



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:16 PM UTC

PDB ID : 8JPU / pdb_00008jpu
Title : Crystal Structure of the acyltransferase domain from the fifth module of the tylosin polyketide synthase
Authors : Huang, S.; Zheng, J.
Deposited on : 2023-06-12
Resolution : 2.50 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

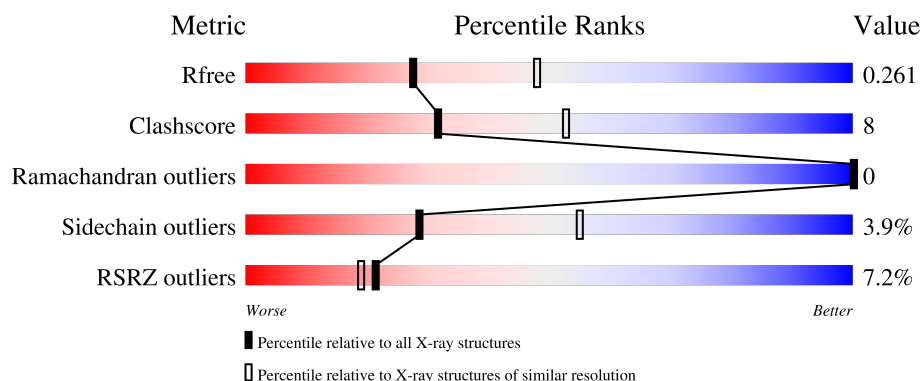
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	431	3% 78% 17% • •
1	B	431	10% 72% 14% • 13%
1	C	431	5% 77% 18% • •
1	D	431	10% 73% 13% • 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11999 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 Ty lactone synthase modules 4 & 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3151	1976	569	592	14			
1	B	375	Total	C	N	O	S	0	0	0
			2821	1770	509	528	14			
1	C	417	Total	C	N	O	S	0	0	0
			3155	1978	570	593	14			
1	D	375	Total	C	N	O	S	0	0	0
			2823	1770	513	526	14			

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



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

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

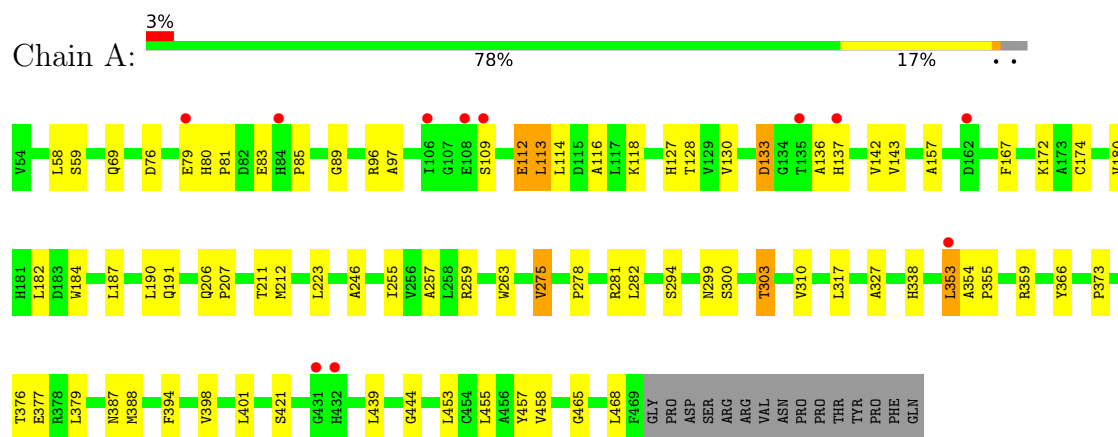
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	4	Total	O	0	0
			4	4		
3	C	7	Total	O	0	0
			7	7		
3	D	9	Total	O	0	0
			9	9		

