



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 PM GMT

PDB ID : 4QSM
Title : Crystal structure of human muscle L-lactate dehydrogenase in complex with inhibitor 2, 3-{[7-(2,4-dimethoxypyrimidin-5-yl)-3-sulfamoylquinolin-4-yl]amino}benzoic acid
Authors : Kolappan, S.; Craig, L.
Deposited on : 2014-07-06
Resolution : 3.00 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

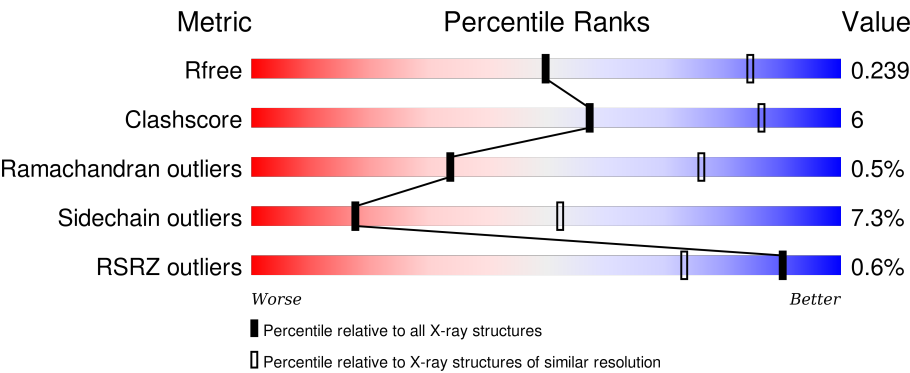
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	337	<div><div></div><div>82%15%..</div></div>
1	B	337	<div><div>%</div><div>77%20%..</div></div>
1	C	337	<div><div></div><div>81%15%..</div></div>
1	D	337	<div><div></div><div>81%16%..</div></div>
1	E	337	<div><div>2%</div><div>80%15%..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	337	<div><div><div>%</div><div><div></div><div>75%</div><div>21%</div><div></div></div><div><div></div><div></div><div>• •</div></div></div></div>
1	G	337	<div><div><div></div><div>83%</div><div>14%</div><div></div></div><div><div></div><div></div><div>• •</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21120 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-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	3	0
			2600	1660	446	481	13			
1	B	331	Total	C	N	O	S	0	2	0
			2584	1650	442	479	13			
1	C	332	Total	C	N	O	S	0	5	0
			2619	1671	448	487	13			
1	D	332	Total	C	N	O	S	0	5	0
			2618	1670	449	486	13			
1	E	331	Total	C	N	O	S	0	3	0
			2593	1655	443	482	13			
1	F	331	Total	C	N	O	S	0	6	0
			2619	1671	451	484	13			
1	G	331	Total	C	N	O	S	0	3	0
			2588	1650	444	481	13			
1	H	331	Total	C	N	O	S	0	0	0
			2567	1639	439	476	13			

There are 48 discrepancies between the modelled and reference sequences:

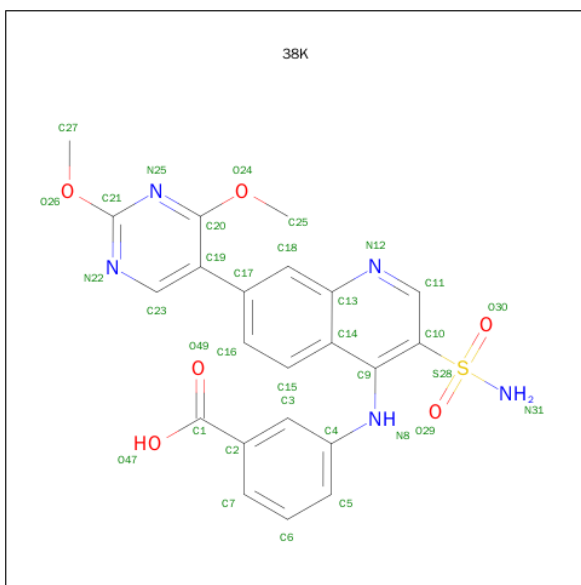
Chain	Residue	Modelled	Actual	Comment	Reference
A	333	HIS	-	EXPRESSION TAG	UNP P00338
A	334	HIS	-	EXPRESSION TAG	UNP P00338
A	335	HIS	-	EXPRESSION TAG	UNP P00338
A	336	HIS	-	EXPRESSION TAG	UNP P00338
A	337	HIS	-	EXPRESSION TAG	UNP P00338
A	338	HIS	-	EXPRESSION TAG	UNP P00338
B	333	HIS	-	EXPRESSION TAG	UNP P00338
B	334	HIS	-	EXPRESSION TAG	UNP P00338
B	335	HIS	-	EXPRESSION TAG	UNP P00338
B	336	HIS	-	EXPRESSION TAG	UNP P00338
B	337	HIS	-	EXPRESSION TAG	UNP P00338
B	338	HIS	-	EXPRESSION TAG	UNP P00338
C	333	HIS	-	EXPRESSION TAG	UNP P00338

