



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 12:20 pm GMT

PDB ID : 5AH2
Title : The sliding clamp of Mycobacterium smegmatis in complex with a natural product.
Authors : Lukat, P.; Kling, A.; Heinz, D.W.; Mueller, R.
Deposited on : 2015-02-04
Resolution : 2.13 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 : 4.02b-467
Mogul : 1.8.4, 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

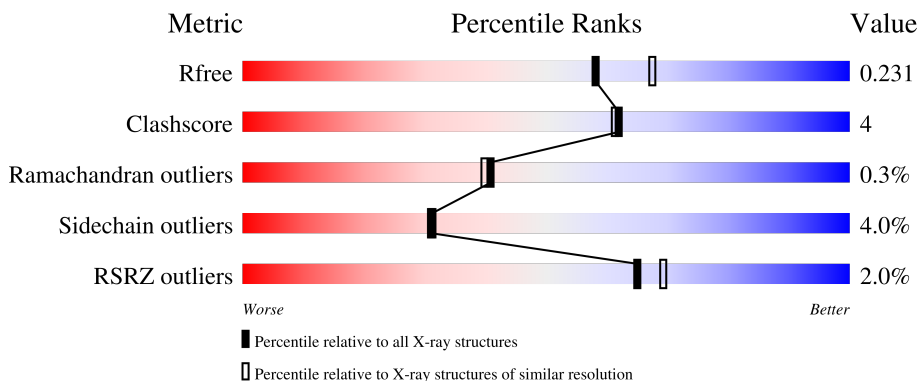
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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.



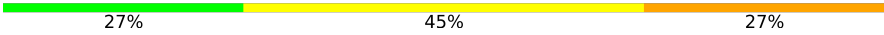
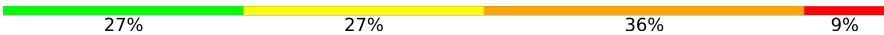

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	401	 2% 85% 10% 5%
1	B	401	 2% 85% 9% 6%
1	C	401	 2% 83% 11% 5%
1	D	401	 2% 83% 11% 5%
2	E	11	 36% 45% 18%

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Mol	Chain	Length	Quality of chain
2	F	11	
2	G	11	
2	H	11	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12271 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 DNA POLYMERASE III SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	Total 2842	C 1804	N 484	O 550	S 4	0	11	0
1	B	377	Total 2791	C 1782	N 472	O 533	S 4	0	10	0
1	C	382	Total 2784	C 1770	N 469	O 541	S 4	0	4	0
1	D	379	Total 2766	C 1765	N 477	O 520	S 4	0	9	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0QND6
A	-2	GLY	-	expression tag	UNP A0QND6
A	-1	GLY	-	expression tag	UNP A0QND6
A	0	ARG	-	expression tag	UNP A0QND6
B	-3	GLY	-	expression tag	UNP A0QND6
B	-2	GLY	-	expression tag	UNP A0QND6
B	-1	GLY	-	expression tag	UNP A0QND6
B	0	ARG	-	expression tag	UNP A0QND6
C	-3	GLY	-	expression tag	UNP A0QND6
C	-2	GLY	-	expression tag	UNP A0QND6
C	-1	GLY	-	expression tag	UNP A0QND6
C	0	ARG	-	expression tag	UNP A0QND6
D	-3	GLY	-	expression tag	UNP A0QND6
D	-2	GLY	-	expression tag	UNP A0QND6
D	-1	GLY	-	expression tag	UNP A0QND6
D	0	ARG	-	expression tag	UNP A0QND6

- Molecule 2 is a protein called GRISELIMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			79	57	10	12			
2	F	11	Total	C	N	O	0	0	0
			79	57	10	12			
2	G	11	Total	C	N	O	0	0	0
			79	57	10	12			
2	H	11	Total	C	N	O	0	0	0
			79	57	10	12			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