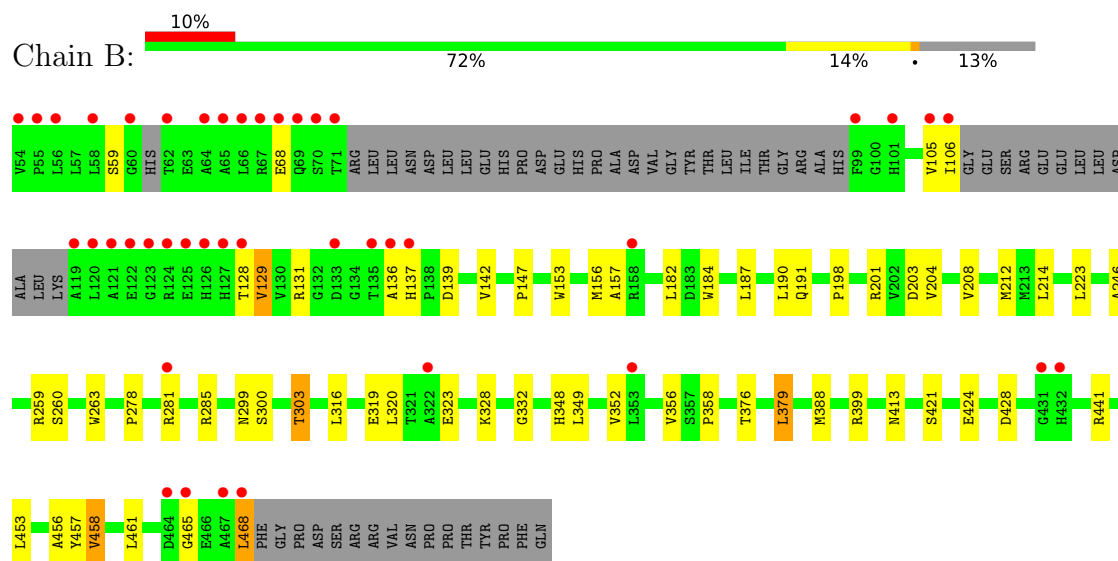
3 Residue-property plots

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.

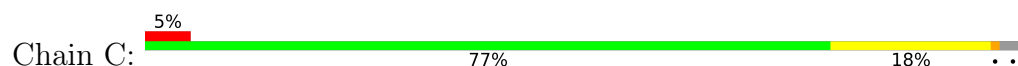
- Molecule 1: Tylactone synthase modules 4 & 5

