Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:56 PM JST

PDB ID	:	6JBM
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 (i) 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 (1)) were used in the production of this report:

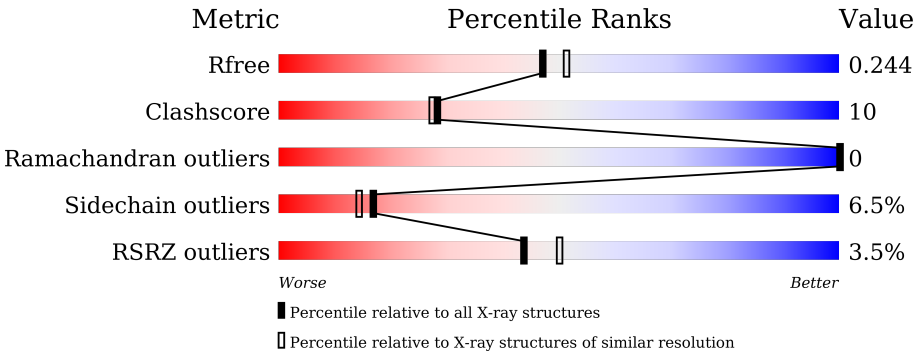
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	3% 74% 16% • 8%
1	B	200	6% 77% 14% • 6%
1	C	200	2% 70% 20% • 8%
1	D	200	2% 68% 22% • 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	502	-	-	X	-
2	SO4	B	504	-	-	X	-

2 Entry composition (i)

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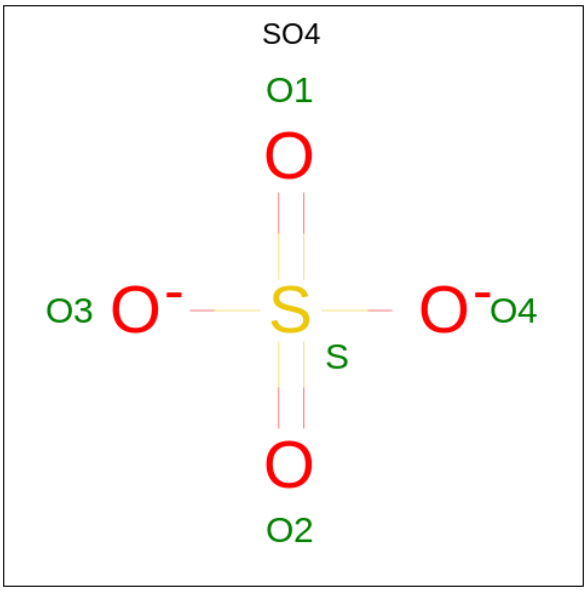
Chain	Residue	Modelled	Actual	Comment	Reference
D	446	HIS	-	expression tag	UNP Q14142
D	447	HIS	-	expression tag	UNP Q14142
D	448	HIS	-	expression tag	UNP Q14142

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

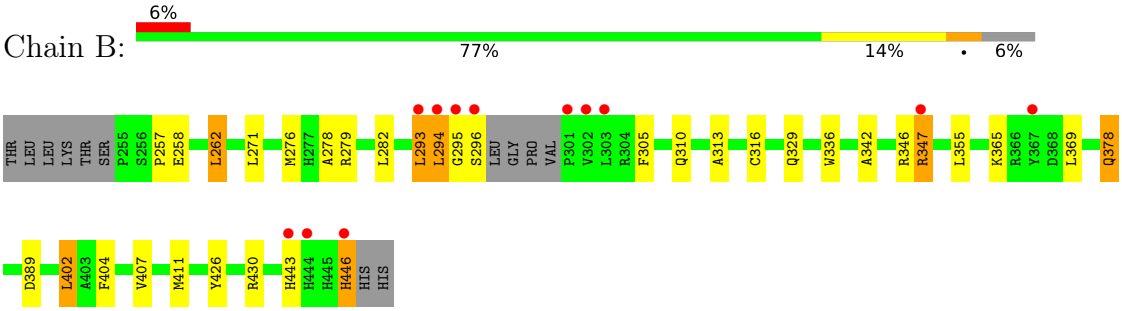
- Molecule 3 is water.

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

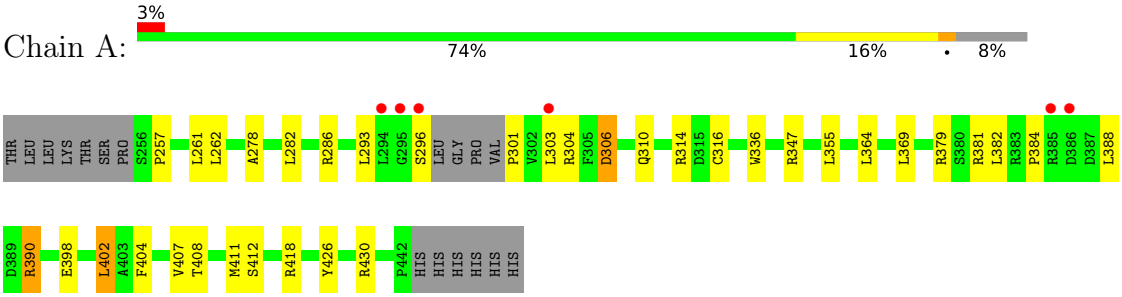
3 Residue-property plots (i)

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.