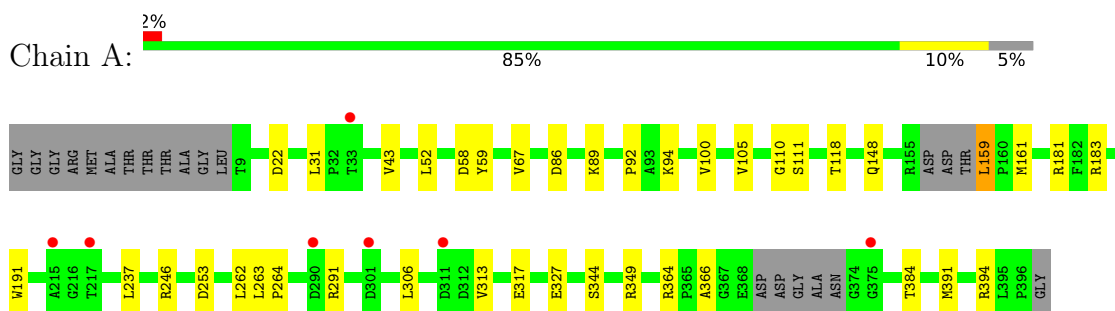
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	273	Total	O	0	0
			273	273		
4	B	190	Total	O	0	0
			190	190		
4	C	183	Total	O	0	0
			183	183		
4	D	124	Total	O	0	0
			124	124		

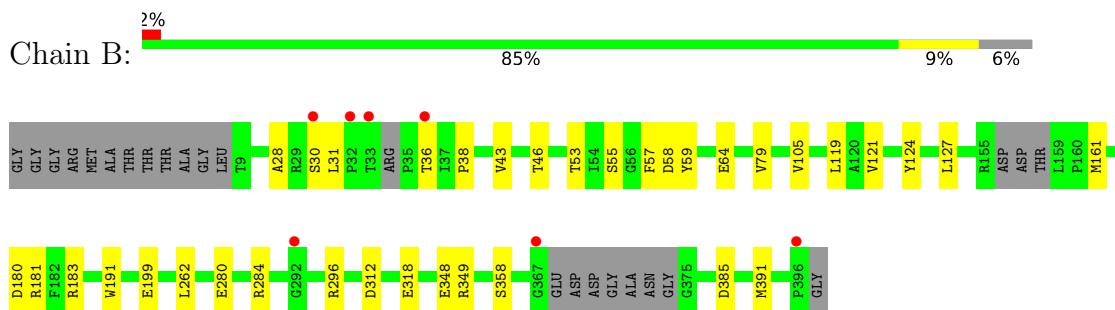
3 Residue-property plots i

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.

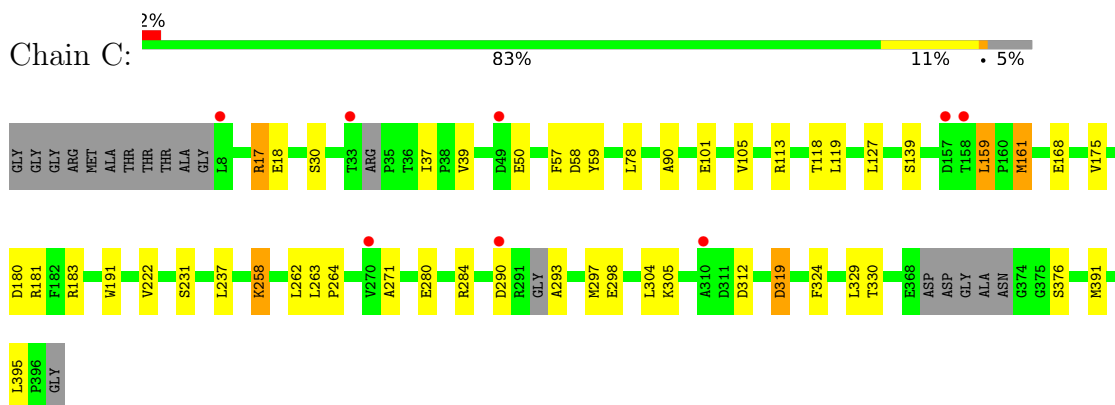
- Molecule 1: DNA POLYMERASE III SUBUNIT BETA



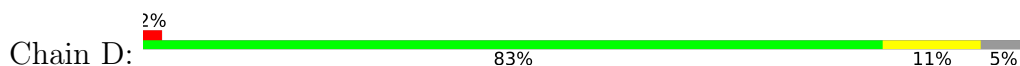
- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