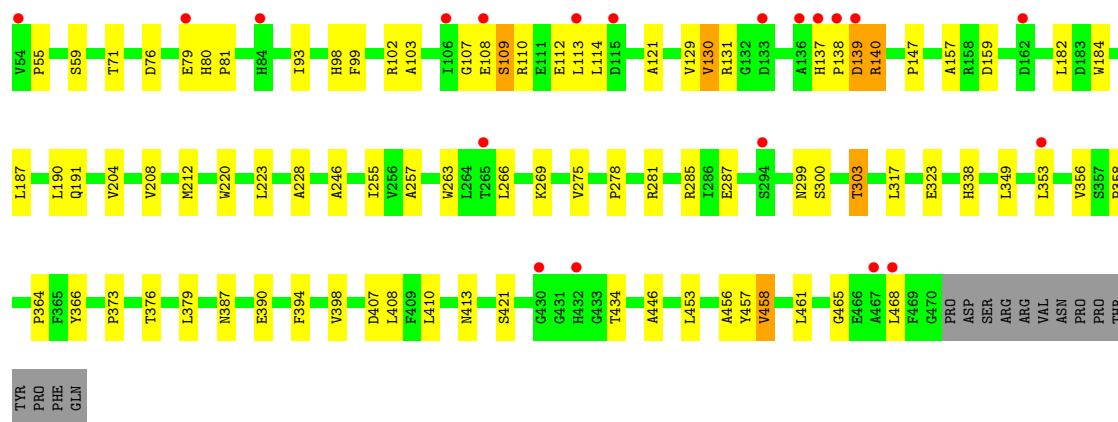


- Molecule 1: Tylactone synthase modules 4 & 5

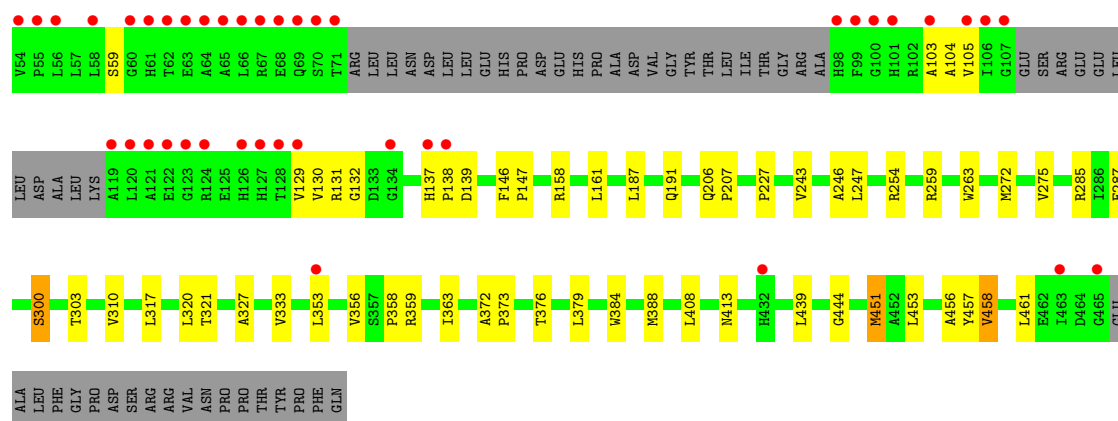
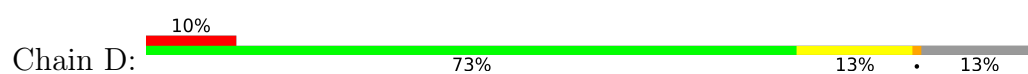


- Molecule 1: Tylactone synthase modules 4 & 5





• Molecule 1: Tylactone synthase modules 4 & 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.95Å 138.38Å 209.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 2.50 39.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.8 (39.46-2.50) 73.9 (39.46-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.202 , 0.263 0.206 , 0.261	Depositor DCC
R_{free} test set	2453 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11999	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% 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: 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	0.49	0/3217	0.86	0/4375
1	B	0.48	0/2876	0.87	0/3907
1	C	0.47	0/3221	0.87	0/4380
1	D	0.48	0/2881	0.86	0/3915
All	All	0.48	0/12195	0.86	0/16577

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3151	0	3121	55	0
1	B	2821	0	2803	44	0
1	C	3155	0	3124	61	0
1	D	2823	0	2799	38	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	7	0	0	0	0
3	D	9	0	0	1	0
All	All	11999	0	11847	193	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 8.