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Chain	Residue	Modelled	Actual	Comment	Reference
C	334	HIS	-	EXPRESSION TAG	UNP P00338
C	335	HIS	-	EXPRESSION TAG	UNP P00338
C	336	HIS	-	EXPRESSION TAG	UNP P00338
C	337	HIS	-	EXPRESSION TAG	UNP P00338
C	338	HIS	-	EXPRESSION TAG	UNP P00338
D	333	HIS	-	EXPRESSION TAG	UNP P00338
D	334	HIS	-	EXPRESSION TAG	UNP P00338
D	335	HIS	-	EXPRESSION TAG	UNP P00338
D	336	HIS	-	EXPRESSION TAG	UNP P00338
D	337	HIS	-	EXPRESSION TAG	UNP P00338
D	338	HIS	-	EXPRESSION TAG	UNP P00338
E	333	HIS	-	EXPRESSION TAG	UNP P00338
E	334	HIS	-	EXPRESSION TAG	UNP P00338
E	335	HIS	-	EXPRESSION TAG	UNP P00338
E	336	HIS	-	EXPRESSION TAG	UNP P00338
E	337	HIS	-	EXPRESSION TAG	UNP P00338
E	338	HIS	-	EXPRESSION TAG	UNP P00338
F	333	HIS	-	EXPRESSION TAG	UNP P00338
F	334	HIS	-	EXPRESSION TAG	UNP P00338
F	335	HIS	-	EXPRESSION TAG	UNP P00338
F	336	HIS	-	EXPRESSION TAG	UNP P00338
F	337	HIS	-	EXPRESSION TAG	UNP P00338
F	338	HIS	-	EXPRESSION TAG	UNP P00338
G	333	HIS	-	EXPRESSION TAG	UNP P00338
G	334	HIS	-	EXPRESSION TAG	UNP P00338
G	335	HIS	-	EXPRESSION TAG	UNP P00338
G	336	HIS	-	EXPRESSION TAG	UNP P00338
G	337	HIS	-	EXPRESSION TAG	UNP P00338
G	338	HIS	-	EXPRESSION TAG	UNP P00338
H	333	HIS	-	EXPRESSION TAG	UNP P00338
H	334	HIS	-	EXPRESSION TAG	UNP P00338
H	335	HIS	-	EXPRESSION TAG	UNP P00338
H	336	HIS	-	EXPRESSION TAG	UNP P00338
H	337	HIS	-	EXPRESSION TAG	UNP P00338
H	338	HIS	-	EXPRESSION TAG	UNP P00338

- Molecule 2 is 3-{[7-(2,4-DIMETHOXYPYRIMIDIN-5-YL)-3-SULFAMOYLQUINOLIN-4-YL]AMINO}BENZOIC ACID (three-letter code: 38K) (formula: C₂₂H₁₉N₅O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	B	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	C	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	D	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	E	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	F	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	G	1	Total	C	N	O	S	0	0
			34	22	5	6	1		
2	H	1	Total	C	N	O	S	0	0
			34	22	5	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	6	Total	O	0	0
			6	6		
3	C	8	Total	O	0	0
			8	8		
3	D	10	Total	O	0	0
			10	10		

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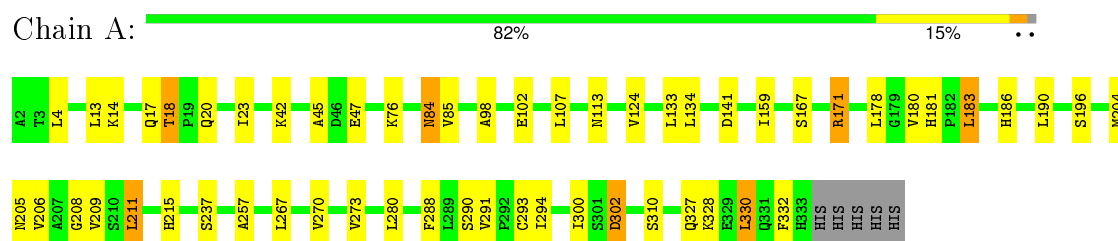
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	6	Total 6	O 6	0	0
3	F	6	Total 6	O 6	0	0
3	G	11	Total 11	O 11	0	0
3	H	6	Total 6	O 6	0	0

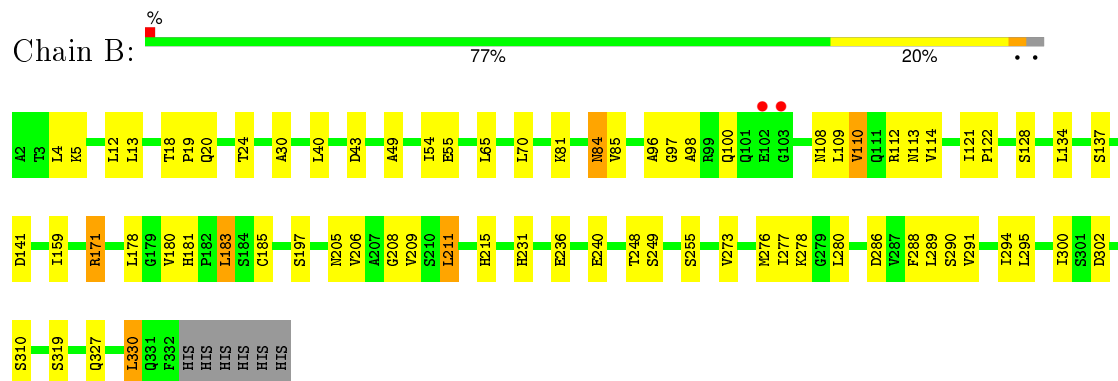
3 Residue-property plots

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.

