



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:04 PM EDT

PDB ID : 5E51 / pdb_00005e51
Title : Crystal structure of Mycobacterium tuberculosis L,D-transpeptidase 1 with Faropenem adduct
Authors : Kumar, P.; Lamichhane, G.; Ginell, S.L.
Deposited on : 2015-10-07
Resolution : 2.25 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

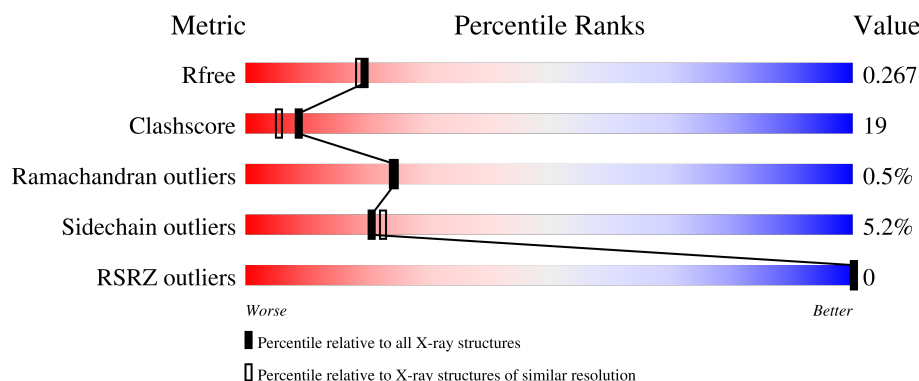
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	223	
1	B	223	
1	C	223	
1	D	223	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5886 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.

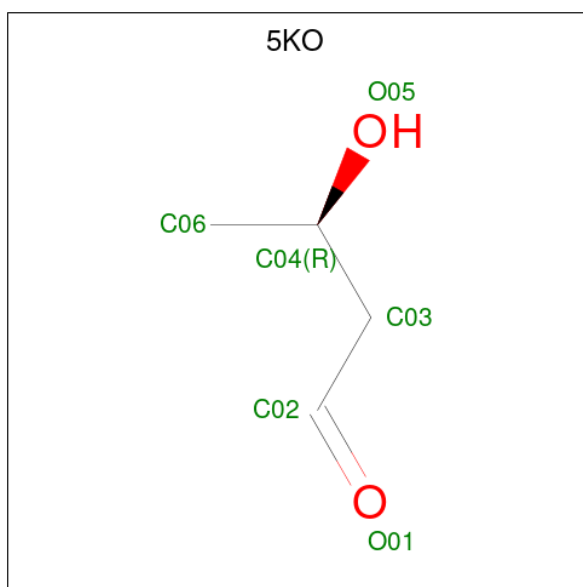
- Molecule 1 is a protein called L,D-transpeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1398	889	246	259	4			
1	B	200	Total	C	N	O	S	0	0	0
			1484	941	265	274	4			
1	C	190	Total	C	N	O	S	0	0	0
			1426	901	260	261	4			
1	D	192	Total	C	N	O	S	0	0	0
			1451	919	258	270	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q7DAG3
A	30	HIS	-	expression tag	UNP Q7DAG3
A	31	MET	-	expression tag	UNP Q7DAG3
B	29	GLY	-	expression tag	UNP Q7DAG3
B	30	HIS	-	expression tag	UNP Q7DAG3
B	31	MET	-	expression tag	UNP Q7DAG3
C	29	GLY	-	expression tag	UNP Q7DAG3
C	30	HIS	-	expression tag	UNP Q7DAG3
C	31	MET	-	expression tag	UNP Q7DAG3
D	29	GLY	-	expression tag	UNP Q7DAG3
D	30	HIS	-	expression tag	UNP Q7DAG3
D	31	MET	-	expression tag	UNP Q7DAG3

- Molecule 2 is (3R)-3-hydroxybutanal (CCD ID: 5KO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		
2	C	1	Total	C	O	0	0
			6	4	2		

