



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:07 AM GMT

PDB ID : 1ZR3
Title : Crystal structure of the macro-domain of human core histone variant macroH2A1.1 (form B)
Authors : Kustatscher, G.; Hothorn, M.; Pugieux, C.; Scheffzek, K.; Ladurner, A.G.
Deposited on : 2005-05-19
Resolution : 1.66 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

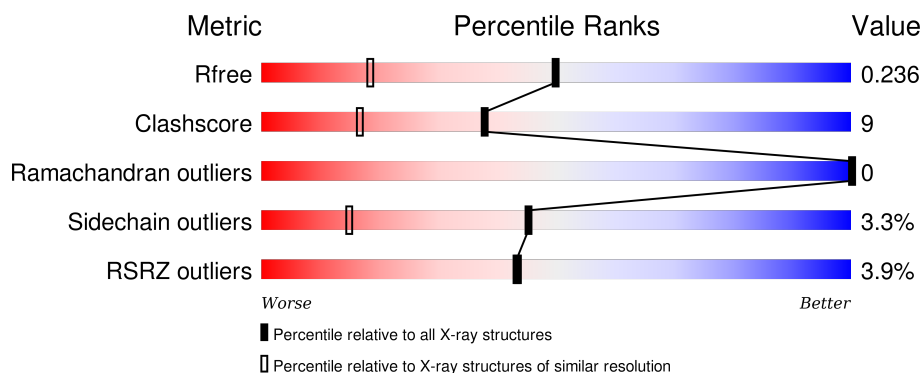
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	211	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 18%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 70% 18% 12% </div> </div>
1	B	211	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 68%, yellow 18%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 70% 18% 12% </div> </div>
1	C	211	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 65%, yellow 18%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 68% 18% 13% </div> </div>
1	D	211	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 8%, green 62%, yellow 16%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 8% 70% 16% 13% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6180 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 histone macroH2A1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	5	0
			1426	916	231	274	5			
1	B	186	Total	C	N	O	S	0	7	0
			1452	932	237	277	6			
1	C	184	Total	C	N	O	S	0	6	0
			1434	922	234	273	5			
1	D	184	Total	C	N	O	S	0	5	0
			1409	903	231	270	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	GLY	-	CLONING ARTIFACT	GB 3493531
A	160	ALA	-	CLONING ARTIFACT	GB 3493531
A	161	MET	-	CLONING ARTIFACT	GB 3493531
B	159	GLY	-	CLONING ARTIFACT	GB 3493531
B	160	ALA	-	CLONING ARTIFACT	GB 3493531
B	161	MET	-	CLONING ARTIFACT	GB 3493531
C	159	GLY	-	CLONING ARTIFACT	GB 3493531
C	160	ALA	-	CLONING ARTIFACT	GB 3493531
C	161	MET	-	CLONING ARTIFACT	GB 3493531
D	159	GLY	-	CLONING ARTIFACT	GB 3493531
D	160	ALA	-	CLONING ARTIFACT	GB 3493531
D	161	MET	-	CLONING ARTIFACT	GB 3493531

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

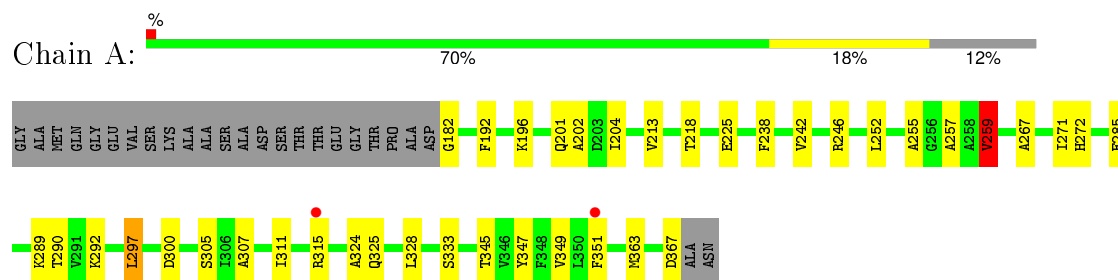
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		
3	B	127	Total	O	0	0
			127	127		
3	C	107	Total	O	0	0
			107	107		
3	D	88	Total	O	0	0
			88	88		