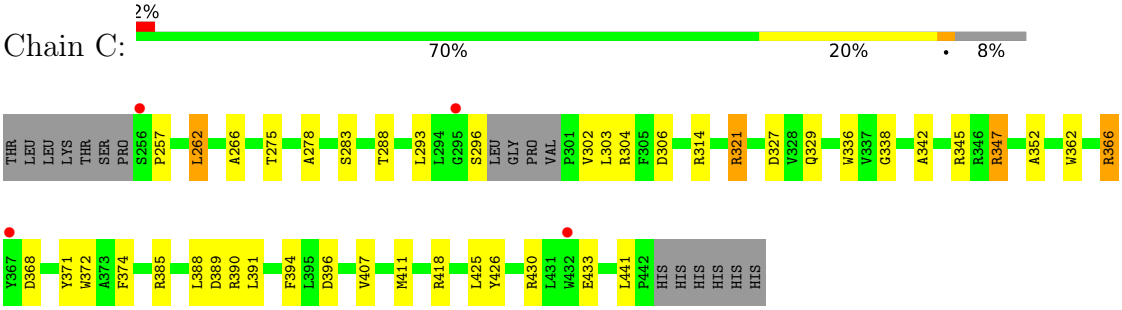
• Molecule 1: Tripartite motif-containing protein 14



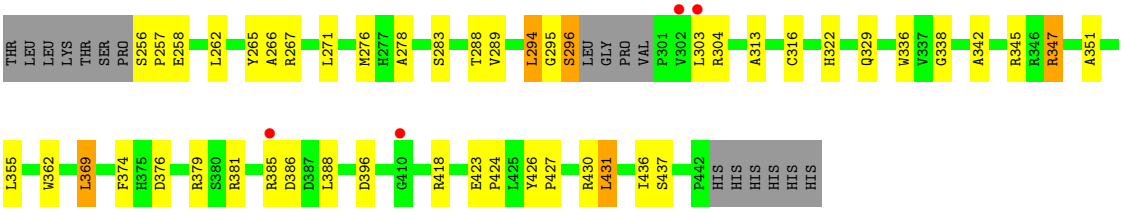
• Molecule 1: Tripartite motif-containing protein 14



• Molecule 1: Tripartite motif-containing protein 14



• Molecule 1: Tripartite motif-containing protein 14


THR LEU LEU LYS THR SER PRO S256 P257 E258 L262 Y265 A266 R267 L271 M276 H277 A278 S283 T288 V289 L294 G295 S296 LEU GLY PRO VAL P301 V302 L303 R304 A313 C316 H322 Q329 W336 V337 G338 A342 R345 R346 R347 A351
L355 W362 L369 F374 H375 D376 R379 S380 R381 R385 D386 D387 L388 D396 G410 R418 E423 P424 L425 Y426 P427 R430 L431 I436 S437 P442 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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) 80.7 (35.40-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.213 , 0.242 0.215 , 0.244	Depositor DCC
R_{free} test set	2294 reflections (4.96%)	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)	0.37 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.196 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/1513	0.69	0/2053
1	B	0.48	0/1572	0.69	0/2133
1	C	0.44	0/1520	0.65	0/2062
1	D	0.52	1/1520 (0.1%)	0.72	1/2062 (0.0%)
All	All	0.48	1/6125 (0.0%)	0.69	1/8310 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	424	PRO	N-CD	5.07	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	423	GLU	C-N-CD	5.56	140.08	128.40

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	27	0
1	B	1526	0	1483	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1479	0	1447	33	0
1	D	1479	0	1447	32	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	116	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 (116) 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:B:279:ARG:HD3	3:B:660:HOH:O	1.77	0.83
1:A:257:PRO:HD2	1:C:433:GLU:CD	2.00	0.81
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:418:ARG:HG2	3:C:636:HOH:O	2.05	0.55
1:A:407:VAL:HA	1:A:411:MET:HE3	1.89	0.54
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: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:276:MET:HE1	1:D:289:VAL:HG23	1.90	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:276:MET:HB2	1:B:276:MET:HE2	1.75	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
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:B:446:HIS:ND1	1:B:446:HIS:C	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:HD13	1:A:404:PHE:CE1	2.55	0.41
1:A:369:LEU:HD13	1:A:369:LEU:HA	1.91	0.41
1:A:407:VAL:HA	1:A:411:MET:CE	2.50	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: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
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 (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	147/164 (90%)	136 (92%)	11 (8%)	13	10
1	B	153/164 (93%)	145 (95%)	8 (5%)	23	21
1	C	148/164 (90%)	139 (94%)	9 (6%)	18	16
1	D	148/164 (90%)	137 (93%)	11 (7%)	13	10
All	All	596/656 (91%)	557 (94%)	39 (6%)	17	14

