



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:27 PM UTC

PDB ID : 6JBM / pdb_00006jbm
Title : Crystal structure of the TRIM14 PRYSPRY domain
Authors : Yin, Y.X.; Yu, Y.; Liang, L.
Deposited on : 2019-01-26
Resolution : 2.10 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

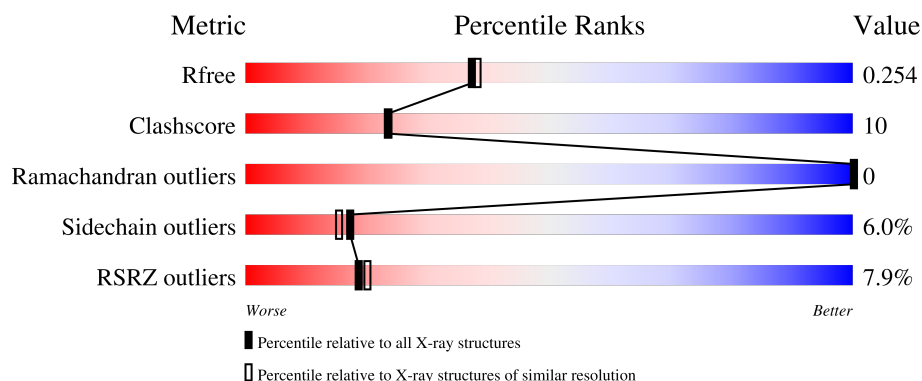
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

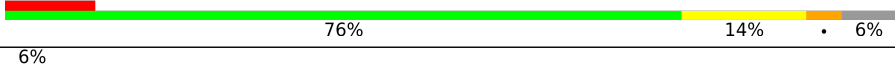
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	200	
1	B	200	
1	C	200	
1	D	200	

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
2	SO4	B	502	-	-	X	-
2	SO4	B	504	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6296 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 Tripartite motif-containing protein 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	188	Total	C	N	O	S	0	0	0
			1526	970	290	260	6			
1	A	183	Total	C	N	O	S	0	0	0
			1472	937	274	255	6			
1	C	183	Total	C	N	O	S	0	0	0
			1479	941	277	255	6			
1	D	183	Total	C	N	O	S	0	0	0
			1479	941	277	255	6			

There are 24 discrepancies between the modelled and reference sequences:

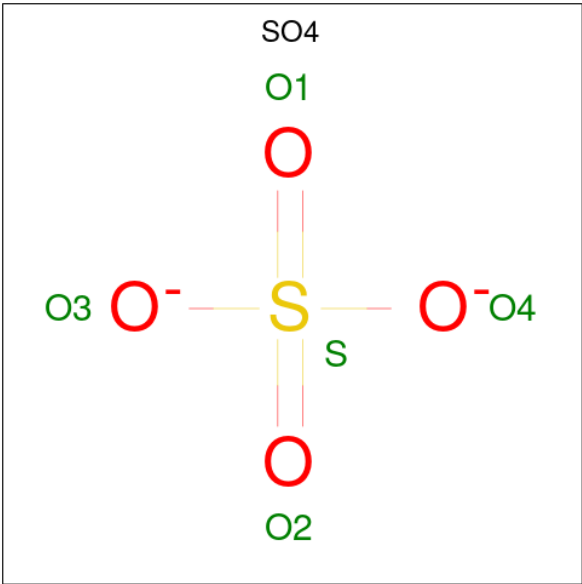
Chain	Residue	Modelled	Actual	Comment	Reference
B	443	HIS	-	expression tag	UNP Q14142
B	444	HIS	-	expression tag	UNP Q14142
B	445	HIS	-	expression tag	UNP Q14142
B	446	HIS	-	expression tag	UNP Q14142
B	447	HIS	-	expression tag	UNP Q14142
B	448	HIS	-	expression tag	UNP Q14142
A	443	HIS	-	expression tag	UNP Q14142
A	444	HIS	-	expression tag	UNP Q14142
A	445	HIS	-	expression tag	UNP Q14142
A	446	HIS	-	expression tag	UNP Q14142
A	447	HIS	-	expression tag	UNP Q14142
A	448	HIS	-	expression tag	UNP Q14142
C	443	HIS	-	expression tag	UNP Q14142
C	444	HIS	-	expression tag	UNP Q14142
C	445	HIS	-	expression tag	UNP Q14142
C	446	HIS	-	expression tag	UNP Q14142
C	447	HIS	-	expression tag	UNP Q14142
C	448	HIS	-	expression tag	UNP Q14142
D	443	HIS	-	expression tag	UNP Q14142
D	444	HIS	-	expression tag	UNP Q14142
D	445	HIS	-	expression tag	UNP Q14142