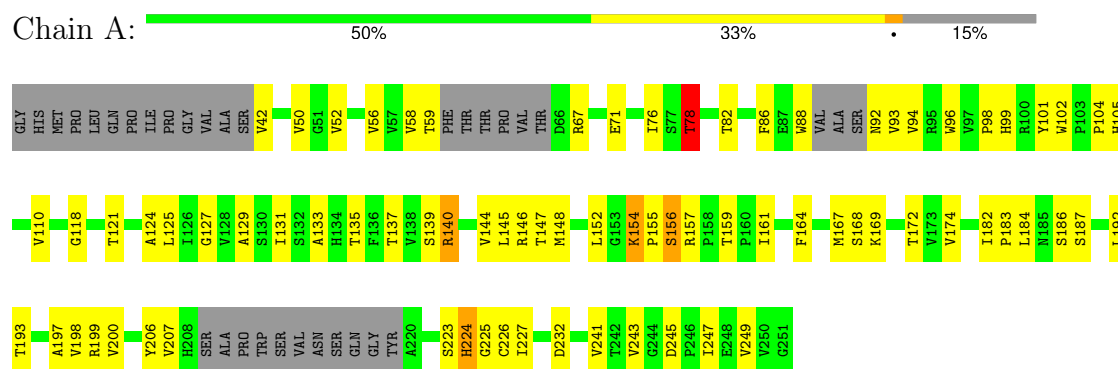
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	19	Total	O	0	0
			19	19		
3	C	39	Total	O	0	0
			39	39		
3	D	27	Total	O	0	0
			27	27		

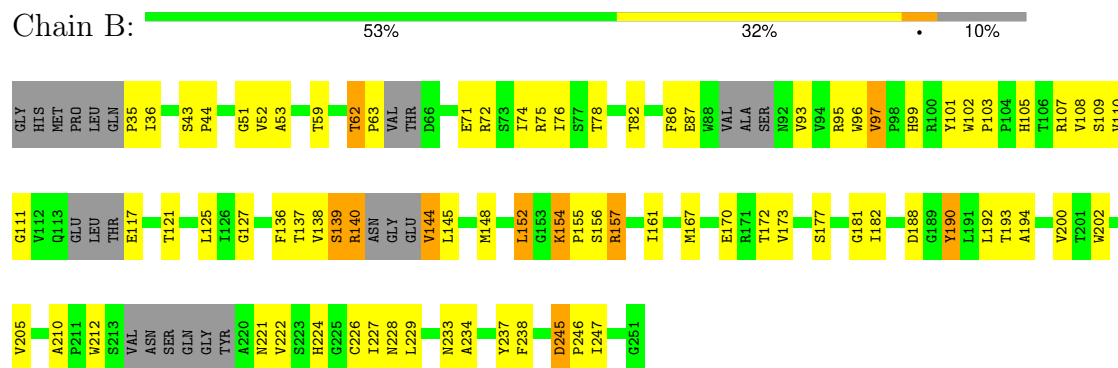
3 Residue-property plots [i](#)

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.