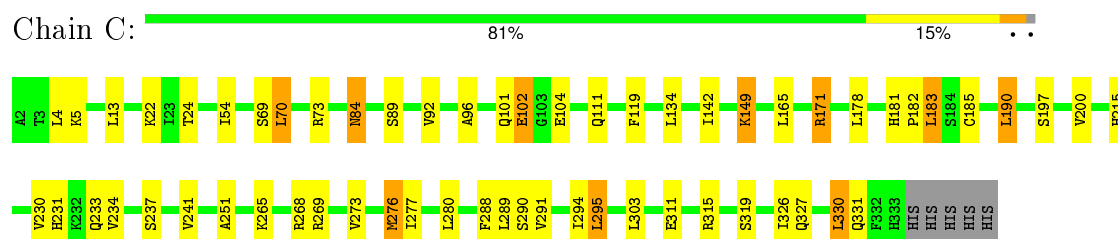
• Molecule 1: L-lactate dehydrogenase A chain



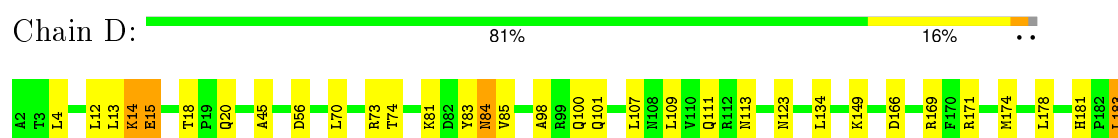
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain

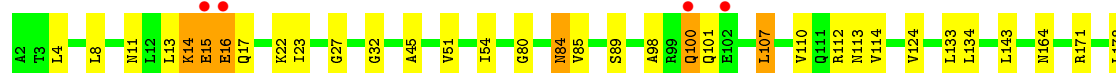
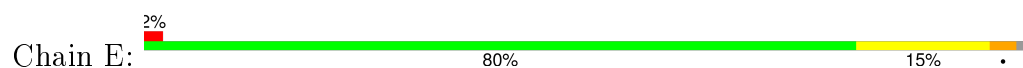


• Molecule 1: L-lactate dehydrogenase A chain

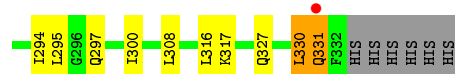
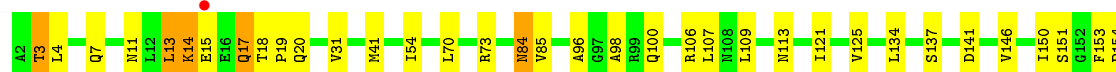




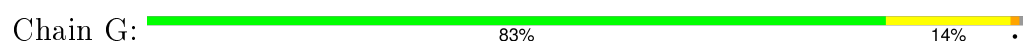
• Molecule 1: L-lactate dehydrogenase A chain



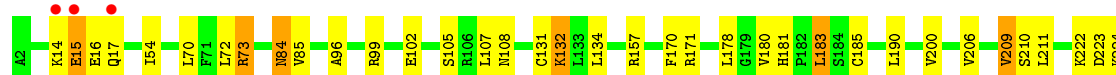
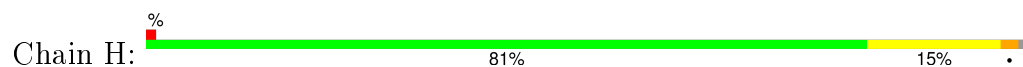
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.31Å 147.31Å 334.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.62 – 3.00 34.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.62-3.00) 100.0 (34.62-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.167 , 0.247 0.169 , 0.239	Depositor DCC
R_{free} test set	4518 reflections (5.62%)	DCC
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.1	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84858 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21120	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: 38K

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	0.56	0/2645	0.77	2/3577 (0.1%)
1	B	0.53	0/2628	0.77	2/3555 (0.1%)
1	C	0.56	0/2664	0.77	1/3604 (0.0%)
1	D	0.57	0/2663	0.79	2/3601 (0.1%)
1	E	0.49	0/2637	0.70	0/3567
1	F	0.53	0/2663	0.73	1/3601 (0.0%)
1	G	0.55	0/2637	0.80	4/3566 (0.1%)
1	H	0.50	0/2611	0.71	0/3532
All	All	0.54	0/21148	0.76	12/28603 (0.0%)

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	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	171	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	141	ASP	CB-CG-OD1	7.12	124.71	118.30
1	F	141	ASP	CB-CG-OD1	6.83	124.45	118.30
1	G	171	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	171	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	171	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	G	12	LEU	CA-CB-CG	5.85	128.76	115.30
1	C	171	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	56	ASP	CB-CG-OD1	5.34	123.10	118.30
1	G	157	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	169	ARG	NE-CZ-NH2	5.10	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	LYS	Peptide
1	F	14	LYS	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	2600	0	2686	29	0
1	B	2584	0	2670	39	0
1	C	2619	0	2695	44	0
1	D	2618	0	2698	28	0
1	E	2593	0	2675	37	0
1	F	2619	0	2707	45	0
1	G	2588	0	2671	21	0
1	H	2567	0	2653	30	0
2	A	34	0	18	0	0
2	B	34	0	18	4	0
2	C	34	0	18	7	0
2	D	34	0	18	1	0
2	E	34	0	18	4	0
2	F	34	0	18	2	0
2	G	34	0	18	7	0
2	H	34	0	18	4	0
3	A	7	0	0	0	0
3	B	6	0	0	0	0
3	C	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	11	0	0	0	0
3	H	6	0	0	0	0
All	All	21120	0	21599	255	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 6.