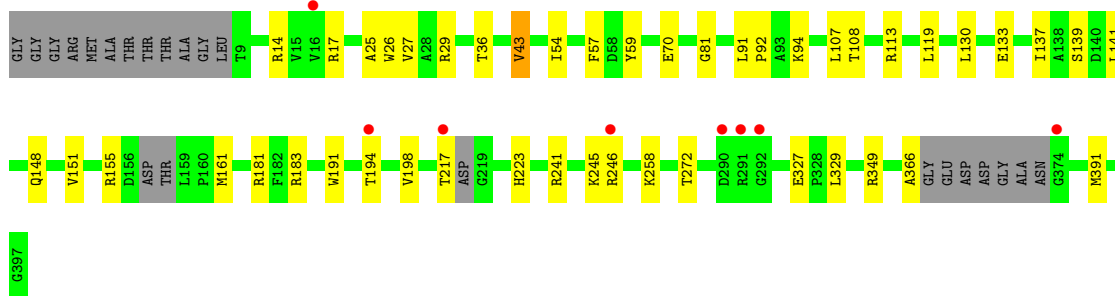


- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

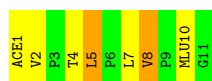


- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

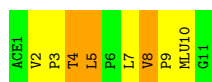
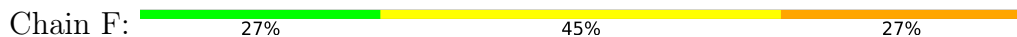




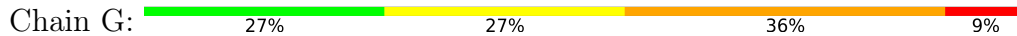
• Molecule 2: GRISELIMYCIN



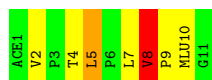
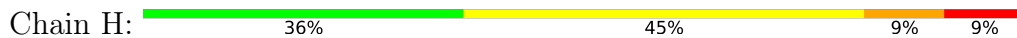
• Molecule 2: GRISELIMYCIN



• Molecule 2: GRISELIMYCIN



• Molecule 2: GRISELIMYCIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.24Å 125.87Å 94.90Å 90.00° 104.42° 90.00°	Depositor
Resolution (Å)	77.71 – 2.13 77.71 – 2.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.71-2.13) 100.0 (77.71-2.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.12Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.182 , 0.231 0.183 , 0.231	Depositor DCC
R_{free} test set	5071 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12271	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: MVA, MLU, NZC, ACE, MP8, NA

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	0.42	0/2906	0.56	0/3965
1	B	0.40	0/2863	0.56	0/3906
1	C	0.39	0/2838	0.54	0/3875
1	D	0.35	0/2835	0.51	0/3872
2	E	0.52	0/24	1.21	0/26
2	F	0.53	0/24	1.39	0/26
2	G	0.56	0/24	1.20	0/26
2	H	0.45	0/24	1.13	0/26
All	All	0.39	0/11538	0.55	0/15722

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	8	MVA	Peptide

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Mol	Chain	Res	Type	Group
2	F	8	MVA	Peptide
2	G	8	MVA	Peptide
2	H	8	MVA	Peptide

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	2842	0	2888	23	0
1	B	2791	0	2865	21	0
1	C	2784	0	2800	27	0
1	D	2766	0	2819	21	0
2	E	79	0	96	6	0
2	F	79	0	96	6	0
2	G	79	0	96	8	0
2	H	79	0	96	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	273	0	0	7	0
4	B	190	0	0	4	0
4	C	183	0	0	4	0
4	D	124	0	0	0	0
All	All	12271	0	11756	103	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 4.