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Chain	Residue	Modelled	Actual	Comment	Reference
D	446	HIS	-	expression tag	UNP Q14142
D	447	HIS	-	expression tag	UNP Q14142
D	448	HIS	-	expression tag	UNP Q14142

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

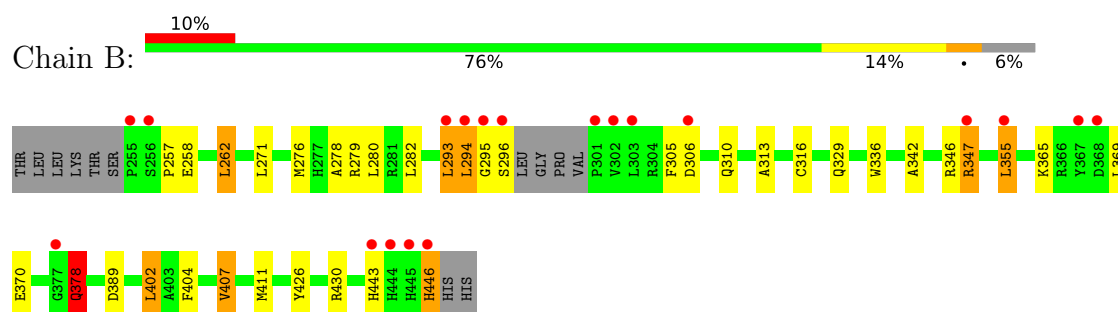
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	84	Total	O	0	0
			84	84		
3	A	62	Total	O	0	0
			62	62		
3	C	52	Total	O	0	0
			52	52		
3	D	82	Total	O	0	0
			82	82		

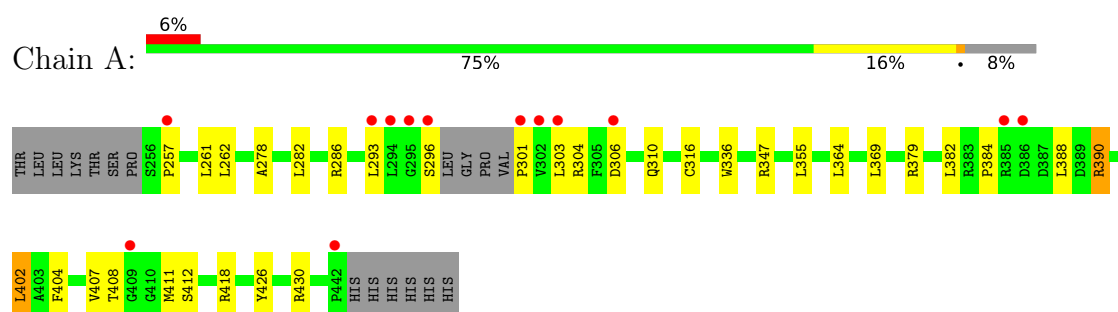
3 Residue-property plots [i](#)

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.