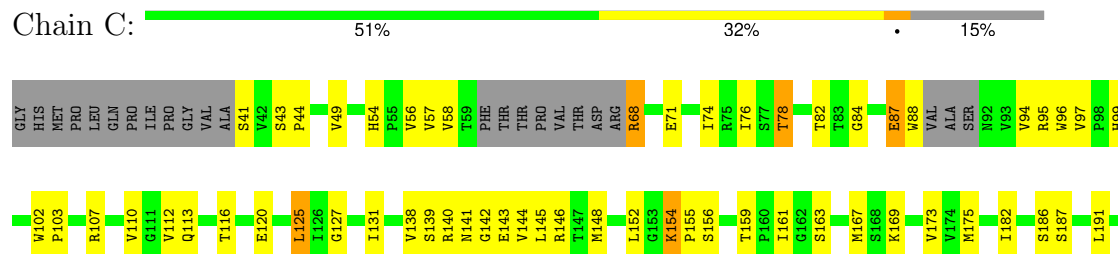
• Molecule 1: L,D-transpeptidase 1

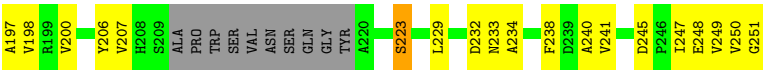


• Molecule 1: L,D-transpeptidase 1

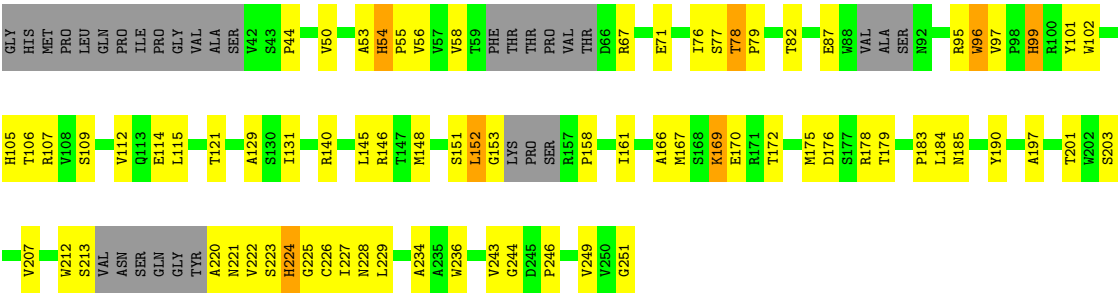


• Molecule 1: L,D-transpeptidase 1





● Molecule 1: L,D-transpeptidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	58.38Å 58.38Å 257.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 2.25 19.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	87.8 (19.88-2.25) 86.6 (19.88-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-5.72 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.258 , 0.296 0.235 , 0.267	Depositor DCC
R_{free} test set	2034 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.478 for -h,-k,l 0.470 for h,-h-k,-l 0.470 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 42244 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5886	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: 5KO

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	0.65	0/1437	1.09	11/1975 (0.6%)
1	B	0.59	0/1526	1.10	14/2093 (0.7%)
1	C	0.65	0/1464	1.20	14/2005 (0.7%)
1	D	0.64	0/1491	1.12	8/2045 (0.4%)
All	All	0.64	0/5918	1.13	47/8118 (0.6%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	PRO	CA-C-N	8.84	128.87	119.76
1	C	103	PRO	C-N-CA	8.84	128.87	119.76
1	C	223	SER	N-CA-C	8.10	123.85	113.88
1	B	157	ARG	CA-C-N	7.80	127.70	120.21
1	B	157	ARG	C-N-CA	7.80	127.70	120.21
1	B	97	VAL	CA-C-N	7.45	127.37	119.85
1	B	97	VAL	C-N-CA	7.45	127.37	119.85
1	C	97	VAL	CA-C-N	7.31	127.07	119.76
1	C	97	VAL	C-N-CA	7.31	127.07	119.76
1	C	182	ILE	CA-C-N	6.91	126.87	120.03
1	C	182	ILE	C-N-CA	6.91	126.87	120.03
1	B	221	ASN	N-CA-C	6.68	119.13	109.71
1	D	78	THR	CA-C-N	6.50	126.73	119.32
1	D	78	THR	C-N-CA	6.50	126.73	119.32
1	A	245	ASP	CA-C-N	6.37	126.39	119.90
1	A	245	ASP	C-N-CA	6.37	126.39	119.90
1	A	154	LYS	CA-C-N	6.11	127.48	119.84
1	A	154	LYS	C-N-CA	6.11	127.48	119.84
1	D	58	VAL	N-CA-C	6.08	116.62	108.11
1	A	78	THR	CA-C-N	5.98	126.13	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	THR	C-N-CA	5.98	126.13	119.32
1	C	154	LYS	CA-C-N	5.81	127.11	119.84
1	C	154	LYS	C-N-CA	5.81	127.11	119.84
1	A	56	VAL	N-CA-C	-5.70	100.21	108.36
1	C	245	ASP	CA-C-N	5.66	125.67	119.90
1	C	245	ASP	C-N-CA	5.66	125.67	119.90
1	B	139	SER	N-CA-C	5.65	118.43	109.50
1	C	113	GLN	CB-CA-C	-5.62	109.59	117.23
1	B	190	TYR	N-CA-C	5.40	116.73	108.52
1	A	118	GLY	N-CA-C	5.37	118.96	110.96
1	D	99	HIS	N-CA-C	5.37	118.99	112.23
1	C	102	TRP	N-CA-C	-5.33	104.00	110.13
1	A	157	ARG	CA-C-N	5.29	125.50	120.31
1	A	157	ARG	C-N-CA	5.29	125.50	120.31
1	C	182	ILE	N-CA-C	5.28	113.75	107.73
1	D	54	HIS	CA-C-N	5.25	125.25	120.21
1	D	54	HIS	C-N-CA	5.25	125.25	120.21
1	D	96	TRP	CA-C-N	-5.25	117.66	123.43
1	D	96	TRP	C-N-CA	-5.25	117.66	123.43
1	B	103	PRO	CA-C-N	5.18	125.10	119.76
1	B	103	PRO	C-N-CA	5.18	125.10	119.76
1	B	154	LYS	CA-C-N	5.11	126.23	119.84
1	B	154	LYS	C-N-CA	5.11	126.23	119.84
1	A	192	LEU	N-CA-C	5.04	117.04	109.23
1	B	72	ARG	N-CA-C	-5.04	106.98	113.23
1	B	245	ASP	CA-C-N	5.02	125.31	119.93
1	B	245	ASP	C-N-CA	5.02	125.31	119.93