All (103) 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:79[B]:VAL:HG11	1:B:105:VAL:HG11	1.71	0.72
1:B:348[A]:GLU:HG2	1:B:349:ARG:HG3	1.72	0.71
1:A:391:MET:HB2	2:E:5:LEU:HD13	1.75	0.69
1:A:92:PRO:HB2	1:A:94:LYS:HD2	1.75	0.69
1:B:181:ARG:HD3	2:F:10:MLU:HD22	1.76	0.68
1:D:391:MET:HB2	2:H:5:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD11	2:E:7:LEU:HD21	1.80	0.62
1:A:181:ARG:HD3	2:E:10:MLU:HD22	1.82	0.61
1:A:364[A]:ARG:NH1	1:A:384:THR:OG1	2.29	0.61
1:B:30:SER:OG	4:B:2016:HOH:O	2.15	0.60
1:A:159:LEU:HD12	1:A:161:MET:HG2	1.83	0.59
1:A:105:VAL:HG23	1:A:118:THR:HG22	1.85	0.58
1:D:14:ARG:NH1	1:D:70:GLU:OE1	2.37	0.57
1:D:349[B]:ARG:HB2	1:D:366:ALA:HB3	1.85	0.57
1:C:391:MET:HB2	2:G:5:LEU:HD13	1.86	0.57
1:B:262:LEU:HD11	2:F:7:LEU:HD21	1.87	0.56
1:D:181:ARG:HD3	2:H:10:MLU:HD22	1.86	0.56
1:B:280:GLU:OE2	1:B:284[A]:ARG:NH2	2.34	0.56
1:B:28:ALA:HA	1:B:31:LEU:HG	1.88	0.56
1:A:246[B]:ARG:NH1	4:A:2100:HOH:O	2.39	0.55
1:B:31:LEU:HD11	1:B:43[B]:VAL:HG23	1.87	0.55
1:B:36:THR:O	1:B:38:PRO:HD3	2.07	0.54
1:C:161:MET:O	4:C:2089:HOH:O	2.19	0.54
1:A:364[B]:ARG:NH1	4:A:2201:HOH:O	2.31	0.53
1:C:37:ILE:HG22	1:C:39:VAL:HG12	1.91	0.53
1:D:92:PRO:HB2	1:D:94:LYS:HG2	1.93	0.51
1:D:91:LEU:HD11	1:D:107:LEU:HD21	1.91	0.51
1:B:124:TYR:OH	4:B:2024:HOH:O	2.19	0.51
1:B:55:SER:HB3	1:B:64:GLU:HG3	1.93	0.51
1:C:113:ARG:NH1	4:C:2045:HOH:O	2.43	0.50
1:B:31:LEU:HD11	1:B:43[A]:VAL:HG13	1.94	0.50
1:A:86:ASP:OD1	4:A:2067:HOH:O	2.20	0.50
1:C:297:MET:HB3	1:C:304:LEU:HD11	1.94	0.49
1:D:26:TRP:CE2	1:D:245:LYS:HD3	2.48	0.49
1:A:22:ASP:OD1	4:A:2015:HOH:O	2.20	0.49
1:D:223:HIS:HB2	1:D:241[A]:ARG:HB2	1.95	0.49
1:A:94:LYS:HD3	1:A:110:GLY:HA3	1.94	0.48
1:A:349[B]:ARG:HB2	1:A:366:ALA:HB3	1.95	0.48
1:C:271:ALA:HB2	1:C:324:PHE:HD1	1.78	0.48
1:A:394:ARG:HB3	2:E:1:ACE:H3	1.96	0.48
2:G:2:MVA:HA	2:G:3:MP8:HD	1.73	0.47
1:B:391:MET:HB2	2:F:5:LEU:HD13	1.97	0.47
1:C:305:LYS:NZ	1:C:319[B]:ASP:OD1	2.37	0.47
1:C:90:ALA:O	4:C:2042:HOH:O	2.19	0.47
1:D:137:ILE:HD11	1:D:141:LEU:HG	1.97	0.46
1:B:284[A]:ARG:HD2	1:B:318:GLU:OE1	2.14	0.46
2:F:10:MLU:HCN3	2:F:10:MLU:HB2	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLN:O	1:D:151:VAL:HG12	2.15	0.46
1:D:272:THR:HG22	1:D:349[A]:ARG:HE	1.81	0.46
1:C:78:LEU:HD23	1:C:119:LEU:HB2	1.97	0.45
1:C:30:SER:OG	4:C:2011:HOH:O	2.21	0.45
1:D:27:VAL:HG21	1:D:54:ILE:HG22	1.98	0.45
1:C:290:ASP:O	1:C:293:ALA:N	2.50	0.45
1:C:280:GLU:OE2	1:C:284:ARG:NH1	2.27	0.45
1:D:25:ALA:O	1:D:29:ARG:HG3	2.17	0.45
1:D:130:LEU:HD13	1:D:246[B]:ARG:NH2	2.31	0.45
2:E:10:MLU:HD23	2:E:10:MLU:HA	1.72	0.45
1:C:181:ARG:HD3	2:G:10:MLU:HD22	1.99	0.44
