15	0.47
1:A:95:LYS:HD2	1:A:98:GLU:OE1	2.15	0.46
1:A:108:PRO:HB3	1:A:119:TYR:CE1	2.50	0.46
1:A:441:LEU:O	1:A:444:SER:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:CYS:O	1:A:504:LYS:HB2	2.15	0.46
1:A:164:PRO:HD3	1:A:178:PHE:HE1	1.81	0.46
1:A:186:THR:O	1:A:187:PHE:C	2.57	0.46
1:A:126:GLU:O	1:A:129:LYS:HG3	2.15	0.46
1:A:269:LEU:HA	1:A:269:LEU:HD12	1.53	0.46
1:A:294:VAL:HG23	1:A:387:TYR:CE1	2.44	0.46
1:A:434:ILE:HD13	1:A:466:ALA:HB1	1.96	0.46
1:A:330:GLU:O	1:A:333:TYR:HB3	2.16	0.46
1:A:145:ALA:HB2	1:A:306:HIS:HB3	1.98	0.45
1:A:325:GLU:HA	1:A:347:PHE:CZ	2.50	0.45
1:A:464:LYS:NZ	1:A:559:GLU:OE1	2.37	0.45
1:A:427:LEU:HD13	1:A:428:LEU:HG	1.93	0.45
1:A:266:LEU:O	1:A:269:LEU:HB2	2.17	0.44
1:A:311:LYS:NZ	7:A:709:HOH:O	2.50	0.44
1:A:134:LYS:NZ	1:A:373:VAL:O	2.44	0.44
1:A:220:GLU:O	1:A:220:GLU:HG3	2.16	0.44
1:A:192:LYS:NZ	1:A:192:LYS:HB3	2.32	0.44
1:A:113:PHE:CZ	1:A:253:TRP:CD2	3.05	0.44
1:A:258:VAL:HG11	1:A:401:VAL:HG11	2.00	0.44
1:A:405:MET:O	1:A:408:TRP:HB3	2.17	0.44
1:A:162:VAL:HG13	1:A:228:THR:HB	1.99	0.44
1:A:325:GLU:HB3	1:A:347:PHE:CE2	2.53	0.44
1:A:362:LEU:HD22	1:A:367:VAL:HG21	2.00	0.44
1:A:297:HIS:C	1:A:299:LEU:N	2.73	0.43
1:A:514:CYS:HB2	1:A:534:CYS:SG	2.57	0.43
1:A:174:ASP:O	1:A:177:THR:HG22	2.18	0.43
1:A:325:GLU:O	1:A:329:LYS:HG3	2.18	0.43
1:A:270:GLU:HG2	1:A:271:THR:HG22	2.00	0.43
1:A:265:THR:HG22	1:A:437:GLU:OE1	2.18	0.43
1:A:456:GLU:HA	1:A:456:GLU:OE1	2.17	0.43
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.88	0.43
1:A:107:ARG:HE	1:A:136:VAL:HG21	1.84	0.43
1:A:193:MET:HE1	1:A:285:MET:HE1	2.02	0.42
1:A:321:ALA:O	1:A:325:GLU:HG3	2.20	0.42
1:A:468:VAL:HG12	1:A:472:ARG:HD2	2.02	0.42
1:A:338:LEU:HD12	1:A:339:SER:H	1.85	0.41
1:A:217:PHE:O	1:A:221:ILE:HG13	2.21	0.41
1:A:231:TYR:CE2	1:A:233:CYS:CA	3.03	0.41
1:A:96:TRP:CZ3	1:A:97:THR:HG22	2.56	0.41
1:A:337:ILE:HD13	1:A:357:PHE:CB	2.50	0.41
1:A:168:ALA:O	1:A:169:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:HE3	1:A:378:GLU:OE1	2.19	0.41
1:A:282:TYR:OH	2:B:27:M3L:CM3	2.65	0.41
1:A:239:ALA:HB3	1:A:306:HIS:NE2	2.35	0.40
1:A:239:ALA:HB3	1:A:306:HIS:CD2	2.56	0.40
1:A:297:HIS:CG	1:A:428:LEU:HD12	2.56	0.40
1:A:175:LYS:CG	1:A:179:PHE:HE1	2.32	0.40
1:A:178:PHE:CD1	1:A:178:PHE:C	2.99	0.40
1:A:199:ALA:O	1:A:203:CYS:N	2.53	0.40
1:A:208:LEU:HD21	7:A:725:HOH:O	2.21	0.40
1:A:326:LYS:O	1:A:330:GLU:HG3	2.21	0.40
1:A:446:LYS:O	1:A:446:LYS:CG	2.70	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	469/490 (96%)	451 (96%)	18 (4%)	0	100	100
2	B	5/12 (42%)	3 (60%)	2 (40%)	0	100	100
All	All	474/502 (94%)	454 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	411/430 (96%)	403 (98%)	8 (2%)	50	75
2	B	3/5 (60%)	3 (100%)	0	100	100
All	All	414/435 (95%)	406 (98%)	8 (2%)	50	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	167	LEU
1	A	255	LEU
1	A	294	VAL
1	A	297	HIS
1	A	350	LEU
1	A	461	ARG
1	A	515	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	423	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	M3L	B	27	2	10,11,12	0.69	0	9,14,16	0.42	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
2	M3L	B	27	2	-	4/9/10/12	-

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
2	B	27	M3L	N-CA-CB-CG
2	B	27	M3L	C-CA-CB-CG
2	B	27	M3L	O-C-CA-CB