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	1398	0	1320	58	0
1	B	1484	0	1416	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1426	0	1378	49	1
1	D	1451	0	1388	57	1
2	A	6	0	0	0	0
2	C	6	0	0	0	0
3	A	30	0	0	4	0
3	B	19	0	0	1	0
3	C	39	0	0	4	1
3	D	27	0	0	3	1
All	All	5886	0	5502	211	2

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 19.

All (211) 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:D:201:THR:HG1	1:D:203:SER:HG	1.21	0.89
1:A:52:VAL:HA	1:A:102:TRP:HD1	1.46	0.80
1:D:105:HIS:N	1:D:121:THR:O	2.16	0.78
1:C:169:LYS:HD2	1:C:241:VAL:HG13	1.68	0.76
1:B:87:GLU:OE1	1:B:95:ARG:NH1	2.19	0.74
1:A:42:VAL:HG22	1:A:58:VAL:HG13	1.70	0.74
1:C:146:ARG:NH2	1:C:233:ASN:OD1	2.21	0.74
1:B:139:SER:HA	1:B:144:VAL:HA	1.71	0.73
1:D:212:TRP:HB2	1:D:220:ALA:HB1	1.69	0.72
1:C:200:VAL:HG13	1:C:247:ILE:HG21	1.72	0.71
1:A:125:LEU:HD12	1:A:140:ARG:HB2	1.73	0.71
1:D:114:GLU:HG3	1:D:115:LEU:HD12	1.73	0.70
1:D:213:SER:HB3	1:D:220:ALA:HA	1.76	0.68
1:A:133:ALA:O	3:A:401:HOH:O	2.12	0.68
1:A:198:VAL:HB	1:A:207:VAL:HB	1.76	0.67
1:C:169:LYS:NZ	1:C:238:PHE:O	2.24	0.66
1:B:107:ARG:NH2	1:B:109:SER:OG	2.28	0.66
1:B:226:CYS:SG	3:B:317:HOH:O	2.30	0.65
1:C:163:SER:O	3:C:403:HOH:O	2.15	0.65
1:D:53:ALA:HB2	1:D:246:PRO:HG3	1.78	0.64
1:A:52:VAL:HB	1:A:102:TRP:H	1.63	0.63
1:C:229:LEU:HB2	1:C:234:ALA:HB2	1.80	0.63
1:D:77:SER:HB3	1:D:109:SER:HB3	1.79	0.63
1:D:67:ARG:O	1:D:71:GLU:HG3	1.99	0.63
1:A:92:ASN:ND2	3:A:403:HOH:O	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LEU:HB2	1:B:234:ALA:HB2	1.80	0.62
1:B:62:THR:HG22	1:B:63:PRO:HD2	1.81	0.61
1:B:154:LYS:NZ	1:B:188:ASP:OD1	2.23	0.61
1:A:159:THR:HG23	1:A:249:VAL:HG11	1.82	0.60
1:B:78:THR:HB	1:B:82:THR:H	1.66	0.60
1:D:102:TRP:CD1	1:D:121:THR:HG21	2.37	0.59
1:C:78:THR:HG21	1:C:82:THR:H	1.67	0.58
1:A:67:ARG:O	1:A:71:GLU:HG3	2.03	0.58
1:A:183:PRO:HG2	1:A:186:SER:HB2	1.86	0.58
1:A:127:GLY:HA2	1:A:137:THR:O	2.04	0.58
1:A:164:PHE:O	1:A:247:ILE:N	2.31	0.58
1:A:168:SER:OG	1:A:199:ARG:NH1	2.37	0.58
1:D:54:HIS:HD2	1:D:55:PRO:HD2	1.67	0.58
1:A:232:ASP:OD1	1:C:232:ASP:HB3	2.03	0.58
1:D:76:ILE:HG13	1:D:96:TRP:CE3	2.39	0.57
1:D:87:GLU:OE1	1:D:95:ARG:NH2	2.33	0.57
1:D:176:ASP:HB3	1:D:179:THR:HG23	1.86	0.57
1:A:52:VAL:HA	1:A:102:TRP:CD1	2.34	0.57
1:A:86:PHE:HD1	1:A:94:VAL:HG21	1.68	0.57
1:C:146:ARG:HG2	1:C:148:MET:HG3	1.87	0.56
1:A:98:PRO:HB2	1:A:101:TYR:O	2.06	0.56