1:D:133:GLU:HB3	1:D:194:THR:HG21	2.00	0.44
2:F:10:MLU:HA	2:F:10:MLU:HD23	1.70	0.44
1:C:139:SER:HB3	1:C:222:VAL:HG13	2.00	0.44
2:G:3:MP8:HA	2:G:4:NZC:H40	1.68	0.44
2:H:10:MLU:HCN3	2:H:10:MLU:HB2	1.65	0.44
1:B:46:THR:HB	1:B:53[A]:THR:OG1	2.18	0.44
1:C:262:LEU:HD11	2:G:7:LEU:CD1	2.48	0.44
1:A:31:LEU:HD11	1:A:43:VAL:HG23	1.99	0.44
1:D:43[B]:VAL:HG23	1:D:81:GLY:HA2	1.99	0.44
1:C:57:PHE:HB2	1:C:127:LEU:HD12	1.99	0.44
1:A:148:GLN:HG2	1:A:344:SER:O	2.18	0.43
1:A:111:SER:HB2	4:A:2079:HOH:O	2.18	0.43
1:C:58:ASP:O	1:C:59:TYR:HB2	2.19	0.43
2:G:4:NZC:H40B	2:G:4:NZC:O	2.18	0.43
1:A:263:LEU:HA	1:A:264:PRO:HD3	1.84	0.43
1:D:43[A]:VAL:HG22	1:D:81:GLY:HA2	2.01	0.43
1:A:100:VAL:HG22	1:A:105:VAL:HG22	1.99	0.43
1:B:57:PHE:HB2	1:B:127:LEU:HD23	2.01	0.43
1:C:168:GLU:HB2	1:C:175:VAL:HB	2.00	0.43
2:F:3:MP8:HA	2:F:4:NZC:H40	1.68	0.42
1:C:258:LYS:HA	1:C:258:LYS:HD2	1.64	0.42
1:B:58:ASP:O	1:B:59:TYR:HB2	2.19	0.42
1:D:108[A]:THR:HG23	1:D:113:ARG:HG2	2.01	0.42
1:C:263:LEU:HA	1:C:264:PRO:HD3	1.88	0.42
1:A:58:ASP:O	1:A:59:TYR:HB2	2.19	0.42
1:B:385:ASP:OD1	4:B:2186:HOH:O	2.21	0.42
2:E:10:MLU:HCN3	2:E:10:MLU:HB2	1.63	0.42
1:A:89:LYS:HG3	4:A:2014:HOH:O	2.20	0.41
1:C:17:ARG:HG3	1:C:18:GLU:N	2.36	0.41
1:B:79[B]:VAL:CG1	1:B:105:VAL:HG11	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:CD1	1:C:161:MET:HG3	2.50	0.41
2:G:7:LEU:HA	2:G:8:MVA:HN1	1.80	0.41
4:A:2183:HOH:O	1:D:161:MET:HG2	2.21	0.41
1:C:180:ASP:O	1:C:181:ARG:HB2	2.20	0.41
1:D:139:SER:OG	1:D:217:THR:OG1	2.37	0.41
2:H:7:LEU:HA	2:H:8:MVA:HN1	1.81	0.41
1:B:161:MET:HG2	4:B:2099:HOH:O	2.20	0.41
1:C:105:VAL:HG23	1:C:118:THR:HG22	2.02	0.41
1:A:52:LEU:HB3	1:A:67[B]:VAL:HG22	2.02	0.41
1:B:180:ASP:O	1:B:181:ARG:HB2	2.21	0.41
1:C:57:PHE:CZ	1:C:59:TYR:HA	2.57	0.40
1:A:306:LEU:O	1:A:317:GLU:HA	2.21	0.40
1:C:262:LEU:HD11	2:G:7:LEU:HD13	2.03	0.40
1:C:298:GLU:HG3	1:C:330:THR:OG1	2.22	0.40
1:D:57:PHE:CZ	1:D:59:TYR:HA	2.57	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	385/401 (96%)	376 (98%)	7 (2%)	2 (0%)	29	25
1	B	379/401 (94%)	371 (98%)	8 (2%)	0	100	100
1	C	378/401 (94%)	367 (97%)	11 (3%)	0	100	100
1	D	380/401 (95%)	371 (98%)	9 (2%)	0	100	100
2	E	3/11 (27%)	2 (67%)	1 (33%)	0	100	100
2	F	3/11 (27%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	G	3/11 (27%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	H	3/11 (27%)	1 (33%)	1 (33%)	1 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1534/1648 (93%)	1490 (97%)	39 (2%)	5 (0%)	41	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	9	PRO
2	G	9	PRO
2	H	9	PRO
1	A	327[A]	GLU
1	A	327[B]	GLU