2	B	27	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	27	M3L	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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
6	SO4	A	608	-	4,4,4	0.26	0	6,6,6	0.17	0
6	SO4	A	605	-	4,4,4	0.30	0	6,6,6	0.23	0
6	SO4	A	610	-	4,4,4	0.28	0	6,6,6	0.17	0
5	OGA	A	604	3	9,9,9	1.60	2 (22%)	8,11,11	1.08	0
6	SO4	A	609	-	4,4,4	0.25	0	6,6,6	0.20	0
6	SO4	A	606	-	4,4,4	0.24	0	6,6,6	0.38	0
6	SO4	A	607	-	4,4,4	0.27	0	6,6,6	0.06	0
6	SO4	A	611	-	4,4,4	0.27	0	6,6,6	0.19	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
5	OGA	A	604	3	-	3/8/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	OGA	C2-C1	-3.37	1.50	1.54
5	A	604	OGA	O2-C1	-2.62	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	OGA	O2-C1-C2-O2'
5	A	604	OGA	O1-C1-C2-O2'
5	A	604	OGA	O1-C1-C2-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	610	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	471/490 (96%)	0.71	76 (16%) 4 3	55, 81, 169, 214	0
2	B	7/12 (58%)	6.41	7 (100%) 0 0	132, 141, 158, 164	0
All	All	478/502 (95%)	0.80	83 (17%) 4 3	55, 81, 169, 214	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	24	ALA	10.8
2	B	31	ALA	9.2
1	A	168	ALA	7.6
2	B	30	PRO	7.1
1	A	337	ILE	6.9
1	A	336	ASP	6.3
1	A	231	TYR	6.2
1	A	167	LEU	6.1
1	A	165	LEU	5.9
1	A	180	MET	5.8
1	A	338	LEU	5.6
2	B	25	ALA	5.6
1	A	487	CYS	5.4
1	A	333	TYR	5.3
1	A	176	VAL	5.3
2	B	29	ALA	5.2
1	A	170	TRP	5.0
1	A	200	ARG	4.9
1	A	563	SER	4.7
1	A	188	ARG	4.4
1	A	352	GLY	4.2
1	A	270	GLU	3.9
1	A	339	SER	3.7
1	A	340	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	515	GLU	3.6
2	B	28	SER	3.6
1	A	294	VAL	3.4
2	B	26	ARG	3.4
1	A	175	LYS	3.4
1	A	349	VAL	3.3
1	A	181	SER	3.3
1	A	178	PHE	3.2
1	A	169	GLU	3.2
1	A	166	ARG	3.1
1	A	179	PHE	3.1
1	A	233	CYS	3.1
1	A	449	ASN	3.0
1	A	347	PHE	3.0
1	A	93	ASP	3.0
1	A	473	PHE	3.0
1	A	350	LEU	3.0
1	A	95	LYS	2.9
1	A	331	CYS	2.9
1	A	517	TYR	2.9
1	A	219	LYS	2.9
1	A	332	VAL	2.8
1	A	172	SER	2.8
1	A	450	LEU	2.8
1	A	360	LYS	2.7
1	A	186	THR	2.7
1	A	150	MET	2.7
1	A	184	THR	2.7
1	A	355	THR	2.5
1	A	297	HIS	2.5
1	A	488	THR	2.5
1	A	348	ASP	2.5
1	A	107	ARG	2.4
1	A	177	THR	2.4
1	A	344	ASP	2.4
1	A	245	GLY	2.4
1	A	446	LYS	2.4
1	A	173	ASP	2.4
1	A	518	SER	2.3
1	A	295	GLU	2.3
1	A	334	ASN	2.3
1	A	171	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	341	ASN	2.3
1	A	237	GLY	2.3
1	A	128	SER	2.2
1	A	447	SER	2.2
1	A	298	TYR	2.2
1	A	495	TYR	2.2
1	A	182	GLY	2.2
1	A	335	ASP	2.2
1	A	157	LYS	2.2
1	A	421	HIS	2.2
1	A	353	LYS	2.1
1	A	296	ASP	2.1
1	A	253	TRP	2.1
1	A	198	PHE	2.1
1	A	346	ALA	2.1
1	A	448	GLU	2.0
1	A	221	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
2	M3L	B	27	12/13	0.83	0.32	119,122,128,130	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($\text{\AA}^2$)	Q<0.9
6	SO4	A	610	5/5	0.67	0.13	105,125,126,129	0
6	SO4	A	609	5/5	0.80	0.14	108,119,127,128	0
6	SO4	A	605	5/5	0.84	0.14	105,115,119,125	0
6	SO4	A	608	5/5	0.85	0.10	122,123,132,137	0
6	SO4	A	611	5/5	0.86	0.11	95,105,112,124	0
6	SO4	A	606	5/5	0.92	0.12	87,87,106,124	0
5	OGA	A	604	10/10	0.93	0.14	72,93,97,100	0
6	SO4	A	607	5/5	0.94	0.13	123,123,124,124	5
3	NI	A	601	1/1	0.99	0.04	69,69,69,69	0
4	ZN	A	603	1/1	0.99	0.04	88,88,88,88	0
4	ZN	A	602	1/1	1.00	0.02	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.