1:D:54:HIS:HB2	1:D:244:GLY:HA3	1.87	0.56
1:C:131:ILE:N	1:C:250:VAL:O	2.35	0.56
1:C:140:ARG:N	1:C:143:GLU:O	2.38	0.56
1:A:200:VAL:O	3:A:402:HOH:O	2.18	0.56
1:D:207:VAL:HG22	1:D:227:ILE:HD11	1.89	0.55
1:D:178:ARG:HD3	1:D:184:LEU:HG	1.87	0.55
1:C:175:MET:O	1:C:191:LEU:HA	2.07	0.55
1:A:154:LYS:C	1:A:156:SER:H	2.15	0.54
1:B:125:LEU:CD1	1:B:140:ARG:HD3	2.37	0.54
1:C:87:GLU:OE1	1:C:95:ARG:NH2	2.40	0.54
1:A:104:PRO:HG3	1:A:124:ALA:HB2	1.88	0.54
1:C:41:SER:O	1:C:58:VAL:HA	2.07	0.54
1:D:50:VAL:HG23	1:D:121:THR:HG22	1.90	0.54
1:B:140:ARG:HG3	1:B:145:LEU:HD11	1.90	0.54
1:A:154:LYS:O	1:A:156:SER:N	2.40	0.54
1:C:197:ALA:HA	1:C:207:VAL:O	2.08	0.53
1:A:86:PHE:CE2	1:A:96:TRP:HD1	2.26	0.53
1:B:52:VAL:O	1:B:102:TRP:N	2.40	0.53
1:B:148:MET:HB2	1:B:233:ASN:ND2	2.24	0.53
1:B:192:LEU:HD13	1:B:210:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:THR:HG23	1:B:93:VAL:HG22	1.91	0.52
1:B:125:LEU:HD12	1:B:140:ARG:HD3	1.91	0.52
1:D:131:ILE:HD12	1:D:161:ILE:HD11	1.90	0.52
1:B:157:ARG:HD2	1:D:161:ILE:HG22	1.90	0.52
1:C:56:VAL:HG21	1:C:76:ILE:HD11	1.91	0.52
1:C:127:GLY:HA3	1:C:138:VAL:HG22	1.91	0.52
1:D:207:VAL:HG13	1:D:227:ILE:HD11	1.91	0.52
1:B:194:ALA:HA	1:B:210:ALA:HB2	1.92	0.52
1:A:78:THR:OG1	1:A:82:THR:N	2.44	0.51
1:A:105:HIS:HA	1:A:121:THR:O	2.09	0.51
1:D:185:ASN:OD1	3:D:302:HOH:O	2.19	0.51
1:B:200:VAL:HB	1:B:205:VAL:HB	1.92	0.51
1:A:232:ASP:HB3	1:C:232:ASP:OD1	2.11	0.51
1:C:141:ASN:H	1:C:142:GLY:HA3	1.75	0.51
1:D:79:PRO:HG2	1:D:106:THR:HG23	1.93	0.51
1:B:136:PHE:O	1:B:148:MET:HG2	2.11	0.50
1:D:78:THR:HG21	1:D:82:THR:OG1	2.11	0.50
1:A:76:ILE:HG13	1:A:96:TRP:CD2	2.47	0.50
1:D:223:SER:C	1:D:225:GLY:H	2.18	0.50
1:D:107:ARG:O	3:D:301:HOH:O	2.19	0.50
1:D:166:ALA:O	1:D:243:VAL:HG13	2.12	0.50
1:C:76:ILE:HD13	1:C:110:VAL:HG13	1.94	0.50
1:D:131:ILE:HB	1:D:251:GLY:HA3	1.92	0.50
1:B:148:MET:HG3	1:B:229:LEU:HD22	1.94	0.50
1:D:226:CYS:SG	3:D:323:HOH:O	2.37	0.50
1:C:49:VAL:HA	1:C:120:GLU:O	2.12	0.50
1:A:88:TRP:CD2	1:A:94:VAL:HB	2.47	0.50
1:A:174:VAL:HA	1:A:193:THR:HA	1.94	0.50
1:D:56:VAL:O	1:D:95:ARG:HA	2.12	0.50
1:B:234:ALA:O	1:B:238:PHE:HB2	2.12	0.49
1:D:170:GLU:HB2	1:D:197:ALA:HB3	1.93	0.49
1:A:88:TRP:CE2	1:A:94:VAL:HB	2.48	0.49
1:A:92:ASN:HA	3:A:427:HOH:O	2.12	0.49
1:A:184:LEU:HB3	1:B:75:ARG:NH1	2.28	0.48
1:D:170:GLU:N	1:D:197:ALA:O	2.32	0.48
1:B:138:VAL:HG21	1:B:237:TYR:HD1	1.79	0.48
1:B:222:VAL:HG21	1:B:228:ASN:HB3	1.94	0.48