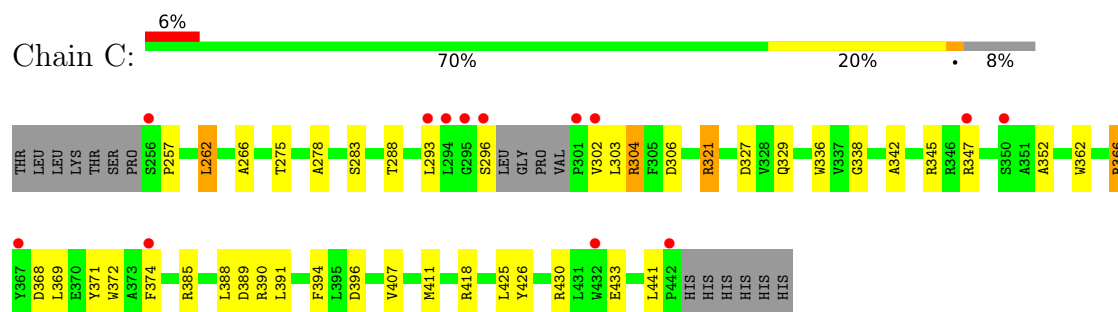
- Molecule 1: Tripartite motif-containing protein 14



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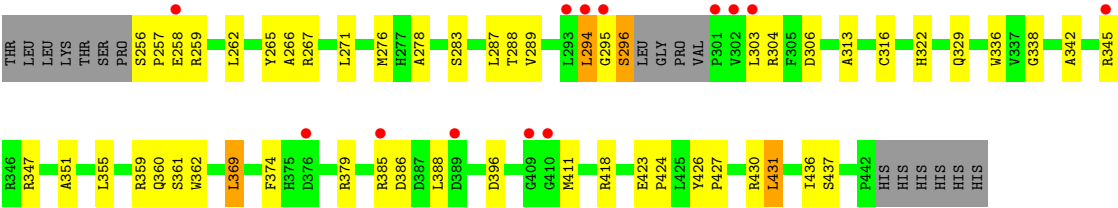


- Molecule 1: Tripartite motif-containing protein 14



- Molecule 1: Tripartite motif-containing protein 14





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.33Å 104.02Å 93.38Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	35.40 – 2.10 35.40 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.0 (35.40-2.10) 85.7 (35.40-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.213 , 0.242 (Not available) , 0.254	Depositor DCC
R_{free} test set	2294 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.196 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6296	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.52	0/1513	0.70	0/2053
1	B	0.52	0/1572	0.81	3/2133 (0.1%)
1	C	0.42	0/1520	0.64	0/2062
1	D	0.60	2/1520 (0.1%)	0.77	5/2062 (0.2%)
All	All	0.52	2/6125 (0.0%)	0.73	8/8310 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	423	GLU	C-N	5.44	1.41	1.33
1	D	424	PRO	N-CD	5.14	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	ASP	N-CA-C	8.17	120.27	111.36
1	B	306	ASP	N-CA-C	6.84	118.81	111.36
1	D	423	GLU	CA-C-N	-6.24	113.36	119.78
1	D	423	GLU	C-N-CA	-6.24	113.36	119.78
1	B	370	GLU	N-CA-C	6.20	119.24	110.50
1	B	378	GLN	N-CA-C	5.72	118.52	110.23
1	D	361	SER	N-CA-C	5.10	116.83	109.07
1	D	360	GLN	N-CA-C	5.02	119.28	113.20

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	1472	0	1435	28	0
1	B	1526	0	1483	36	0
1	C	1479	0	1447	35	0
1	D	1479	0	1447	33	0
2	A	15	0	0	0	0
2	B	20	0	0	8	0
2	C	5	0	0	0	0
2	D	20	0	0	1	0
3	A	62	0	0	1	0
3	B	84	0	0	2	0
3	C	52	0	0	5	0
3	D	82	0	0	2	0
All	All	6296	0	5812	120	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 10.