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	297/306 (97%)	290 (98%)	7 (2%)	49	52
1	B	293/306 (96%)	285 (97%)	8 (3%)	44	47
1	C	287/306 (94%)	271 (94%)	16 (6%)	21	18
1	D	283/306 (92%)	271 (96%)	12 (4%)	30	29
2	E	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	F	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	G	3/3 (100%)	1 (33%)	2 (67%)	0	0
2	H	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1172/1236 (95%)	1124 (96%)	48 (4%)	31	30

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

Mol	Chain	Res	Type
1	A	159	LEU
1	A	183	ARG
1	A	191	TRP
1	A	237	LEU
1	A	253	ASP

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Mol	Chain	Res	Type
1	A	291	ARG
1	A	313	VAL
1	B	119	LEU
1	B	121	VAL
1	B	183	ARG
1	B	191	TRP
1	B	199	GLU
1	B	296	ARG
1	B	312	ASP
1	B	358	SER
1	C	17	ARG
1	C	50	GLU
1	C	101	GLU
1	C	159	LEU
1	C	161	MET
1	C	183	ARG
1	C	191	TRP
1	C	231	SER
1	C	237	LEU
1	C	258	LYS
1	C	312	ASP
1	C	319[A]	ASP
1	C	319[B]	ASP
1	C	329	LEU
1	C	376	SER
1	C	395	LEU
1	D	17	ARG
1	D	36	THR
1	D	43[A]	VAL
1	D	43[B]	VAL
1	D	119	LEU
1	D	155	ARG
1	D	183	ARG
1	D	191	TRP
1	D	198	VAL
1	D	258	LYS
1	D	327	GLU
1	D	329	LEU
2	E	5	LEU
2	F	5	LEU
2	G	5	LEU
2	G	7	LEU

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Mol	Chain	Res	Type
2	H	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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	MVA	H	2	2	6,7,8	0.71	0	7,8,10	2.83	1 (14%)
2	MP8	E	3	2	5,8,9	0.49	0	3,10,12	1.02	0
2	MP8	E	6	2	5,8,9	0.41	0	3,10,12	1.07	0
2	NZC	E	4	2	6,7,8	0.84	0	6,8,10	1.38	1 (16%)
2	MP8	G	6	2	5,8,9	0.49	0	3,10,12	0.76	0
2	MVA	H	8	2	6,7,8	0.72	0	7,8,10	1.41	1 (14%)
2	MLU	H	10	2	7,8,9	0.57	0	6,9,11	0.90	0
2	MVA	F	8	2	6,7,8	0.61	0	7,8,10	1.37	1 (14%)
2	NZC	G	4	2	6,7,8	0.99	0	6,8,10	0.99	0
2	NZC	F	4	2	6,7,8	0.94	0	6,8,10	1.30	1 (16%)
2	MLU	E	10	2	7,8,9	0.56	0	6,9,11	0.89	0
2	MVA	G	2	2	6,7,8	0.82	0	7,8,10	2.67	2 (28%)
2	MLU	G	10	2	7,8,9	0.57	0	6,9,11	1.10	1 (16%)
2	MP8	F	3	2	5,8,9	0.55	0	3,10,12	0.76	0
2	MVA	F	2	2	6,7,8	0.73	0	7,8,10	2.09	2 (28%)
2	MP8	F	6	2	5,8,9	0.48	0	3,10,12	1.08	0
2	MVA	E	2	2	6,7,8	0.79	0	7,8,10	2.39	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MP8	H	6	2	5,8,9	0.48	0	3,10,12	0.90	0
2	MLU	F	10	2	7,8,9	0.40	0	6,9,11	1.15	0
2	MP8	H	3	2	5,8,9	0.41	0	3,10,12	1.47	0
2	MVA	E	8	2	6,7,8	0.73	0	7,8,10	1.47	2 (28%)
2	NZC	H	4	2	6,7,8	0.93	0	6,8,10	1.33	1 (16%)
2	MP8	G	3	2	5,8,9	0.53	0	3,10,12	0.95	0
2	MVA	G	8	2	6,7,8	0.80	0	7,8,10	2.18	2 (28%)