1:D:175:MET:HB3	1:D:190:TYR:CE1	2.48	0.48
1:B:161:ILE:HD12	1:D:158:PRO:HD2	1.94	0.48
1:A:131:ILE:HD12	1:A:161:ILE:HD11	1.96	0.48
1:C:198:VAL:HB	1:C:207:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:CE1	1:B:96:TRP:HD1	2.31	0.48
1:C:141:ASN:N	1:C:142:GLY:HA3	2.29	0.48
1:B:210:ALA:O	1:B:212:TRP:HD1	1.95	0.47
1:B:154:LYS:C	1:B:156:SER:H	2.22	0.47
1:B:181:GLY:HA3	1:D:99:HIS:CE1	2.48	0.47
1:D:44:PRO:HG3	1:D:54:HIS:CE1	2.49	0.47
1:A:139:SER:HA	1:A:144:VAL:HA	1.96	0.47
1:B:52:VAL:HG23	1:B:101:TYR:HB3	1.97	0.47
1:C:127:GLY:HA2	1:C:138:VAL:HA	1.96	0.47
1:D:146:ARG:HD2	1:D:236:TRP:CE3	2.50	0.47
1:A:76:ILE:HG13	1:A:96:TRP:CE3	2.49	0.47
1:C:43:SER:O	1:C:56:VAL:HA	2.15	0.47
1:B:152:LEU:HD23	1:B:227:ILE:HG23	1.97	0.47
1:A:154:LYS:HE2	1:A:223:SER:HA	1.97	0.47
1:C:223:SER:OG	3:C:402:HOH:O	2.00	0.47
1:A:146:ARG:HG2	1:A:148:MET:HG3	1.98	0.46
1:A:200:VAL:HG22	1:A:247:ILE:HD13	1.97	0.46
1:B:105:HIS:N	1:B:121:THR:OG1	2.48	0.46
1:D:146:ARG:HG2	1:D:148:MET:CG	2.46	0.46
1:A:174:VAL:HG22	1:A:193:THR:OG1	2.15	0.46
1:A:224:HIS:HB3	1:A:226:CYS:SG	2.56	0.46
1:B:43:SER:HA	1:B:44:PRO:C	2.40	0.46
1:B:71:GLU:HG2	1:B:86:PHE:CE2	2.51	0.45
1:B:167:MET:HE1	1:B:202:TRP:CD1	2.51	0.45
1:C:186:SER:O	3:C:404:HOH:O	2.20	0.45
1:D:112:VAL:HG23	1:D:115:LEU:HB2	1.98	0.45
1:A:50:VAL:HG12	1:A:243:VAL:HG23	1.98	0.45
1:A:146:ARG:HG2	1:A:148:MET:CG	2.46	0.45
1:C:43:SER:HA	1:C:44:PRO:C	2.41	0.45
1:C:84:GLY:HA3	1:C:96:TRP:CZ2	2.50	0.45
1:C:154:LYS:C	1:C:156:SER:H	2.24	0.45
1:C:159:THR:HG22	1:C:249:VAL:HG11	1.99	0.45
1:B:136:PHE:N	1:B:148:MET:O	2.43	0.45
1:B:51:GLY:HA3	1:B:245:ASP:N	2.32	0.45
1:D:161:ILE:HA	1:D:249:VAL:HB	1.99	0.45
1:B:127:GLY:HA2	1:B:137:THR:O	2.16	0.45
1:D:167:MET:HE2	1:D:167:MET:HB3	1.84	0.45
1:B:53:ALA:H	1:B:246:PRO:HD3	1.82	0.45
1:C:78:THR:CG2	1:C:82:THR:H	2.29	0.45
1:D:224:HIS:HB3	1:D:226:CYS:SG	2.58	0.44
1:A:161:ILE:HG23	1:A:249:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:SER:HB2	1:D:228:ASN:HB3	1.99	0.44
1:A:86:PHE:HD1	1:A:94:VAL:CG2	2.29	0.44
1:A:59:THR:OG1	1:A:93:VAL:HG22	2.18	0.44
1:A:140:ARG:CB	1:A:145:LEU:HD11	2.47	0.44
1:A:169:LYS:HD2	1:A:241:VAL:HG13	2.00	0.44
1:A:161:ILE:HA	1:A:249:VAL:HB	2.00	0.44
1:A:198:VAL:O	1:A:207:VAL:N	2.31	0.44
1:B:181:GLY:CA	1:D:99:HIS:CE1	3.01	0.44
1:B:222:VAL:HG21	1:B:228:ASN:CB	2.47	0.44
1:D:153:GLY:HA2	1:D:225:GLY:HA2	2.00	0.44