All (120) 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:B:293:LEU:HD22	2:B:502:SO4:O2	1.63	0.98
1:B:294:LEU:HD11	1:D:418:ARG:NH2	1.84	0.91
1:D:256:SER:N	1:D:257:PRO:CD	2.35	0.87
1:A:257:PRO:HD2	1:C:433:GLU:CD	2.00	0.85
1:B:279:ARG:HD3	3:B:660:HOH:O	1.77	0.83
1:B:347:ARG:HD3	2:B:504:SO4:O1	1.81	0.81
1:B:347:ARG:HG2	2:B:504:SO4:O2	1.81	0.80
1:C:278:ALA:HB1	1:C:296:SER:HA	1.67	0.77
1:B:294:LEU:HD11	1:D:418:ARG:HH22	1.45	0.76
1:D:385:ARG:HG3	1:D:386:ASP:N	1.99	0.76
1:C:388:LEU:HD23	1:C:391:LEU:HD21	1.69	0.74
1:A:257:PRO:CD	1:C:433:GLU:OE1	2.36	0.74
1:D:345:ARG:HD2	1:D:347:ARG:NH2	2.03	0.73
1:C:418:ARG:CG	3:C:636:HOH:O	2.40	0.69
1:D:256:SER:N	1:D:257:PRO:HD3	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:PRO:HG2	1:C:262:LEU:HD21	1.74	0.69
1:A:257:PRO:HG2	1:C:433:GLU:HG3	1.74	0.68
1:D:294:LEU:HD12	1:D:295:GLY:H	1.59	0.68
1:C:266:ALA:HB1	1:C:441:LEU:HB3	1.75	0.66
1:C:418:ARG:HG3	3:C:636:HOH:O	1.97	0.65
1:B:347:ARG:HD3	2:B:504:SO4:S	2.37	0.65
1:A:278:ALA:HB1	1:A:296:SER:HA	1.79	0.65
1:A:390:ARG:HB2	1:A:408:THR:HG23	1.78	0.65
1:B:258:GLU:HG3	3:B:642:HOH:O	1.96	0.65
1:A:336:TRP:CE3	1:A:430:ARG:HG2	2.32	0.65
1:A:257:PRO:HD3	1:C:433:GLU:OE1	1.97	0.64
1:C:321:ARG:HG2	1:C:394:PHE:CZ	2.32	0.64
1:C:262:LEU:HD23	1:C:411:MET:HE2	1.80	0.63
1:C:347:ARG:HD2	1:C:347:ARG:H	1.63	0.63
1:A:336:TRP:HB2	1:A:430:ARG:HB3	1.79	0.63
1:D:329:GLN:NE2	3:D:601:HOH:O	2.31	0.62
1:B:336:TRP:NE1	1:B:365:LYS:HD2	2.15	0.61
1:A:257:PRO:HD2	1:C:433:GLU:OE1	1.99	0.61
1:D:345:ARG:HD2	1:D:347:ARG:CZ	2.32	0.59
1:D:278:ALA:O	1:D:296:SER:HB2	2.03	0.59
1:B:257:PRO:HG2	1:B:262:LEU:HD21	1.85	0.58
1:B:293:LEU:CD2	2:B:502:SO4:O2	2.46	0.58
1:D:336:TRP:HB2	1:D:430:ARG:HB3	1.84	0.58
1:B:407:VAL:HB	1:B:411:MET:SD	2.44	0.57
1:B:310:GLN:HE21	1:B:430:ARG:HD2	1.70	0.56
1:D:351:ALA:HB2	2:D:504:SO4:O4	2.06	0.56
1:B:305:PHE:HA	1:B:346:ARG:O	2.05	0.56
1:D:374:PHE:CE2	1:D:379:ARG:HD3	2.40	0.56
1:A:257:PRO:CD	1:C:433:GLU:CD	2.76	0.56
1:D:256:SER:N	1:D:257:PRO:HD2	2.20	0.55