All (193) 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:C:190:LEU:HD22	1:C:212:MET:HE3	1.29	1.13
1:C:157:ALA:HB2	1:C:212:MET:HE1	1.38	1.02
1:C:157:ALA:HB2	1:C:212:MET:CE	1.94	0.97
1:C:278:PRO:HD2	1:C:281:ARG:HD3	1.50	0.93
1:C:157:ALA:CB	1:C:212:MET:HE1	2.02	0.90
1:D:103:ALA:HB2	1:D:131:ARG:HD2	1.57	0.86
1:A:180:VAL:HG12	1:B:328:LYS:HD3	1.57	0.84
1:C:190:LEU:HD22	1:C:212:MET:CE	2.12	0.80
1:B:157:ALA:HB2	1:B:212:MET:HE1	1.64	0.79
1:A:303:THR:HG21	1:A:421:SER:OG	1.88	0.74
1:B:106:ILE:O	1:B:128:THR:HB	1.87	0.74
1:B:299:ASN:HB2	1:B:303:THR:HG22	1.69	0.74
1:D:132:GLY:N	1:D:458:VAL:HG11	2.05	0.72
1:A:259:ARG:NH2	2:A:500:SO4:O2	2.23	0.71
1:D:131:ARG:O	1:D:131:ARG:HG3	1.91	0.70
1:B:190:LEU:HD22	1:B:212:MET:HE3	1.73	0.70
1:A:180:VAL:CG1	1:B:328:LYS:HD3	2.22	0.70
1:A:223:LEU:HD13	1:A:453:LEU:HD11	1.75	0.69
1:A:157:ALA:HB2	1:A:212:MET:CE	2.22	0.69
1:C:408:LEU:HD13	1:C:434:THR:HB	1.73	0.69
1:B:157:ALA:HB2	1:B:212:MET:CE	2.21	0.68
1:A:299:ASN:HB2	1:A:303:THR:HG22	1.75	0.68
1:A:157:ALA:HB2	1:A:212:MET:HE1	1.77	0.67
1:D:451:MET:HE2	1:D:451:MET:HA	1.76	0.67
1:A:278:PRO:HD2	1:A:281:ARG:HD3	1.77	0.67
1:B:105:VAL:HG22	1:B:129:VAL:HG22	1.76	0.67
1:D:137:HIS:CD2	1:D:138:PRO:HD2	2.30	0.67
1:B:187:LEU:O	1:B:191:GLN:HG2	1.96	0.66
1:C:109:SER:O	1:C:112:GLU:HB2	1.96	0.65
1:A:300:SER:OG	1:A:303:THR:HB	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:HIS:HB3	1:C:138:PRO:HD2	1.79	0.65
1:C:465:GLY:HA2	1:C:468:LEU:CD2	2.27	0.64
1:C:157:ALA:HB2	1:C:212:MET:HE3	1.81	0.62
1:B:157:ALA:CB	1:B:212:MET:HE1	2.30	0.62
1:C:59:SER:HB3	1:C:457:TYR:OH	2.00	0.61
1:C:140:ARG:HD2	1:C:407:ASP:OD2	2.01	0.61
1:B:190:LEU:HD21	1:B:208:VAL:HG13	1.84	0.60
1:A:96:ARG:HG2	1:A:97:ALA:O	2.02	0.59
1:C:303:THR:HG21	1:C:421:SER:OG	2.01	0.59
1:D:439:LEU:HD22	1:D:444:GLY:HA2	1.83	0.59
1:D:137:HIS:CG	1:D:138:PRO:HD2	2.37	0.59
1:B:376:THR:HB	1:B:379:LEU:HD22	1.84	0.59
1:A:354:ALA:HB3	1:B:441:ARG:HD3	1.85	0.58
1:A:109:SER:HB2	1:A:112:GLU:OE1	2.04	0.58
1:C:147:PRO:HG2	1:C:413:ASN:ND2	2.18	0.58
1:B:190:LEU:CD2	1:B:212:MET:HE3	2.33	0.57
1:D:456:ALA:HB1	1:D:461:LEU:HD12	1.87	0.57
1:C:278:PRO:CD	1:C:281:ARG:HD3	2.32	0.57
1:D:285:ARG:HD2	1:D:320:LEU:HD21	1.87	0.56
1:B:137:HIS:CE1	1:B:139:ASP:HB2	2.40	0.56