1:B:154:LYS:O	1:B:156:SER:N	2.51	0.44
1:D:146:ARG:HE	1:D:146:ARG:HB2	1.56	0.44
1:C:154:LYS:O	1:C:156:SER:N	2.51	0.43
1:B:35:PRO:HB3	1:B:36:ILE:HA	2.00	0.43
1:D:54:HIS:CD2	1:D:55:PRO:HD2	2.51	0.43
1:D:183:PRO:HB2	1:D:185:ASN:OD1	2.18	0.43
1:B:53:ALA:N	1:B:246:PRO:HD3	2.33	0.43
1:B:177:SER:HB3	1:B:190:TYR:CZ	2.54	0.43
1:C:154:LYS:HE2	1:C:223:SER:HA	2.00	0.43
1:C:125:LEU:HD13	1:C:240:ALA:HB1	2.00	0.43
1:D:169:LYS:HE3	1:D:169:LYS:HB2	1.71	0.43
1:D:213:SER:HB3	1:D:221:ASN:H	1.83	0.43
1:D:229:LEU:HB2	1:D:234:ALA:HB2	2.00	0.43
1:A:152:LEU:HB3	1:A:159:THR:CG2	2.49	0.43
1:B:76:ILE:HG13	1:B:96:TRP:CE2	2.54	0.42
1:B:200:VAL:HG22	1:B:247:ILE:HD13	2.00	0.42
1:A:76:ILE:CD1	1:A:110:VAL:HG13	2.49	0.42
1:C:44:PRO:HG3	1:C:54:HIS:CE1	2.54	0.42
1:C:167:MET:HE2	1:C:167:MET:HB3	1.81	0.42
1:D:54:HIS:HB2	1:D:244:GLY:CA	2.50	0.42
1:D:129:ALA:HB1	1:D:152:LEU:HD22	2.02	0.42
1:C:197:ALA:HB1	1:C:206:TYR:CD2	2.53	0.42
1:A:152:LEU:HD23	1:A:227:ILE:HG23	2.01	0.42
1:C:140:ARG:CB	1:C:145:LEU:HD11	2.50	0.42
1:C:68:ARG:NE	1:C:71:GLU:OE1	2.52	0.42
1:B:74:ILE:HA	1:B:111:GLY:O	2.20	0.42
1:C:131:ILE:HB	1:C:251:GLY:HA3	2.02	0.42
1:C:198:VAL:N	1:C:207:VAL:O	2.42	0.42
1:D:102:TRP:CG	1:D:121:THR:HG21	2.54	0.42
1:A:223:SER:C	1:A:225:GLY:H	2.27	0.42
1:B:210:ALA:HB3	1:B:212:TRP:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:THR:HG23	1:B:193:THR:CG2	2.50	0.41
1:C:173:VAL:HG13	1:C:175:MET:HE3	2.01	0.41
1:A:137:THR:OG1	1:A:147:THR:HG23	2.19	0.41
1:A:129:ALA:HA	1:A:135:THR:O	2.20	0.41
1:A:167:MET:SD	1:A:199:ARG:HD3	2.60	0.41
1:B:105:HIS:HA	1:B:121:THR:O	2.20	0.41
1:B:177:SER:HB2	1:B:182:ILE:HB	2.02	0.41
1:A:197:ALA:HB1	1:A:206:TYR:CD2	2.56	0.41
1:C:57:VAL:HG22	1:C:95:ARG:CB	2.51	0.41
1:C:125:LEU:HD23	1:C:139:SER:O	2.21	0.41
1:A:167:MET:HE2	1:A:167:MET:HB3	1.75	0.41
1:B:170:GLU:OE1	1:B:173:VAL:HB	2.20	0.41
1:D:227:ILE:O	1:D:227:ILE:HG13	2.21	0.41
1:A:92:ASN:HB3	1:A:93:VAL:H	1.65	0.41
1:C:74:ILE:HG12	1:C:112:VAL:HG22	2.02	0.41
1:C:139:SER:OG	1:C:144:VAL:HG12	2.21	0.40
1:D:161:ILE:HG23	1:D:249:VAL:O	2.21	0.40
1:B:102:TRP:CH2	1:B:108:VAL:HG11	2.56	0.40
1:C:88:TRP:CH2	1:C:94:VAL:HB	2.56	0.40
1:C:248:GLU:OE2	3:C:405:HOH:O	2.22	0.40
1:D:145:LEU:HB2	1:D:236:TRP:HH2	1.86	0.40
1:D:212:TRP:CE2	1:D:222:VAL:HG13	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:426:HOH:O	3:D:315:HOH:O[1_445]	2.09	0.11
1:C:116:THR:OG1	1:D:178:ARG:NH2[1_445]	2.12	0.08