1:A:369:LEU:HB2	3:A:625:HOH:O	2.06	0.55
1:D:259:ARG:HA	1:D:411:MET:HE2	1.87	0.55
1:C:418:ARG:HG2	3:C:636:HOH:O	2.05	0.55
1:A:390:ARG:HB3	1:A:407:VAL:HB	1.90	0.54
1:C:257:PRO:HG2	1:C:262:LEU:CD2	2.38	0.53
1:D:276:MET:HE1	1:D:289:VAL:HG23	1.89	0.53
1:D:278:ALA:HB2	1:D:304:ARG:NH1	2.23	0.53
1:B:310:GLN:HE22	1:B:355:LEU:H	1.56	0.53
1:D:431:LEU:HD22	1:D:436:ILE:HD12	1.92	0.52
1:B:329:GLN:HG2	1:B:389:ASP:OD1	2.09	0.52
1:B:336:TRP:HB2	1:B:430:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:CG	2:B:504:SO4:O2	2.56	0.52
1:C:283:SER:HB2	1:C:288:THR:HB	1.90	0.52
1:D:342:ALA:HB2	1:D:426:TYR:CE2	2.44	0.52
1:C:329:GLN:HB2	1:C:389:ASP:OD2	2.10	0.51
1:B:443:HIS:CE1	1:A:418:ARG:HB3	2.45	0.51
1:B:276:MET:HE2	1:B:280:LEU:HB3	1.92	0.51
1:A:293:LEU:H	1:A:293:LEU:HD12	1.75	0.51
1:A:261:LEU:HD23	1:C:293:LEU:HD13	1.94	0.50
1:B:276:MET:HE2	1:B:280:LEU:CB	2.42	0.50
1:B:402:LEU:HD13	1:B:404:PHE:HE1	1.76	0.50
1:C:321:ARG:HD3	1:C:396:ASP:OD2	2.12	0.49
1:B:378:GLN:O	1:B:378:GLN:HG3	2.12	0.49
1:B:402:LEU:HD13	1:B:404:PHE:CE1	2.47	0.49
1:B:347:ARG:HD3	2:B:504:SO4:O2	2.12	0.49
1:A:306:ASP:HB2	1:A:347:ARG:HA	1.94	0.49
1:A:316:CYS:HB3	1:A:426:TYR:CZ	2.49	0.48
1:D:313:ALA:HB3	1:D:427:PRO:HD2	1.94	0.48
1:D:288:THR:HG22	1:D:437:SER:CB	2.44	0.48
1:D:267:ARG:HD3	1:D:322:HIS:HB3	1.96	0.47
1:B:446:HIS:ND1	1:B:446:HIS:C	2.73	0.47
1:D:288:THR:HG22	1:D:437:SER:HB2	1.97	0.47
1:B:271:LEU:HA	1:B:313:ALA:HA	1.97	0.46
1:D:265:TYR:O	1:D:267:ARG:HD2	2.14	0.46
1:D:266:ALA:O	1:D:267:ARG:NH1	2.42	0.46
1:C:338:GLY:HA3	1:C:362:TRP:O	2.16	0.46
1:C:336:TRP:HB2	1:C:430:ARG:HB3	1.98	0.45
1:B:271:LEU:HB2	1:B:282:LEU:HD11	1.98	0.45
1:B:279:ARG:HG3	1:B:295:GLY:HA3	1.99	0.45
1:B:443:HIS:HE1	1:A:418:ARG:HB3	1.81	0.45
1:C:306:ASP:OD1	1:C:347:ARG:HA	2.16	0.45
1:A:316:CYS:HB3	1:A:426:TYR:CE1	2.52	0.45
1:C:345:ARG:NH2	1:D:396:ASP:OD2	2.41	0.45
1:C:366:ARG:NH1	1:C:368:ASP:O	2.40	0.45
1:C:366:ARG:HB2	1:C:371:TYR:CE1	2.52	0.44
1:C:372:TRP:HB3	1:C:374:PHE:CE1	2.52	0.44
1:C:385:ARG:HB3	3:C:612:HOH:O	2.18	0.44