All (255) 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:70[A]:LEU:O	1:C:70[A]:LEU:HD13	1.45	1.11
2:H:501:38K:H12	2:H:501:38K:H5	1.11	1.08
2:H:501:38K:H12	2:H:501:38K:C5	1.95	0.96
1:E:107[A]:LEU:C	1:E:107[A]:LEU:HD12	1.88	0.93
2:C:501:38K:H5	2:C:501:38K:H12	1.48	0.92
1:E:107[A]:LEU:O	1:E:107[A]:LEU:HD12	1.68	0.92
1:G:96:ALA:HA	2:G:501:38K:H1	1.45	0.81
1:B:84:ASN:HD22	1:B:85:VAL:N	1.79	0.80
1:C:70[A]:LEU:HD13	1:C:70[A]:LEU:C	2.02	0.79
1:A:327:GLN:HA	1:A:330:LEU:HD22	1.66	0.77
1:E:181:HIS:CE1	1:E:183:LEU:HD22	2.20	0.76
2:E:501:38K:H12	2:E:501:38K:C5	2.17	0.74
1:F:96:ALA:HA	2:F:501:38K:H1	1.53	0.73
2:C:501:38K:C5	2:C:501:38K:H12	2.19	0.72
2:E:501:38K:C15	2:E:501:38K:C5	2.69	0.71
1:G:98:ALA:H	1:G:113:ASN:HD21	1.38	0.71
2:G:501:38K:H5	2:G:501:38K:H12	1.72	0.70
1:A:181:HIS:CE1	1:A:183:LEU:HD22	2.28	0.69
1:D:84:ASN:HD22	1:D:85:VAL:N	1.91	0.69
1:D:111:GLN:HE22	1:D:331:GLN:H	1.39	0.68
1:E:84:ASN:HD22	1:E:85:VAL:N	1.91	0.68
1:F:269:ARG:HD3	1:H:183:LEU:HD23	1.75	0.68
1:B:181:HIS:CE1	1:B:183:LEU:HD22	2.30	0.67
1:H:181:HIS:CE1	1:H:183:LEU:HD22	2.30	0.67
1:A:294[A]:ILE:HD12	1:A:302:ASP:HB2	1.78	0.66
1:F:84:ASN:HD22	1:F:85:VAL:N	1.93	0.66
1:F:327:GLN:HA	1:F:330:LEU:HD22	1.78	0.65
1:D:277:ILE:HD11	1:D:289:LEU:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:ASN:HD22	1:H:85:VAL:N	1.94	0.65
1:E:205:ASN:HD22	1:E:208:GLY:H	1.44	0.65
1:C:70[A]:LEU:CD1	1:C:70[A]:LEU:C	2.64	0.65
1:E:171:ARG:HD2	1:E:185:CYS:O	1.97	0.65
1:F:31:VAL:HG22	1:F:252:ILE:HG21	1.79	0.64
1:G:111:GLN:HE22	1:G:331:GLN:H	1.45	0.64
1:E:107[A]:LEU:C	1:E:107[A]:LEU:CD1	2.63	0.63
1:G:84:ASN:HD22	1:G:85:VAL:N	1.96	0.63
1:E:4:LEU:HD13	1:F:215:HIS:HB2	1.80	0.63
1:D:181:HIS:CE1	1:D:183:LEU:HD22	2.33	0.63
2:B:501:38K:C7	1:H:102:GLU:HG3	2.30	0.62
1:C:70[A]:LEU:O	1:C:70[A]:LEU:CD1	2.36	0.61
1:H:96:ALA:HA	2:H:501:38K:H1	1.64	0.61
1:H:273:VAL:O	1:H:290:SER:HA	1.99	0.61
1:F:13:LEU:HB2	1:F:15:GLU:HG2	1.82	0.61
1:H:190:LEU:HD22	1:H:200:VAL:HG21	1.83	0.61
1:G:100:GLN:HB2	1:G:109:LEU:HD22	1.81	0.61
1:F:171:ARG:HD2	1:F:185:CYS:O	2.01	0.61
1:B:327:GLN:HA	1:B:330:LEU:HD22	1.82	0.60
1:H:171:ARG:HD2	1:H:185:CYS:O	2.02	0.60
1:C:96:ALA:HB2	2:C:501:38K:H2	1.66	0.59
1:B:110:VAL:O	1:B:114:VAL:HG23	2.02	0.59
1:D:171:ARG:HD2	1:D:185:CYS:O	2.02	0.59
1:F:181:HIS:CE1	1:F:183:LEU:HD22	2.37	0.59
1:E:183:LEU:HD13	1:F:70:LEU:HD12	1.85	0.59
1:A:4:LEU:HD13	1:B:215:HIS:HB2	1.85	0.59
1:C:111:GLN:HE22	1:C:331[B]:GLN:H	1.51	0.58
1:A:102:GLU:HG2	2:G:501:38K:C5	2.34	0.58
1:A:267:LEU:O	1:C:181:HIS:HB2	2.04	0.58
1:A:84:ASN:HD22	1:A:85:VAL:N	2.02	0.58
1:C:171:ARG:HD2	1:C:185:CYS:O	2.04	0.57
1:D:83:TYR:HB2	1:D:123:ASN:HD22	1.70	0.57
1:H:293:CYS:HB3	1:H:300:ILE:HG23	1.86	0.57
1:B:100:GLN:HB2	1:B:109:LEU:HD22	1.86	0.56
1:E:331:GLN:HE21	1:E:331:GLN:HA	1.70	0.56
1:D:205:ASN:HD22	1:D:208:GLY:H	1.54	0.56
1:F:18:THR:HG22	1:F:19:PRO:O	2.05	0.56
1:E:215:HIS:HB2	1:F:4:LEU:HD13	1.86	0.56