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	MVA	H	2	2	-	1/6/8/10	-
2	MP8	E	3	2	-	0/0/11/13	0/1/1/1
2	MP8	E	6	2	-	0/0/11/13	0/1/1/1
2	NZC	E	4	2	-	1/5/8/10	-
2	MP8	G	6	2	-	0/0/11/13	0/1/1/1
2	MVA	H	8	2	-	5/6/8/10	-
2	MLU	H	10	2	-	2/5/8/10	-
2	MVA	F	8	2	-	2/6/8/10	-
2	NZC	G	4	2	-	1/5/8/10	-
2	NZC	F	4	2	-	1/5/8/10	-
2	MLU	E	10	2	-	3/5/8/10	-
2	MVA	G	2	2	-	5/6/8/10	-
2	MLU	G	10	2	-	2/5/8/10	-
2	MP8	F	3	2	-	0/0/11/13	0/1/1/1
2	MVA	F	2	2	-	2/6/8/10	-
2	MP8	F	6	2	-	0/0/11/13	0/1/1/1
2	MVA	E	2	2	-	3/6/8/10	-
2	MP8	H	6	2	-	0/0/11/13	0/1/1/1
2	MLU	F	10	2	-	2/5/8/10	-
2	MP8	H	3	2	-	0/0/11/13	0/1/1/1
2	MVA	E	8	2	-	1/6/8/10	-
2	NZC	H	4	2	-	1/5/8/10	-
2	MP8	G	3	2	-	0/0/11/13	0/1/1/1
2	MVA	G	8	2	-	1/6/8/10	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	MVA	CB-CA-N	-6.78	102.34	111.17
2	E	2	MVA	CB-CA-N	-5.49	104.02	111.17
2	G	2	MVA	CG2-CB-CA	4.98	118.84	111.21
2	G	2	MVA	CB-CA-C	4.48	118.66	113.04
2	G	8	MVA	CB-CA-N	-4.06	105.88	111.17
2	F	2	MVA	CB-CA-N	-3.70	106.35	111.17
2	G	8	MVA	CB-CA-C	-3.50	108.66	113.04
2	H	8	MVA	CB-CA-C	-3.18	109.06	113.04
2	F	2	MVA	CB-CA-C	-3.08	109.17	113.04
2	F	8	MVA	CB-CA-N	-2.99	107.28	111.17
2	E	8	MVA	CB-CA-N	-2.52	107.89	111.17
2	E	8	MVA	CB-CA-C	-2.43	110.00	113.04
2	E	4	NZC	C-CA-N	2.38	118.83	110.88
2	H	4	NZC	C-CA-N	2.32	118.65	110.88
2	G	10	MLU	O-C-CA	-2.31	118.71	124.78
2	F	4	NZC	C-CA-N	2.31	118.61	110.88

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	MVA	N-CA-CB-CG2
2	E	4	NZC	CB-CA-N-C40
2	F	4	NZC	CB-CA-N-C40
2	F	8	MVA	N-CA-CB-CG1
2	G	2	MVA	CB-CA-N-CN
2	G	2	MVA	N-CA-CB-CG1
2	G	2	MVA	N-CA-CB-CG2
2	G	2	MVA	C-CA-CB-CG1
2	G	2	MVA	C-CA-CB-CG2
2	G	4	NZC	CB-CA-N-C40
2	H	4	NZC	CB-CA-N-C40
2	H	8	MVA	N-CA-CB-CG1
2	H	8	MVA	N-CA-CB-CG2
2	H	8	MVA	C-CA-CB-CG1
2	E	10	MLU	C-CA-CB-CG
2	F	10	MLU	C-CA-CB-CG
2	G	10	MLU	C-CA-CB-CG
2	H	10	MLU	C-CA-CB-CG
2	F	10	MLU	N-CA-CB-CG
2	E	10	MLU	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	H	10	MLU	N-CA-CB-CG
2	G	10	MLU	N-CA-CB-CG
2	H	8	MVA	C-CA-CB-CG2
2	E	2	MVA	N-CA-CB-CG1
2	E	2	MVA	CB-CA-N-CN
2	E	8	MVA	CB-CA-N-CN
2	F	2	MVA	CB-CA-N-CN
2	F	8	MVA	CB-CA-N-CN
2	G	8	MVA	CB-CA-N-CN
2	H	2	MVA	CB-CA-N-CN
2	H	8	MVA	CB-CA-N-CN
2	E	10	MLU	CA-CB-CG-CD2
2	F	2	MVA	N-CA-CB-CG2