1:B:137:HIS:NE2	1:B:139:ASP:HB2	2.20	0.56
1:D:254:ARG:NH1	1:D:353:LEU:O	2.39	0.56
1:A:59:SER:HB3	1:A:457:TYR:OH	2.06	0.56
1:C:182:LEU:HD21	1:C:257:ALA:HB1	1.88	0.55
1:C:366:TYR:CE2	1:C:373:PRO:HG3	2.42	0.55
1:B:399:ARG:NH2	1:B:428:ASP:OD2	2.39	0.55
1:B:223:LEU:HD13	1:B:453:LEU:HD22	1.87	0.55
1:C:394:PHE:O	1:C:398:VAL:HG23	2.06	0.55
1:C:223:LEU:HD13	1:C:453:LEU:HD11	1.89	0.54
1:D:372:ALA:HB1	1:D:373:PRO:HD2	1.89	0.54
1:A:263:TRP:NE1	1:A:388:MET:HE3	2.22	0.54
1:B:356:VAL:HG23	1:B:358:PRO:HD3	1.89	0.54
1:A:157:ALA:CB	1:A:212:MET:HE1	2.38	0.54
1:B:203:ASP:HA	1:B:260:SER:HB2	1.91	0.53
1:B:303:THR:HG21	1:B:421:SER:OG	2.08	0.53
1:D:132:GLY:H	1:D:458:VAL:HG11	1.73	0.53
1:C:59:SER:HB2	1:C:99:PHE:H	1.74	0.53
1:D:158:ARG:NH1	3:D:601:HOH:O	2.38	0.53
1:D:147:PRO:HG2	1:D:413:ASN:ND2	2.24	0.52
1:C:465:GLY:HA2	1:C:468:LEU:HD23	1.90	0.52
1:D:132:GLY:O	1:D:458:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:GLY:CA	1:C:113:LEU:HD11	2.40	0.51
1:A:130:VAL:HG11	1:A:455:LEU:HD23	1.93	0.51
1:B:246:ALA:HB1	1:B:376:THR:HB	1.91	0.51
1:B:182:LEU:HD13	1:B:184:TRP:CZ2	2.46	0.51
1:C:55:PRO:HG2	1:C:468:LEU:HD12	1.93	0.51
1:D:246:ALA:O	1:D:359:ARG:HG2	2.11	0.51
1:B:465:GLY:HA2	1:B:468:LEU:HD23	1.92	0.50
1:A:109:SER:O	1:A:112:GLU:HB2	2.11	0.50
1:B:278:PRO:HD2	1:B:281:ARG:HD3	1.94	0.50
1:C:266:LEU:HA	1:C:269:LYS:HD2	1.93	0.50
1:C:228:ALA:O	1:C:364:PRO:HD2	2.10	0.50
1:D:259:ARG:NH2	2:D:500:SO4:O3	2.44	0.50
1:A:366:TYR:CE2	1:A:373:PRO:HG3	2.47	0.50
1:A:206:GLN:HB2	1:A:207:PRO:HD3	1.94	0.50
1:C:109:SER:O	1:C:112:GLU:N	2.46	0.49
1:A:465:GLY:HA2	1:A:468:LEU:CD2	2.43	0.49
1:A:275:VAL:HG21	1:A:282:LEU:HD13	1.94	0.49
1:B:349:LEU:HD11	1:B:388:MET:SD	2.52	0.49
1:C:79:GLU:O	1:C:80:HIS:CG	2.65	0.49
1:D:247:LEU:HD11	1:D:384:TRP:CZ2	2.48	0.48
1:A:81:PRO:C	1:A:83:GLU:H	2.22	0.48
1:C:107:GLY:HA3	1:C:113:LEU:HD21	1.94	0.48
1:D:376:THR:HB	1:D:379:LEU:HD22	1.95	0.48
1:B:131:ARG:C	1:B:458:VAL:HG11	2.38	0.48
1:C:190:LEU:HD21	1:C:208:VAL:HG13	1.95	0.48
1:C:76:ASP:O	1:C:80:HIS:HB2	2.13	0.48
1:A:190:LEU:HD22	1:A:212:MET:HE3	1.95	0.47
1:A:167:PHE:HZ	1:A:212:MET:HE1	1.78	0.47
1:D:59:SER:HB3	1:D:457:TYR:OH	2.15	0.47
1:A:338:HIS:HE1	1:A:387:ASN:O	1.98	0.47
1:C:338:HIS:CE1	1:C:387:ASN:O	2.68	0.47