1:B:236:GLU:O	1:B:240:GLU:HG2	2.06	0.56
1:A:183:LEU:HD13	1:B:70:LEU:HD12	1.87	0.56
1:G:294:ILE:HD12	1:G:302:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ARG:HD2	1:G:185:CYS:O	2.05	0.56
1:B:84:ASN:C	1:B:84:ASN:HD22	2.08	0.55
1:E:124:VAL:HG11	1:E:133:LEU:HD21	1.87	0.55
1:A:102:GLU:HG2	2:G:501:38K:H5	1.88	0.55
1:C:84:ASN:C	1:C:84:ASN:HD22	2.10	0.54
1:F:98:ALA:H	1:F:113:ASN:HD21	1.56	0.54
1:C:119:PHE:CD1	2:C:501:38K:H18	2.43	0.54
1:H:206:VAL:O	1:H:209:VAL:HG13	2.08	0.54
1:B:30:ALA:HB1	1:B:249:SER:HB3	1.90	0.54
1:B:55:GLU:HG3	1:B:81:LYS:HD2	1.89	0.54
1:F:281:TYR:CE2	1:F:308:LEU:HD12	2.43	0.54
2:G:501:38K:H5	2:G:501:38K:C15	2.38	0.54
1:B:96:ALA:HA	2:B:501:38K:H1	1.73	0.54
1:E:198:VAL:HG11	1:E:312:GLU:HG2	1.90	0.54
1:C:215:HIS:HB2	1:D:4:LEU:HD13	1.90	0.54
1:C:268:ARG:HA	1:C:295:LEU:O	2.07	0.53
1:F:241:VAL:HG11	1:F:248:THR:HG22	1.89	0.53
1:F:294[A]:ILE:HD13	1:H:180:VAL:HG22	1.90	0.53
2:H:501:38K:C15	2:H:501:38K:H5	2.07	0.53
1:H:105:SER:OG	1:H:108:ASN:HB2	2.09	0.53
1:H:131:CYS:O	1:H:157:ARG:HD2	2.08	0.53
1:B:24:THR:OG1	1:B:49:ALA:HB3	2.09	0.53
1:C:24:THR:HB	1:C:92:VAL:HG22	1.90	0.53
1:A:270:VAL:HA	1:A:293:CYS:O	2.09	0.52
1:G:183:LEU:HD13	1:H:70:LEU:HD12	1.91	0.52
1:E:325:GLY:HA2	1:E:328:LYS:HD2	1.90	0.52
1:F:154:PRO:HB2	1:F:156:ASN:OD1	2.09	0.52
1:E:98:ALA:HB1	1:E:112:ARG:NH1	2.24	0.52
1:B:277[A]:ILE:HD11	1:B:289:LEU:HD12	1.91	0.52
2:F:501:38K:H3	2:F:501:38K:H2	1.56	0.52
1:C:181:HIS:CE1	1:C:183:LEU:HD22	2.44	0.52
1:F:11:ASN:OD1	1:F:14:LYS:HG3	2.10	0.52
1:D:100:GLN:HE22	1:D:109:LEU:HD22	1.74	0.52
1:G:148:TRP:CZ2	1:G:276:MET:HE1	2.44	0.51
1:G:205:ASN:HA	1:G:211:LEU:HD13	1.90	0.51
1:H:294:ILE:HD12	1:H:302:ASP:HB2	1.92	0.51
1:B:40:LEU:HD11	1:B:65:LEU:HD13	1.93	0.51
1:C:70[B]:LEU:HD12	1:D:183:LEU:HD13	1.93	0.51
1:B:294:ILE:HD12	1:B:302:ASP:HB2	1.93	0.51
1:B:84:ASN:HD22	1:B:85:VAL:H	1.57	0.51
1:D:327:GLN:HA	1:D:330:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HG	1:B:4:LEU:HD21	1.93	0.50
1:C:276:MET:HG2	1:C:288:PHE:CE2	2.47	0.50
1:H:277:ILE:HD13	1:H:283:ILE:HG21	1.93	0.50
1:E:16:GLU:HG3	1:H:298:ASN:HD21	1.77	0.50
1:C:327:GLN:HA	1:C:330:LEU:HD22	1.93	0.50
1:G:96:ALA:CA	2:G:501:38K:H1	2.19	0.50
1:A:205:ASN:HD22	1:A:208:GLY:H	1.59	0.50
1:F:13:LEU:HB2	1:F:15:GLU:CG	2.42	0.50
1:E:107[A]:LEU:O	1:E:107[A]:LEU:CD1	2.53	0.50
1:G:4:LEU:HD21	1:H:211:LEU:HG	1.93	0.50
1:G:160:GLY:HA3	1:G:274:SER:HB3	1.94	0.50
1:B:159:ILE:HG23	1:B:300:ILE:HD11	1.93	0.50
1:C:197:SER:OG	1:C:231:HIS:HE1	1.95	0.49
1:E:164:ASN:HA	1:E:272:PRO:HG2	1.94	0.49
1:C:230:VAL:O	1:C:234:VAL:HG23	2.12	0.49
1:A:186:HIS:O	1:A:204:MET:HA	2.13	0.49
1:E:190:LEU:HD22	1:E:200:VAL:HG21	1.94	0.49
1:F:186:HIS:O	1:F:204:MET:HA	2.13	0.49
1:B:18:THR:HG22	1:B:19:PRO:O	2.13	0.48
1:A:98:ALA:H	1:A:113:ASN:ND2	2.11	0.48
1:C:96:ALA:CB	2:C:501:38K:H2	2.26	0.48
2:E:501:38K:H5	2:E:501:38K:C15	2.42	0.48
1:E:206:VAL:O	1:E:209:VAL:HG13	2.13	0.48
1:A:180:VAL:HG22	1:C:294:ILE:HD13	1.96	0.48