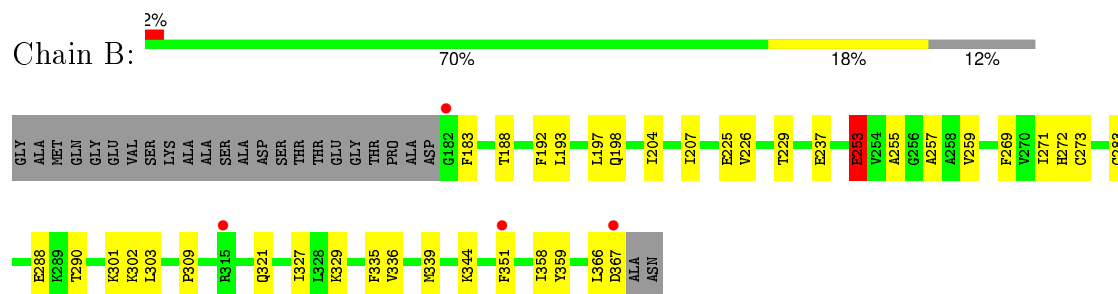
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

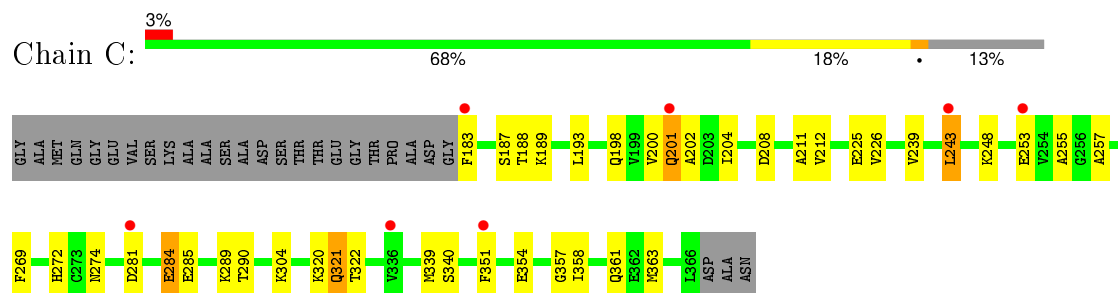
- Molecule 1: histone macroH2A1.1



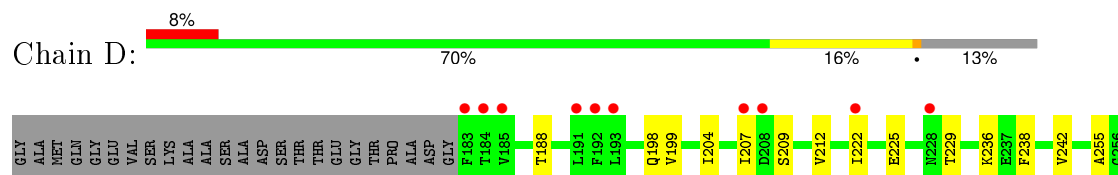
- Molecule 1: histone macroH2A1.1

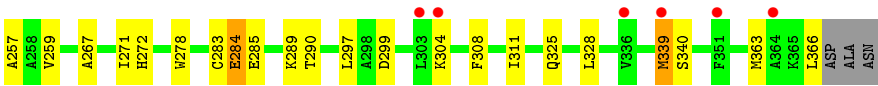


- Molecule 1: histone macroH2A1.1



- Molecule 1: histone macroH2A1.1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.90Å 89.20Å 92.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.28 – 1.66 64.29 – 1.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.28-1.66) 98.3 (64.29-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.232 0.195 , 0.236	Depositor DCC
R_{free} test set	3905 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.1	EDS
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 78097 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6180	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MES

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	1.07	2/1459 (0.1%)	0.91	4/1971 (0.2%)
1	B	1.07	4/1476 (0.3%)	0.87	0/1992
1	C	0.99	0/1461	0.87	1/1972 (0.1%)
1	D	1.03	5/1432 (0.3%)	0.84	0/1935
All	All	1.04	11/5828 (0.2%)	0.87	5/7870 (0.1%)

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
1	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	340	SER	CB-OG	14.16	1.60	1.42
1	A	285	GLU	CD-OE2	6.62	1.32	1.25
1	B	273	CYS	CB-SG	-6.49	1.71	1.82
1	D	283	CYS	CB-SG	-6.33	1.71	1.82
1	B	253	GLU	CG-CD	5.99	1.60	1.51
1	D	299	ASP	CG-OD1	5.67	1.38	1.25
1	B	283	CYS	CB-SG	-5.47	1.72	1.81
1	B	359	TYR	CD2-CE2	-5.30	1.31	1.39
1	D	339	MET	C-O	5.16	1.33	1.23
1	D	278	TRP	CB-CG	-5.12	1.41	1.50
1	A	196	LYS	CG-CD	5.03	1.69	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LYS	CA-CB-CG	6.83	128.42	113.40
1	C	243	LEU	CB-CG-CD1	6.56	122.15	111.00
1	A	259[A]	VAL	CB-CA-C	-5.27	101.38	111.40
1	A	259[B]	VAL	CB-CA-C	-5.27	101.38	111.40
1	A	363	MET	CG-SD-CE	5.06	108.30	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	366	LEU	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	1426	0	1462	27	2
1	B	1452	0	1486	30	0
1	C	1434	0	1473	25	2
1	D	1409	0	1429	30	0
2	A	12	0	12	1	0
3	A	125	0	0	3	0
3	B	127	0	0	7	0
3	C	107	0	0	1	0
3	D	88	0	0	3	0
All	All	6180	0	5862	107	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 9.