1:A:394:PHE:O	1:A:398:VAL:HG23	2.14	0.47
1:A:174:CYS:HB2	1:A:211:THR:HG23	1.95	0.47
1:B:285:ARG:NH2	1:B:323:GLU:OE1	2.45	0.47
1:D:130:VAL:O	1:D:131:ARG:C	2.57	0.47
1:B:68:GLU:O	1:B:68:GLU:HG3	2.14	0.47
1:C:159:ASP:OD2	1:C:446:ALA:N	2.38	0.47
1:D:187:LEU:O	1:D:191:GLN:HG2	2.15	0.47
1:A:255:ILE:HA	1:A:353:LEU:HD21	1.96	0.47
1:C:299:ASN:HB2	1:C:303:THR:HG22	1.97	0.47
1:C:112:GLU:N	1:C:112:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:HIS:CB	1:C:138:PRO:HD2	2.45	0.46
1:D:103:ALA:HB2	1:D:131:ARG:CD	2.38	0.46
1:A:143:VAL:HG21	1:A:401:LEU:HD22	1.98	0.46
1:A:187:LEU:O	1:A:191:GLN:HG2	2.15	0.46
1:B:147:PRO:HG2	1:B:413:ASN:ND2	2.30	0.46
1:D:130:VAL:O	1:D:132:GLY:N	2.48	0.46
1:D:146:PHE:CZ	1:D:243:VAL:HG21	2.51	0.46
1:D:227:PRO:HB2	1:D:363:ILE:HD12	1.98	0.46
1:B:348:HIS:O	1:B:352:VAL:HG22	2.15	0.46
1:C:338:HIS:HE1	1:C:387:ASN:O	1.97	0.46
1:D:451:MET:HA	1:D:451:MET:CE	2.45	0.46
1:B:59:SER:HB3	1:B:457:TYR:OH	2.17	0.46
1:C:130:VAL:HG12	1:C:458:VAL:HG21	1.98	0.46
1:C:107:GLY:CA	1:C:113:LEU:HD21	2.47	0.45
1:C:190:LEU:CD2	1:C:212:MET:HE3	2.21	0.45
1:C:71:THR:HG22	1:C:121:ALA:HB1	1.97	0.45
1:A:109:SER:H	1:A:112:GLU:HB2	1.80	0.45
1:A:355:PRO:HG2	1:B:332:GLY:HA3	1.99	0.45
1:A:439:LEU:HD22	1:A:444:GLY:HA2	1.98	0.45
1:A:182:LEU:HD21	1:A:257:ALA:HB1	1.99	0.45
1:C:103:ALA:HB2	1:C:131:ARG:HD2	1.99	0.45
1:A:133:ASP:OD1	1:A:133:ASP:N	2.48	0.45
1:B:465:GLY:HA2	1:B:468:LEU:CD2	2.47	0.45
1:A:127:HIS:CD2	1:A:128:THR:HG23	2.52	0.44
1:B:136:ALA:O	1:B:137:HIS:C	2.60	0.44
1:C:187:LEU:O	1:C:191:GLN:HG2	2.17	0.44
1:B:201:ARG:HB3	1:B:204:VAL:HG23	1.99	0.44
1:C:102:ARG:HD3	1:C:457:TYR:CZ	2.53	0.44
1:C:255:ILE:HA	1:C:353:LEU:CD2	2.47	0.44
1:A:76:ASP:O	1:A:80:HIS:HB2	2.17	0.44
1:A:182:LEU:HD13	1:A:184:TRP:CZ2	2.52	0.44
1:A:113:LEU:O	1:A:116:ALA:N	2.51	0.44
1:B:153:TRP:CH2	1:B:156:MET:HA	2.53	0.43
1:C:113:LEU:O	1:C:114:LEU:C	2.61	0.43
1:C:81:PRO:HA	1:C:110:ARG:HH22	1.83	0.43
1:A:85:PRO:O	1:A:89:GLY:N	2.40	0.43
1:B:153:TRP:CZ2	1:B:156:MET:HA	2.54	0.43
1:A:58:LEU:HD22	1:A:69:GLN:HG3	2.01	0.43
1:A:377:GLU:CD	1:B:198:PRO:HG3	2.43	0.43
1:A:172:LYS:HG2	1:A:187:LEU:HD11	2.01	0.43
1:D:105:VAL:HG22	1:D:129:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD12	1:A:114:LEU:N	2.34	0.42