1:D:45:ALA:O	1:D:74:THR:HG23	2.13	0.48
1:C:111:GLN:HE22	1:C:331[A]:GLN:H	1.62	0.47
1:C:273:VAL:O	1:C:290:SER:HA	2.13	0.47
1:B:181:HIS:HB2	1:D:267:LEU:O	2.14	0.47
1:A:23:ILE:HD12	1:A:45:ALA:HB2	1.97	0.47
1:D:13:LEU:HG	1:D:15:GLU:HG2	1.96	0.47
1:H:230:VAL:O	1:H:234:VAL:HG23	2.14	0.47
1:F:190:LEU:HD22	1:F:200:VAL:HG21	1.95	0.47
1:H:14:LYS:HG3	1:H:15:GLU:N	2.30	0.47
1:G:111:GLN:HE22	1:G:331:GLN:N	2.11	0.47
1:F:233:GLN:O	1:F:237:SER:OG	2.30	0.47
1:D:84:ASN:C	1:D:84:ASN:HD22	2.17	0.47
1:D:98:ALA:H	1:D:113:ASN:ND2	2.13	0.47
1:F:331:GLN:HE21	1:F:331:GLN:HB2	1.58	0.47
1:A:141:ASP:HB3	1:A:288:PHE:O	2.14	0.47
1:A:183:LEU:HD23	1:C:269:ARG:HD3	1.97	0.46
1:F:183:LEU:HD23	1:H:269:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:VAL:O	1:F:209:VAL:HG12	2.16	0.46
1:B:205:ASN:HD22	1:B:208:GLY:H	1.64	0.46
1:B:108:ASN:O	1:B:112:ARG:HG3	2.16	0.46
1:D:111:GLN:HE22	1:D:331:GLN:N	2.11	0.46
1:A:206:VAL:O	1:A:209:VAL:HG12	2.16	0.46
1:F:84:ASN:HD22	1:F:85:VAL:H	1.63	0.46
1:C:277:ILE:HD11	1:C:289:LEU:HD12	1.96	0.46
1:H:132:LYS:NZ	1:H:297:GLN:O	2.41	0.46
1:F:294[A]:ILE:CD1	1:H:180:VAL:HG22	2.46	0.46
1:H:271:HIS:CD2	1:H:295:LEU:HD22	2.51	0.46
1:F:241:VAL:CG1	1:F:248:THR:HG22	2.46	0.45
1:F:205:ASN:HD22	1:F:208:GLY:H	1.64	0.45
1:C:165:LEU:HD11	1:C:251:ALA:HB1	1.99	0.45
1:H:331:GLN:HE21	1:H:331:GLN:HA	1.81	0.45
1:F:159:ILE:HG23	1:F:300:ILE:HD11	1.99	0.45
1:C:70[B]:LEU:HD11	1:D:171:ARG:NH2	2.31	0.45
1:E:4:LEU:HD13	1:F:215:HIS:CB	2.46	0.45
1:H:14:LYS:O	1:H:16:GLU:N	2.49	0.45
1:B:180:VAL:HG22	1:D:294:ILE:HD13	1.99	0.45
1:H:170:PHE:HD2	1:H:234:VAL:HG21	1.82	0.45
1:G:273:VAL:O	1:G:290:SER:HA	2.17	0.45
1:E:303:LEU:HD12	1:E:303:LEU:C	2.38	0.45
1:E:27:GLY:O	1:E:32:GLY:HA3	2.17	0.45
1:E:331:GLN:HE21	1:E:331:GLN:CA	2.27	0.44
1:D:317:LYS:HE2	1:D:321:ASP:OD2	2.18	0.44
1:F:121:ILE:O	1:F:125:VAL:HG13	2.17	0.44
1:B:278:LYS:HE2	1:B:286:ASP:OD2	2.17	0.44
1:E:51:VAL:HG13	1:E:80:GLY:O	2.17	0.44
1:D:98:ALA:H	1:D:113:ASN:HD21	1.65	0.44
1:B:273:VAL:O	1:B:290:SER:HA	2.18	0.44
1:B:121:ILE:HB	1:B:122:PRO:HD3	2.00	0.44
1:C:233:GLN:O	1:C:237:SER:OG	2.32	0.44
1:B:276:MET:HG2	1:B:288:PHE:CE2	2.53	0.44
2:G:501:38K:H2	2:G:501:38K:H3	1.64	0.44
1:E:84:ASN:C	1:E:84:ASN:HD22	2.20	0.44
1:A:4:LEU:HD21	1:B:211:LEU:HG	1.99	0.44
1:E:98:ALA:HB1	1:E:112:ARG:HH12	1.83	0.44
1:A:215:HIS:HB2	1:B:4:LEU:HD13	2.00	0.44
1:F:3:THR:O	1:F:7:GLN:HG3	2.18	0.44
1:G:294:ILE:HD12	1:G:302:ASP:CB	2.48	0.43
1:C:190:LEU:HD22	1:C:200:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:GLN:NE2	1:G:17:GLN:HB2	2.33	0.43
1:A:167:SER:O	1:A:171:ARG:HG3	2.18	0.43
1:B:97:GLY:H	2:B:501:38K:H1	1.65	0.43
1:B:43:ASP:HB3	1:C:265:LYS:HE2	2.00	0.43
1:C:22:LYS:HB3	1:C:89:SER:HA	1.99	0.43
1:F:232[B]:LYS:HD2	1:F:232[B]:LYS:HA	1.85	0.43
1:E:11:ASN:HD21	1:E:14:LYS:HG3	1.84	0.43
1:A:84:ASN:HD22	1:A:84:ASN:C	2.22	0.43
1:E:267:LEU:O	1:G:181:HIS:HB2	2.19	0.43
1:C:183:LEU:HD21	1:D:73:ARG:NH2	2.34	0.42