1:D:271:LEU:HA	1:D:313:ALA:HA	2.00	0.44
1:B:342:ALA:HB2	1:B:426:TYR:CE2	2.53	0.43
1:C:385:ARG:CB	3:C:612:HOH:O	2.67	0.43
1:C:342:ALA:HB2	1:C:426:TYR:CE2	2.54	0.43
1:A:282:LEU:HG	1:A:286:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLN:HG2	1:A:430:ARG:HB2	2.01	0.43
1:B:316:CYS:HB3	1:B:426:TYR:CE1	2.53	0.43
1:C:345:ARG:HD2	1:C:352:ALA:CB	2.48	0.43
1:D:316:CYS:HB3	1:D:426:TYR:CZ	2.53	0.42
1:B:279:ARG:HG3	1:B:295:GLY:CA	2.49	0.42
1:C:327:ASP:OD1	1:C:329:GLN:HB3	2.20	0.42
1:D:283:SER:HB3	1:D:288:THR:OG1	2.19	0.42
1:D:338:GLY:HA3	1:D:362:TRP:O	2.20	0.42
1:D:369:LEU:HD22	1:D:369:LEU:N	2.34	0.42
1:B:347:ARG:NH1	2:B:504:SO4:O1	2.52	0.41
1:D:345:ARG:HB2	3:D:671:HOH:O	2.19	0.41
1:A:402:LEU:HD13	1:A:404:PHE:CE1	2.55	0.41
1:A:407:VAL:HA	1:A:411:MET:CE	2.50	0.41
1:A:369:LEU:HD13	1:A:369:LEU:HA	1.91	0.41
1:B:278:ALA:HB1	1:B:296:SER:HA	2.02	0.41
1:C:407:VAL:HG22	1:C:411:MET:SD	2.60	0.41
1:A:364:LEU:HG	1:A:382:LEU:HD11	2.02	0.41
1:A:411:MET:HA	1:A:411:MET:HE2	2.02	0.41
1:B:294:LEU:HD13	1:B:295:GLY:N	2.36	0.41
1:A:301:PRO:HA	1:A:304:ARG:HB3	2.04	0.40
1:A:384:PRO:CB	1:A:388:LEU:HD21	2.51	0.40
1:C:275:THR:HA	1:C:304:ARG:HA	2.02	0.40
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.89	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	179/200 (90%)	176 (98%)	3 (2%)	0	100	100
1	B	184/200 (92%)	180 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	179/200 (90%)	172 (96%)	7 (4%)	0	100	100
1	D	179/200 (90%)	176 (98%)	3 (2%)	0	100	100
All	All	721/800 (90%)	704 (98%)	17 (2%)	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	147/164 (90%)	140 (95%)	7 (5%)	23	23
1	B	153/164 (93%)	143 (94%)	10 (6%)	15	13
1	C	148/164 (90%)	139 (94%)	9 (6%)	17	15
1	D	148/164 (90%)	138 (93%)	10 (7%)	14	12
All	All	596/656 (91%)	560 (94%)	36 (6%)	17	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	262	LEU
1	B	293	LEU
1	B	294	LEU
1	B	347	ARG
1	B	355	LEU
1	B	369	LEU
1	B	378	GLN
1	B	402	LEU
1	B	407	VAL
1	B	446	HIS
1	A	262	LEU
1	A	303	LEU
1	A	355	LEU
1	A	379	ARG