1:C:103:ALA:CB	1:C:131:ARG:HD2	2.48	0.42
1:C:285:ARG:NH2	1:C:323:GLU:OE1	2.49	0.42
1:A:79:GLU:O	1:A:80:HIS:CG	2.71	0.42
1:C:108:GLU:HB2	1:C:112:GLU:HG2	2.01	0.42
1:B:182:LEU:HD13	1:B:184:TRP:CE2	2.55	0.42
1:B:456:ALA:HB1	1:B:461:LEU:HD12	2.00	0.42
1:D:206:GLN:HB2	1:D:207:PRO:HD3	2.01	0.42
1:A:255:ILE:HG12	1:A:353:LEU:HD11	2.01	0.42
1:C:356:VAL:C	1:C:358:PRO:HD3	2.44	0.42
1:C:465:GLY:HA2	1:C:468:LEU:HD21	1.99	0.42
1:A:157:ALA:HB2	1:A:212:MET:HE3	2.01	0.42
1:C:93:ILE:O	1:C:98:HIS:HE1	2.03	0.42
1:C:139:ASP:N	1:C:139:ASP:OD1	2.52	0.42
1:C:349:LEU:HG	1:C:353:LEU:HD12	2.02	0.42
1:C:456:ALA:HB1	1:C:461:LEU:HD12	2.01	0.42
1:D:300:SER:HB3	1:D:303:THR:HB	2.01	0.42
1:C:246:ALA:HB1	1:C:376:THR:HB	2.01	0.41
1:B:316:LEU:O	1:B:320:LEU:HG	2.20	0.41
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.95	0.41
1:D:246:ALA:HB1	1:D:376:THR:HB	2.03	0.41
1:C:113:LEU:H	1:C:113:LEU:HD22	1.86	0.41
1:C:184:TRP:CH2	1:C:204:VAL:HA	2.55	0.41
1:C:109:SER:O	1:C:110:ARG:C	2.63	0.41
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.91	0.41
1:D:130:VAL:HG12	1:D:132:GLY:H	1.85	0.41
1:A:136:ALA:O	1:A:137:HIS:C	2.62	0.41
1:A:465:GLY:HA2	1:A:468:LEU:HD21	2.03	0.41
1:C:220:TRP:CE2	1:C:410:LEU:HD21	2.56	0.41
1:A:112:GLU:OE1	1:A:112:GLU:N	2.53	0.40
1:A:338:HIS:CE1	1:A:387:ASN:O	2.73	0.40
1:B:285:ARG:HD3	1:B:320:LEU:HD21	2.03	0.40
1:B:319:GLU:O	1:B:323:GLU:HG3	2.21	0.40
1:D:263:TRP:NE1	1:D:388:MET:HE3	2.36	0.40
1:D:356:VAL:HG23	1:D:358:PRO:HD3	2.02	0.40
1:D:104:ALA:O	1:D:129:VAL:HA	2.21	0.40
1:D:272:MET:HG3	1:D:333:VAL:HG11	2.02	0.40
1:D:317:LEU:HD22	1:D:327:ALA:HB1	2.04	0.40
1:A:317:LEU:HD22	1:A:327:ALA:HB1	2.04	0.40
1:A:246:ALA:HB1	1:A:376:THR:HB	2.03	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	414/431 (96%)	398 (96%)	16 (4%)	0	100	100
1	B	367/431 (85%)	353 (96%)	14 (4%)	0	100	100
1	C	415/431 (96%)	402 (97%)	13 (3%)	0	100	100
1	D	369/431 (86%)	355 (96%)	14 (4%)	0	100	100
All	All	1565/1724 (91%)	1508 (96%)	57 (4%)	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	325/339 (96%)	312 (96%)	13 (4%)	28	54
1	B	290/339 (86%)	279 (96%)	11 (4%)	29	56
1	C	325/339 (96%)	311 (96%)	14 (4%)	26	51
1	D	290/339 (86%)	280 (97%)	10 (3%)	32	60
All	All	1230/1356 (91%)	1182 (96%)	48 (4%)	28	55