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	8	MVA	1	0
2	H	10	MLU	2	0
2	G	4	NZC	2	0
2	F	4	NZC	1	0
2	E	10	MLU	3	0
2	G	2	MVA	1	0
2	G	10	MLU	1	0
2	F	3	MP8	1	0
2	F	10	MLU	3	0
2	G	3	MP8	2	0
2	G	8	MVA	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	380/401 (94%)	0.19	7 (1%) 68 72	21, 36, 68, 94	0
1	B	377/401 (94%)	0.18	7 (1%) 66 71	22, 37, 67, 96	0
1	C	382/401 (95%)	0.24	8 (2%) 63 68	25, 43, 75, 104	0
1	D	379/401 (94%)	0.30	8 (2%) 63 68	27, 48, 80, 102	0
2	E	4/11 (36%)	0.28	0 100 100	28, 33, 38, 50	0
2	F	4/11 (36%)	-0.00	0 100 100	31, 32, 47, 56	0
2	G	4/11 (36%)	0.17	0 100 100	31, 36, 46, 52	0
2	H	4/11 (36%)	0.00	0 100 100	32, 33, 48, 56	0
All	All	1534/1648 (93%)	0.23	30 (1%) 65 69	21, 41, 73, 104	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	374	GLY	5.5
1	D	292	GLY	5.1
1	C	290	ASP	3.9
1	B	36	THR	3.7
1	D	290	ASP	3.6
1	C	157	ASP	3.1
1	B	32	PRO	3.0
1	D	194	THR	2.7
1	B	292	GLY	2.7
1	B	33	THR	2.6
1	A	301	ASP	2.6
1	B	30	SER	2.5
1	D	291	ARG	2.5
1	B	396	PRO	2.5
1	A	290	ASP	2.4
1	D	217	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	367	GLY	2.4
1	A	311	ASP	2.4
1	A	33	THR	2.3
1	C	310	ALA	2.3
1	D	16	VAL	2.3
1	A	375	GLY	2.2
1	C	270	VAL	2.2
1	C	158	THR	2.2
1	A	217	THR	2.1
1	C	49	ASP	2.1
1	C	8	LEU	2.0
1	D	246[A]	ARG	2.0
1	C	33	THR	2.0
1	A	215	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MVA	F	8	8/9	0.85	0.17	53,56,56,57	0
2	MVA	G	2	8/9	0.87	0.16	31,33,36,37	0
2	MVA	H	8	8/9	0.87	0.20	54,61,63,65	0
2	MVA	E	8	8/9	0.90	0.16	44,48,52,55	0
2	MVA	G	8	8/9	0.91	0.19	50,57,58,63	0
2	MP8	H	6	8/9	0.92	0.13	35,38,41,42	0
2	MVA	H	2	8/9	0.92	0.10	33,35,37,38	0
2	MP8	F	6	8/9	0.93	0.10	36,39,42,43	0
2	MP8	H	3	8/9	0.93	0.13	25,29,30,32	0
2	MP8	G	6	8/9	0.93	0.09	39,41,45,46	0
2	MVA	E	2	8/9	0.93	0.15	30,32,35,36	0
2	MLU	H	10	9/10	0.93	0.16	35,48,54,55	0
2	NZC	E	4	8/9	0.94	0.14	28,29,30,30	0
2	MP8	F	3	8/9	0.94	0.15	27,28,30,31	0
2	NZC	G	4	8/9	0.94	0.12	24,27,29,32	0
2	NZC	F	4	8/9	0.94	0.12	28,31,32,33	0
2	MLU	G	10	9/10	0.94	0.19	46,48,53,54	0
2	MP8	E	6	8/9	0.94	0.15	29,34,36,38	0
2	MVA	F	2	8/9	0.95	0.11	31,33,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLU	E	10	9/10	0.95	0.10	40,49,52,53	0
2	MP8	E	3	8/9	0.95	0.14	25,28,29,29	0
2	MP8	G	3	8/9	0.95	0.12	26,29,32,32	0
2	MLU	F	10	9/10	0.96	0.14	36,44,48,50	0
2	NZC	H	4	8/9	0.98	0.12	27,28,31,31	0

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, 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(\AA^2)	Q<0.9
3	NA	A	1398	1/1	0.92	0.19	45,45,45,45	0
3	NA	C	1398	1/1	0.93	0.42	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.