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Mol	Chain	Res	Type
1	A	390	ARG
1	A	402	LEU
1	A	412	SER
1	C	262	LEU
1	C	302	VAL
1	C	303	LEU
1	C	304	ARG
1	C	321	ARG
1	C	366	ARG
1	C	369	LEU
1	C	390	ARG
1	C	425	LEU
1	D	258	GLU
1	D	262	LEU
1	D	287	LEU
1	D	294	LEU
1	D	296	SER
1	D	355	LEU
1	D	359	ARG
1	D	369	LEU
1	D	388	LEU
1	D	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	GLN
1	B	443	HIS
1	C	329	GLN

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

12 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	$\# Z > 2$
2	SO4	D	501	-	4,4,4	1.31	0	6,6,6	0.63	0
2	SO4	D	504	-	4,4,4	0.28	0	6,6,6	0.52	0
2	SO4	D	503	-	4,4,4	0.38	0	6,6,6	0.38	0
2	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.22	0
2	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.39	0
2	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.28	0
2	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.29	0
2	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.29	0
2	SO4	B	504	-	4,4,4	0.26	0	6,6,6	0.36	0
2	SO4	A	502	-	4,4,4	0.40	0	6,6,6	0.39	0
2	SO4	C	501	-	4,4,4	0.22	0	6,6,6	0.37	0
2	SO4	B	503	-	4,4,4	0.38	0	6,6,6	0.49	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.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	504	SO4	1	0
2	B	502	SO4	2	0
2	B	504	SO4	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	183/200 (91%)	0.21	13 (7%) 22 23	15, 25, 44, 68	0
1	B	188/200 (94%)	0.38	19 (10%) 12 13	12, 24, 42, 65	0
1	C	183/200 (91%)	0.44	13 (7%) 22 23	15, 28, 43, 60	0
1	D	183/200 (91%)	0.46	13 (7%) 22 23	16, 30, 45, 62	0
All	All	737/800 (92%)	0.38	58 (7%) 18 20	12, 27, 45, 68	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	PRO	6.3
1	B	303	LEU	5.1
1	B	443	HIS	4.8
1	C	301	PRO	4.2
1	C	296	SER	3.9
1	A	295	GLY	3.9
1	B	296	SER	3.8
1	B	444	HIS	3.7
1	B	368	ASP	3.7
1	B	293	LEU	3.6
1	B	302	VAL	3.6
1	B	295	GLY	3.6
1	C	367	TYR	3.6
1	C	295	GLY	3.5
1	C	442	PRO	3.4
1	A	302	VAL	3.3
1	B	294	LEU	3.2
1	B	446	HIS	3.2
1	A	296	SER	3.2
1	C	432	TRP	3.1
1	C	256	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	367	TYR	3.1
1	B	445	HIS	3.1
1	D	295	GLY	3.1
1	A	409	GLY	3.0
1	A	301	PRO	3.0
1	A	306	ASP	2.9
1	D	301	PRO	2.9
1	D	303	LEU	2.9
1	B	255	PRO	2.9
1	C	374	PHE	2.9
1	A	294	LEU	2.8
1	C	293	LEU	2.7
1	A	293	LEU	2.6
1	D	302	VAL	2.6
1	D	410	GLY	2.6
1	A	386	ASP	2.6
1	B	377	GLY	2.5
1	D	294	LEU	2.5
1	B	355	LEU	2.5
1	A	303	LEU	2.5
1	A	442	PRO	2.4
1	C	294	LEU	2.4
1	D	258	GLU	2.4
1	B	256	SER	2.4
1	C	302	VAL	2.3
1	D	409	GLY	2.3
1	B	347	ARG	2.3
1	D	345	ARG	2.3
1	B	306	ASP	2.3
1	C	347	ARG	2.2
1	D	376	ASP	2.2
1	A	385	ARG	2.1
1	D	293	LEU	2.1
1	D	385	ARG	2.1
1	C	350	SER	2.1
1	D	389	ASP	2.0
1	A	257	PRO	2.0

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

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(Å ²)	Q<0.9
2	SO4	B	502	5/5	0.74	0.14	55,58,68,72	0
2	SO4	D	504	5/5	0.80	0.22	50,57,60,65	0
2	SO4	A	503	5/5	0.84	0.16	40,47,51,63	0
2	SO4	B	503	5/5	0.89	0.12	48,50,55,55	0
2	SO4	C	501	5/5	0.90	0.19	34,42,45,50	0
2	SO4	D	502	5/5	0.90	0.10	47,50,55,57	0
2	SO4	B	504	5/5	0.90	0.17	45,48,57,58	0
2	SO4	D	503	5/5	0.91	0.11	37,42,45,53	0
2	SO4	A	501	5/5	0.91	0.10	32,41,47,47	0
2	SO4	A	502	5/5	0.94	0.15	35,37,38,49	0
2	SO4	B	501	5/5	0.95	0.16	44,46,48,48	0
2	SO4	D	501	5/5	0.97	0.11	33,34,38,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.