1:C:142:ILE:HD13	1:C:326:ILE:HG21	2.00	0.42
1:E:14:LYS:O	1:E:15:GLU:HG3	2.19	0.42
1:A:124:VAL:HG11	1:A:133:LEU:HD21	2.00	0.42
1:C:101:GLN:O	1:C:102:GLU:O	2.37	0.42
1:H:84:ASN:HD22	1:H:85:VAL:H	1.67	0.42
1:D:190:LEU:HD22	1:D:200:VAL:HG21	2.02	0.42
1:F:100:GLN:HA	1:F:109:LEU:HD13	2.01	0.42
1:E:113:ASN:HB3	1:E:143:LEU:HD21	2.02	0.42
1:B:110:VAL:HG22	1:B:330:LEU:HD11	2.02	0.42
1:G:189:VAL:CG1	1:G:197:SER:HB2	2.50	0.42
1:E:22:LYS:HB3	1:E:89:SER:HA	2.02	0.42
2:E:501:38K:C4	2:E:501:38K:H12	2.48	0.42
1:A:273:VAL:O	1:A:290:SER:HA	2.20	0.42
1:B:98:ALA:H	1:B:113:ASN:ND2	2.18	0.42
1:F:277:ILE:HD11	1:F:289:LEU:HD12	2.00	0.42
1:B:12:LEU:O	1:B:13:LEU:C	2.58	0.42
1:E:16:GLU:HG3	1:H:298:ASN:ND2	2.34	0.42
1:A:159:ILE:HG12	1:A:300:ILE:CD1	2.50	0.42
1:B:171:ARG:HD2	1:B:185:CYS:O	2.20	0.42
1:C:311:GLU:O	1:C:315:ARG:HG2	2.19	0.42
1:B:197:SER:OG	1:B:231:HIS:HE1	2.03	0.41
2:C:501:38K:H11	2:C:501:38K:H15	2.01	0.41
1:B:98:ALA:H	1:B:113:ASN:HD21	1.67	0.41
1:B:206:VAL:O	1:B:209:VAL:HG12	2.20	0.41
1:C:84:ASN:C	1:C:84:ASN:ND2	2.73	0.41
1:C:70[A]:LEU:HD22	1:D:183:LEU:HD13	2.01	0.41
1:A:98:ALA:H	1:A:113:ASN:HD21	1.68	0.41
1:E:8:LEU:HD11	1:F:209:VAL:HG13	2.01	0.41
1:C:237:SER:O	1:C:241:VAL:HG23	2.20	0.41
1:G:12:LEU:O	1:G:14:LYS:NZ	2.47	0.41
1:F:146:VAL:HG12	1:F:150:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:GLN:HB2	1:G:297:GLN:HE21	1.84	0.41
1:C:149:LYS:HA	1:C:149:LYS:HD3	1.89	0.41
1:C:4:LEU:O	1:C:5:LYS:C	2.58	0.41
2:B:501:38K:C15	2:B:501:38K:C5	2.99	0.41
1:D:14:LYS:O	1:D:15:GLU:O	2.38	0.41
1:E:15:GLU:O	1:E:17:GLN:N	2.54	0.41
1:F:151:SER:OG	1:F:153:PHE:HB2	2.21	0.41
1:C:119:PHE:HD1	2:C:501:38K:H18	1.81	0.41
2:D:501:38K:H3	2:D:501:38K:H2	1.69	0.41
1:E:23:ILE:HD12	1:E:45:ALA:HB2	2.02	0.41
1:H:72:LEU:C	1:H:73:ARG:HD2	2.40	0.41
1:F:165:LEU:HD11	1:F:251:ALA:HB1	2.01	0.41
1:C:181:HIS:ND1	1:C:182:PRO:HD2	2.35	0.41
1:C:215:HIS:CB	1:D:4:LEU:HD13	2.50	0.41
1:F:84:ASN:HD22	1:F:84:ASN:C	2.25	0.40
1:F:98:ALA:H	1:F:113:ASN:ND2	2.17	0.40
1:F:242:ILE:HG12	1:F:247:TYR:HA	2.02	0.40
1:D:278:LYS:HE2	1:D:286:ASP:OD2	2.21	0.40
1:A:42:LYS:HD3	1:A:257:ALA:HB1	2.03	0.40
1:A:47:GLU:HA	1:A:76:LYS:O	2.21	0.40
1:E:110:VAL:O	1:E:114:VAL:HG23	2.21	0.40
1:C:183:LEU:HD13	1:D:70:LEU:HD12	2.04	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	333/337 (99%)	320 (96%)	11 (3%)	2 (1%)	30	72
1	B	331/337 (98%)	309 (93%)	22 (7%)	0	100	100
1	C	335/337 (99%)	316 (94%)	18 (5%)	1 (0%)	46	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	46	84
1	E	332/337 (98%)	300 (90%)	28 (8%)	4 (1%)	16	56
1	F	335/337 (99%)	319 (95%)	15 (4%)	1 (0%)	46	84
1	G	332/337 (98%)	314 (95%)	17 (5%)	1 (0%)	46	84
1	H	329/337 (98%)	318 (97%)	9 (3%)	2 (1%)	30	72
All	All	2662/2696 (99%)	2514 (94%)	136 (5%)	12 (0%)	34	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	102	GLU
1	D	15	GLU
1	H	15	GLU
1	A	17	GLN
1	E	100	GLN
1	E	278	LYS
1	E	16	GLU
1	F	137	SER
1	H	223	ASP
1	E	249	SER
1	A	18	THR
1	G	249	SER