All (107) 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:222:ILE:HG22	1:D:222:ILE:O	1.71	0.90
1:B:225:GLU:O	1:B:229[A]:THR:HG23	1.76	0.85
1:D:222:ILE:HD11	1:D:242:VAL:HG11	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CZ	1:A:367:ASP:HB3	2.12	0.83
1:C:239:VAL:O	1:C:243:LEU:HD13	1.80	0.82
1:D:259[A]:VAL:HG12	1:D:271:ILE:HG12	1.63	0.80
1:D:259[A]:VAL:CG1	1:D:271:ILE:HG12	2.15	0.77
1:C:357:GLY:O	1:C:361[A]:GLN:HG3	1.86	0.75
1:A:192:PHE:CE2	1:A:367:ASP:HB3	2.22	0.75
1:B:193[A]:LEU:HD21	1:B:339[A]:MET:CE	2.19	0.73
1:B:193[A]:LEU:HD21	1:B:339[A]:MET:HE1	1.72	0.72
1:A:218[A]:THR:HG23	3:A:596:HOH:O	1.90	0.69
1:D:222:ILE:HG21	1:D:238:PHE:HE2	1.57	0.69
1:D:222:ILE:CG2	1:D:222:ILE:O	2.42	0.68
1:C:225:GLU:HG3	1:C:226:VAL:HG23	1.74	0.67
1:B:344[A]:LYS:HE3	3:B:482:HOH:O	1.95	0.66
1:C:201:GLN:OE1	1:C:201:GLN:HA	1.96	0.66
1:A:292:LYS:NZ	1:A:333:SER:HB3	2.11	0.65
1:A:300:ASP:O	1:B:302:LYS:HE3	1.97	0.64
1:A:292:LYS:HZ1	1:A:333:SER:HB3	1.63	0.64
1:B:237:GLU:HG2	3:B:468:HOH:O	1.99	0.62
1:B:259[A]:VAL:HG12	1:B:271:ILE:HG12	1.82	0.61
1:D:204:ILE:O	1:D:207:ILE:HG22	1.99	0.61
1:A:225:GLU:OE1	1:A:351:PHE:CD2	2.55	0.60
1:B:192:PHE:CZ	1:B:367:ASP:HB3	2.36	0.59
1:D:222:ILE:HD11	1:D:242:VAL:CG1	2.32	0.59
1:B:193[A]:LEU:HD21	1:B:339[A]:MET:SD	2.44	0.58
1:C:320:LYS:NZ	1:C:354:GLU:OE1	2.23	0.57
1:B:204:ILE:O	1:B:207:ILE:HG22	2.07	0.54
1:B:183:PHE:HE2	1:C:248[A]:LYS:HG2	1.73	0.53
1:D:204:ILE:HG12	1:D:212[A]:VAL:HG13	1.89	0.53
1:D:188:THR:HG23	1:D:198:GLN:HG2	1.89	0.53
1:A:289:LYS:HE3	3:A:532:HOH:O	2.09	0.53
1:B:188:THR:HG23	1:B:198:GLN:HG2	1.91	0.52
1:C:320:LYS:HB3	1:C:358:ILE:HD13	1.91	0.52
1:C:351:PHE:CE1	3:C:400:HOH:O	2.63	0.51
1:B:183:PHE:CD2	1:C:248[A]:LYS:HE2	2.46	0.50
1:A:259[B]:VAL:HG22	1:A:271:ILE:HG12	1.93	0.50
1:D:257:ALA:HA	1:D:272:HIS:O	2.13	0.49
1:D:222:ILE:CG2	1:D:238:PHE:HE2	2.24	0.49
1:C:201:GLN:O	1:C:202:ALA:HB2	2.12	0.49
1:B:335:PHE:O	1:B:339[A]:MET:HE2	2.13	0.49
1:C:357:GLY:O	1:C:361[A]:GLN:CG	2.59	0.48
1:C:255:ALA:HA	1:C:290:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ILE:HB	3:D:433:HOH:O	2.14	0.48
1:D:255:ALA:HA	1:D:290:THR:OG1	2.14	0.48
1:A:324:ALA:O	1:A:328:LEU:HD23	2.13	0.47
1:A:238:PHE:O	1:A:242:VAL:HG23	2.15	0.47
1:A:257:ALA:HA	1:A:272:HIS:O	2.14	0.47
1:B:336[A]:VAL:HG13	3:B:461:HOH:O	2.15	0.47
1:B:253:GLU:H	1:B:253:GLU:CD	2.17	0.47
1:A:202:ALA:O	1:A:351:PHE:CD1	2.68	0.47
1:B:226:VAL:HG21	1:B:309:PRO:HG3	1.96	0.47