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	182/223 (82%)	173 (95%)	8 (4%)	1 (0%)	24	24
1	B	188/223 (84%)	175 (93%)	12 (6%)	1 (0%)	24	24
1	C	182/223 (82%)	173 (95%)	8 (4%)	1 (0%)	24	24
1	D	182/223 (82%)	169 (93%)	12 (7%)	1 (0%)	24	24
All	All	734/892 (82%)	690 (94%)	40 (5%)	4 (0%)	24	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	PRO
1	D	101	TYR
1	C	155	PRO
1	B	155	PRO

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	147/186 (79%)	139 (95%)	8 (5%)	20	21
1	B	159/186 (86%)	150 (94%)	9 (6%)	18	19
1	C	153/186 (82%)	144 (94%)	9 (6%)	18	18
1	D	157/186 (84%)	151 (96%)	6 (4%)	29	36
All	All	616/744 (83%)	584 (95%)	32 (5%)	21	22

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	99	HIS
1	A	140	ARG
1	A	156	SER
1	A	172	THR
1	A	182	ILE
1	A	187	SER

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Mol	Chain	Res	Type
1	A	224	HIS
1	B	62	THR
1	B	97	VAL
1	B	99	HIS
1	B	110	VAL
1	B	117	GLU
1	B	140	ARG
1	B	144	VAL
1	B	152	LEU
1	B	224	HIS
1	C	68	ARG
1	C	78	THR
1	C	87	GLU
1	C	99	HIS
1	C	107	ARG
1	C	125	LEU
1	C	152	LEU
1	C	161	ILE
1	C	187	SER
1	D	97	VAL
1	D	140	ARG
1	D	152	LEU
1	D	169	LYS
1	D	172	THR
1	D	224	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	HIS
1	C	228	ASN
1	D	54	HIS
1	D	85	HIS
1	D	92	ASN

5.3.3 RNA ⓘ

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](#)

2 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	5KO	C	301	1	5,5,5	0.74	0	5,5,5	1.11	1 (20%)
2	5KO	A	301	1	5,5,5	0.84	0	5,5,5	1.14	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5KO	C	301	1	-	2/3/3/3	-
2	5KO	A	301	1	-	2/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	5KO	O01-C02-C03	-2.32	118.63	125.38
2	C	301	5KO	O01-C02-C03	-2.07	119.34	125.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	5KO	C02-C03-C04-O05
2	A	301	5KO	C02-C03-C04-C06
2	C	301	5KO	C02-C03-C04-O05
2	C	301	5KO	C02-C03-C04-C06

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	190/223 (85%)	-0.71	0 100 100	13, 20, 44, 62	0
1	B	200/223 (89%)	-0.47	0 100 100	16, 29, 59, 127	0
1	C	190/223 (85%)	-0.68	0 100 100	13, 22, 39, 74	0
1	D	192/223 (86%)	-0.65	0 100 100	11, 23, 36, 46	0
All	All	772/892 (86%)	-0.63	0 100 100	11, 23, 49, 127	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	5KO	C	301	6/6	0.96	0.06	20,22,26,26	0
2	5KO	A	301	6/6	0.98	0.06	20,21,22,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.