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	113	LEU

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Mol	Chain	Res	Type
1	A	118	LYS
1	A	133	ASP
1	A	142	VAL
1	A	275	VAL
1	A	294	SER
1	A	303	THR
1	A	310	VAL
1	A	353	LEU
1	A	359	ARG
1	A	379	LEU
1	A	458	VAL
1	B	129	VAL
1	B	142	VAL
1	B	214	LEU
1	B	259	ARG
1	B	263	TRP
1	B	300	SER
1	B	303	THR
1	B	379	LEU
1	B	424	GLU
1	B	458	VAL
1	B	468	LEU
1	C	109	SER
1	C	129	VAL
1	C	130	VAL
1	C	139	ASP
1	C	140	ARG
1	C	263	TRP
1	C	275	VAL
1	C	287	GLU
1	C	300	SER
1	C	303	THR
1	C	317	LEU
1	C	379	LEU
1	C	390	GLU
1	C	458	VAL
1	D	139	ASP
1	D	275	VAL
1	D	287	GLU
1	D	300	SER
1	D	310	VAL
1	D	321	THR

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Mol	Chain	Res	Type
1	D	408	LEU
1	D	451	MET
1	D	453	LEU
1	D	458	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	98	HIS
1	A	413	ASN
1	B	69	GLN
1	B	413	ASN
1	B	437	HIS
1	B	459	ASN
1	C	69	GLN
1	C	98	HIS
1	C	206	GLN
1	C	348	HIS
1	D	69	GLN
1	D	413	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	500	-	4,4,4	0.49	0	6,6,6	0.08	0
2	SO4	A	500	-	4,4,4	0.31	0	6,6,6	0.15	0
2	SO4	B	500	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	C	500	-	4,4,4	0.31	0	6,6,6	0.13	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	SO4	1	0
2	A	500	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	416/431 (96%)	0.09	11 (2%) 57 52	17, 37, 96, 141	0
1	B	375/431 (87%)	0.31	42 (11%) 10 8	20, 38, 126, 176	0
1	C	417/431 (96%)	0.12	20 (4%) 35 31	22, 40, 90, 145	0
1	D	375/431 (87%)	0.31	41 (10%) 10 9	19, 36, 127, 212	0
All	All	1583/1724 (91%)	0.20	114 (7%) 21 19	17, 39, 115, 212	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	LEU	7.7
1	D	70	SER	5.6
1	D	56	LEU	4.8
1	D	55	PRO	4.3
1	B	468	LEU	4.3
1	B	127	HIS	4.3
1	D	64	ALA	4.1
1	D	58	LEU	4.0
1	D	119	ALA	4.0
1	B	66	LEU	4.0
1	B	54	VAL	4.0
1	D	54	VAL	3.9
1	D	126	HIS	3.8
1	B	56	LEU	3.7
1	B	465	GLY	3.7
1	B	70	SER	3.7
1	D	71	THR	3.7
1	D	121	ALA	3.7
1	B	99	PHE	3.7
1	A	353	LEU	3.6
1	B	62	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	68	GLU	3.5
1	D	65	ALA	3.5
1	B	119	ALA	3.5
1	B	432	HIS	3.5
1	B	353	LEU	3.4
1	D	129	VAL	3.4
1	B	64	ALA	3.4
1	A	135	THR	3.4
1	A	431	GLY	3.3
1	D	62	THR	3.2
1	C	467	ALA	3.1
1	D	99	PHE	3.1
1	D	107	GLY	3.1
1	D	103	ALA	3.1
1	D	465	GLY	3.1
1	D	106	ILE	3.1
1	D	120	LEU	3.1
1	B	106	ILE	3.1
1	B	120	LEU	3.0
1	C	133	ASP	3.0
1	B	68	GLU	3.0
1	A	84	HIS	2.9
1	B	135	THR	2.9
1	A	137	HIS	2.9
1	D	128	THR	2.9
1	B	467	ALA	2.8
1	C	106	ILE	2.8
1	B	71	THR	2.8
1	C	136	ALA	2.8
1	A	79	GLU	2.8
1	D	124	ARG	2.8
1	B	55	PRO	2.7
1	B	58	LEU	2.7
1	D	353	LEU	2.7
1	B	137	HIS	2.7
1	D	63	GLU	2.7
1	C	54	VAL	2.7
1	D	122	GLU	2.6
1	B	128	THR	2.6
1	C	84	HIS	2.6
1	B	123	GLY	2.6
1	C	137	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	123	GLY	2.5
1	D	101	HIS	2.5
1	B	431	GLY	2.5
1	C	108	GLU	2.5
1	D	69	GLN	2.5
1	D	105	VAL	2.5
1	D	127	HIS	2.5
1	D	432	HIS	2.5
1	D	138	PRO	2.4
1	C	353	LEU	2.4
1	D	98	HIS	2.4
1	B	60	GLY	2.4
1	B	69	GLN	2.4
1	C	79	GLU	2.4
1	C	162	ASP	2.4
1	B	121	ALA	2.4
1	A	109	SER	2.3
1	D	67	ARG	2.3
1	D	137	HIS	2.3
1	C	294	SER	2.3
1	B	126	HIS	2.3
1	B	136	ALA	2.3
1	C	430	GLY	2.3
1	B	133	ASP	2.3
1	A	432	HIS	2.3
1	D	61	HIS	2.3
1	D	100	GLY	2.3
1	B	122	GLU	2.3
1	C	138	PRO	2.3
1	D	134	GLY	2.2
1	B	101	HIS	2.2
1	C	139	ASP	2.2
1	B	65	ALA	2.2
1	B	464	ASP	2.2
1	C	432	HIS	2.2
1	B	322	ALA	2.1
1	C	113	LEU	2.1
1	A	106	ILE	2.1
1	D	463	ILE	2.1
1	B	158	ARG	2.1
1	C	265	THR	2.1
1	D	60	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	125	GLU	2.1
1	B	67	ARG	2.1
1	C	115	ASP	2.1
1	B	105	VAL	2.0
1	B	124	ARG	2.0
1	B	281	ARG	2.0
1	A	108	GLU	2.0
1	C	468	LEU	2.0
1	A	162	ASP	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 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
2	SO4	C	500	5/5	0.96	0.10	44,46,55,65	0
2	SO4	D	500	5/5	0.96	0.10	40,41,45,55	0
2	SO4	A	500	5/5	0.97	0.09	32,34,38,48	0
2	SO4	B	500	5/5	0.97	0.07	42,44,46,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.