1:B:351:PHE:HZ	3:B:418:HOH:O	1.98	0.47
1:A:315:ARG:HG2	2:A:500:MES:H72	1.98	0.46
1:A:182:GLY:N	3:A:525:HOH:O	2.49	0.46
1:D:204:ILE:HG12	1:D:212[A]:VAL:CG1	2.44	0.46
1:D:236:LYS:HD2	3:D:409:HOH:O	2.15	0.46
1:D:259[A]:VAL:HG12	1:D:271:ILE:CG1	2.42	0.46
1:C:321:GLN:HG3	1:C:322:THR:N	2.29	0.46
1:C:189:LYS:HE3	1:C:363:MET:O	2.16	0.46
1:D:259[A]:VAL:HG13	1:D:297:LEU:HD13	1.97	0.46
1:A:351:PHE:N	1:A:351:PHE:CD1	2.83	0.46
1:C:211:ALA:HA	1:C:269:PHE:O	2.16	0.46
1:A:218[A]:THR:HG22	1:A:252:LEU:O	2.16	0.46
1:D:284[A]:GLU:H	1:D:284[A]:GLU:CD	2.19	0.45
1:C:225:GLU:HG3	1:C:226:VAL:N	2.31	0.45
1:B:259[B]:VAL:CG1	1:B:269:PHE:HB3	2.47	0.45
1:A:259[A]:VAL:CG1	1:A:271:ILE:HG12	2.47	0.45
1:B:321:GLN:HA	1:B:358:ILE:HG21	1.98	0.45
1:B:192:PHE:CE2	1:B:367:ASP:HB3	2.52	0.45
1:B:257:ALA:HA	1:B:272:HIS:O	2.17	0.45
1:A:259[B]:VAL:HG23	1:A:297:LEU:HG	1.98	0.45
1:B:255:ALA:HA	1:B:290:THR:OG1	2.17	0.45
1:A:292:LYS:HZ1	1:A:333:SER:CB	2.28	0.44
1:A:255:ALA:HA	1:A:290:THR:OG1	2.17	0.44
1:D:285:GLU:O	1:D:289:LYS:HG3	2.18	0.44
1:A:204:ILE:HA	1:A:349:VAL:HG11	1.98	0.44
1:B:288:GLU:OE1	1:B:329:LYS:HE3	2.17	0.44
1:A:213:VAL:HG11	1:A:311:ILE:HD11	2.00	0.44
1:C:204:ILE:HG12	1:C:212:VAL:HG13	1.99	0.43
1:B:327:ILE:HD13	3:B:405:HOH:O	2.18	0.43
1:C:257:ALA:HA	1:C:272:HIS:O	2.17	0.43
1:B:339[A]:MET:HE1	3:B:447:HOH:O	2.19	0.43
1:A:307:ALA:HA	1:A:347:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LYS:HB2	1:B:303:LEU:HG	2.01	0.42
1:D:188:THR:HG23	1:D:198:GLN:CG	2.49	0.42
1:D:225:GLU:O	1:D:229:THR:HG23	2.20	0.42
1:B:259[A]:VAL:HG22	3:B:444:HOH:O	2.19	0.42
1:C:193[A]:LEU:HD21	1:C:339:MET:SD	2.60	0.42
1:A:305:SER:HA	1:A:345:THR:O	2.20	0.42
1:B:183:PHE:CE2	1:C:248[A]:LYS:HD3	2.54	0.42
1:D:199:VAL:HG23	1:D:363:MET:HE1	2.02	0.42
1:D:259[B]:VAL:CG2	1:D:297:LEU:HD13	2.50	0.41
1:D:222:ILE:HD12	3:D:380:HOH:O	2.20	0.41
1:C:188:THR:HG23	1:C:198:GLN:HG2	2.02	0.41
1:C:284[A]:GLU:OE2	1:C:285:GLU:HG3	2.20	0.41
1:D:259[B]:VAL:HG22	1:D:297:LEU:HD13	2.02	0.41
1:D:308:PHE:HD2	1:D:311:ILE:CD1	2.34	0.41
1:B:183:PHE:CE2	1:C:248[A]:LYS:HG2	2.53	0.40
1:C:204:ILE:HG22	1:C:351:PHE:HZ	1.86	0.40
1:D:328:LEU:HD12	1:D:366:LEU:HD11	2.04	0.40
1:D:209:SER:O	1:D:267:ALA:HA	2.22	0.40
1:C:183:PHE:HB2	1:C:200:VAL:CG1	2.52	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)
1:A:201:GLN:OE1	1:C:361[A]:GLN:OE1[2_455]	1.76	0.44
1:A:201:GLN:OE1	1:C:361[A]:GLN:CD[2_455]	2.08	0.12