All (39) 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	369	LEU
1	B	378	GLN
1	B	402	LEU
1	B	446	HIS
1	A	262	LEU
1	A	303	LEU
1	A	306	ASP
1	A	314	ARG
1	A	355	LEU
1	A	379	ARG
1	A	381	ARG
1	A	390	ARG
1	A	398	GLU
1	A	402	LEU
1	A	412	SER
1	C	262	LEU
1	C	302	VAL
1	C	303	LEU
1	C	314	ARG
1	C	321	ARG
1	C	347	ARG
1	C	366	ARG
1	C	390	ARG
1	C	425	LEU
1	D	258	GLU
1	D	262	LEU

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Mol	Chain	Res	Type
1	D	294	LEU
1	D	296	SER
1	D	347	ARG
1	D	355	LEU
1	D	369	LEU
1	D	376	ASP
1	D	381	ARG
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	D	360	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	501	-	4,4,4	0.12	0	6,6,6	0.39	0
2	SO4	D	504	-	4,4,4	0.20	0	6,6,6	0.57	0
2	SO4	B	501	-	4,4,4	0.36	0	6,6,6	0.20	0
2	SO4	B	504	-	4,4,4	0.25	0	6,6,6	0.37	0
2	SO4	A	502	-	4,4,4	0.51	0	6,6,6	0.40	0
2	SO4	A	503	-	4,4,4	0.12	0	6,6,6	0.29	0
2	SO4	B	503	-	4,4,4	0.32	0	6,6,6	0.48	0
2	SO4	D	502	-	4,4,4	0.17	0	6,6,6	0.25	0
2	SO4	A	501	-	4,4,4	0.30	0	6,6,6	0.39	0
2	SO4	D	501	-	4,4,4	1.49	0	6,6,6	0.66	0
2	SO4	D	503	-	4,4,4	0.36	0	6,6,6	0.38	0
2	SO4	B	502	-	4,4,4	0.21	0	6,6,6	0.30	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	504	SO4	6	0
2	B	502	SO4	2	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, 95^{th} 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%)	-0.02	6 (3%)	46	53	15, 25, 44, 68	0
1	B	188/200 (94%)	0.20	12 (6%)	19	24	12, 24, 42, 65	0
1	C	183/200 (91%)	0.15	4 (2%)	62	66	15, 28, 43, 60	0
1	D	183/200 (91%)	0.06	4 (2%)	62	66	16, 30, 45, 62	0
All	All	737/800 (92%)	0.10	26 (3%)	44	50	12, 27, 45, 68	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	LEU	5.6
1	B	302	VAL	5.1
1	B	443	HIS	4.4
1	B	301	PRO	4.2
1	C	432	TRP	3.6
1	C	295	GLY	3.5
1	B	296	SER	3.5
1	C	256	SER	3.4
1	C	367	TYR	3.1
1	A	295	GLY	3.0
1	B	444	HIS	2.9
1	B	295	GLY	2.8
1	B	446	HIS	2.7
1	B	367	TYR	2.5
1	A	303	LEU	2.5
1	D	302	VAL	2.5
1	A	294	LEU	2.4
1	D	385	ARG	2.3
1	B	294	LEU	2.3
1	B	347	ARG	2.3
1	B	293	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	296	SER	2.1
1	D	303	LEU	2.1
1	D	410	GLY	2.1
1	A	386	ASP	2.0
1	A	385	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	0.87	0.24	55,58,68,72	0
2	SO4	D	504	5/5	0.89	0.24	50,57,60,65	0
2	SO4	A	503	5/5	0.91	0.19	40,47,51,63	0
2	SO4	B	503	5/5	0.94	0.10	48,50,55,55	0
2	SO4	D	503	5/5	0.94	0.10	37,42,45,53	0
2	SO4	A	501	5/5	0.94	0.10	32,41,47,47	0
2	SO4	B	504	5/5	0.95	0.17	45,48,57,58	0
2	SO4	C	501	5/5	0.96	0.18	34,42,45,50	0
2	SO4	D	502	5/5	0.96	0.08	47,50,55,57	0
2	SO4	A	502	5/5	0.97	0.13	35,37,38,49	0
2	SO4	D	501	5/5	0.99	0.09	33,34,38,45	0
2	SO4	B	501	5/5	0.99	0.14	44,46,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.