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	189/211 (90%)	184 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	191/211 (90%)	187 (98%)	4 (2%)	0	100	100
1	C	188/211 (89%)	181 (96%)	7 (4%)	0	100	100
1	D	186/211 (88%)	181 (97%)	5 (3%)	0	100	100
All	All	754/844 (89%)	733 (97%)	21 (3%)	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	158/169 (94%)	154 (98%)	4 (2%)	55	26
1	B	160/169 (95%)	158 (99%)	2 (1%)	76	57
1	C	158/169 (94%)	146 (92%)	12 (8%)	16	2
1	D	154/169 (91%)	149 (97%)	5 (3%)	46	16
All	All	630/676 (93%)	607 (96%)	23 (4%)	45	13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259[A]	VAL
1	A	259[B]	VAL
1	A	297	LEU
1	A	325	GLN
1	B	197	LEU
1	B	253	GLU
1	C	187	SER
1	C	201	GLN
1	C	208	ASP
1	C	253	GLU
1	C	274	ASN
1	C	281	ASP
1	C	284[A]	GLU

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Mol	Chain	Res	Type
1	C	284[B]	GLU
1	C	289	LYS
1	C	304	LYS
1	C	321	GLN
1	C	340	SER
1	D	284[A]	GLU
1	D	284[B]	GLU
1	D	304	LYS
1	D	325	GLN
1	D	339	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	B	198	GLN
1	B	263	HIS
1	B	361	GLN
1	C	274	ASN
1	D	228	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	MES	A	500	-	11,12,12	0.36	0	14,16,16	5.12	7 (50%)

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	MES	A	500	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	MES	O2S-S-C8	-13.21	95.64	106.91
2	A	500	MES	O1S-S-C8	-9.19	99.06	106.91
2	A	500	MES	O1-C6-C5	-2.50	106.11	111.84
2	A	500	MES	O3S-S-O1S	2.05	116.39	111.61
2	A	500	MES	C7-N4-C3	3.34	119.82	111.27
2	A	500	MES	O3S-S-O2S	4.16	121.29	111.61
2	A	500	MES	C5-N4-C3	7.79	125.77	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	MES	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/211 (88%)	0.35	2 (1%) 82 85	29, 34, 40, 52	0
1	B	186/211 (88%)	0.35	4 (2%) 65 67	29, 33, 41, 49	0
1	C	184/211 (87%)	0.50	7 (3%) 44 44	26, 34, 43, 49	0
1	D	184/211 (87%)	0.67	16 (8%) 13 11	26, 34, 42, 49	0
All	All	740/844 (87%)	0.47	29 (3%) 43 43	26, 34, 42, 52	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	PHE	9.1
1	A	315	ARG	5.2
1	A	351	PHE	5.0
1	D	351	PHE	4.7
1	C	183	PHE	4.7
1	B	182	GLY	4.6
1	C	201	GLN	4.5
1	D	339	MET	4.4
1	B	351	PHE	4.4
1	D	185	VAL	4.1
1	C	243	LEU	3.4
1	D	336	VAL	3.1
1	D	303	LEU	2.9
1	B	367	ASP	2.8
1	C	281	ASP	2.8
1	D	191	LEU	2.7
1	D	192	PHE	2.6
1	D	183	PHE	2.6
1	D	207	ILE	2.5
1	D	193	LEU	2.4
1	D	364	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	253	GLU	2.2
1	D	222	ILE	2.2
1	D	208	ASP	2.1
1	D	228	ASN	2.1
1	D	184	THR	2.1
1	B	315	ARG	2.1
1	C	336	VAL	2.1
1	D	304	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MES	A	500	12/12	0.94	0.25	1.58	29,40,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.