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	291/293 (99%)	272 (94%)	19 (6%)	21	58
1	B	289/293 (99%)	270 (93%)	19 (7%)	21	57
1	C	293/293 (100%)	272 (93%)	21 (7%)	18	53
1	D	293/293 (100%)	266 (91%)	27 (9%)	11	40
1	E	290/293 (99%)	268 (92%)	22 (8%)	16	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	293/293 (100%)	270 (92%)	23 (8%)	16	49
1	G	290/293 (99%)	269 (93%)	21 (7%)	18	53
1	H	287/293 (98%)	266 (93%)	21 (7%)	17	52
All	All	2326/2344 (99%)	2153 (93%)	173 (7%)	17	52

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	18	THR
1	A	20	GLN
1	A	84	ASN
1	A	107	LEU
1	A	134	LEU
1	A	178	LEU
1	A	183	LEU
1	A	190	LEU
1	A	196	SER
1	A	211	LEU
1	A	237	SER
1	A	280	LEU
1	A	291	VAL
1	A	302	ASP
1	A	310	SER
1	A	328	LYS
1	A	330	LEU
1	A	332	PHE
1	B	5	LYS
1	B	20	GLN
1	B	54	ILE
1	B	84	ASN
1	B	110	VAL
1	B	128	SER
1	B	134	LEU
1	B	137	SER
1	B	178	LEU
1	B	183	LEU
1	B	211	LEU
1	B	248	THR
1	B	255	SER
1	B	280	LEU

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Mol	Chain	Res	Type
1	B	291	VAL
1	B	295	LEU
1	B	310	SER
1	B	319	SER
1	B	330	LEU
1	C	13	LEU
1	C	54	ILE
1	C	69	SER
1	C	70[A]	LEU
1	C	70[B]	LEU
1	C	73	ARG
1	C	84	ASN
1	C	104	GLU
1	C	134	LEU
1	C	149	LYS
1	C	178	LEU
1	C	183	LEU
1	C	190	LEU
1	C	276	MET
1	C	280	LEU
1	C	291	VAL
1	C	295	LEU
1	C	303[A]	LEU
1	C	303[B]	LEU
1	C	319	SER
1	C	330	LEU
1	D	12	LEU
1	D	14	LYS
1	D	18	THR
1	D	20	GLN
1	D	81	LYS
1	D	84	ASN
1	D	101	GLN
1	D	107	LEU
1	D	134	LEU
1	D	149	LYS
1	D	166	ASP
1	D	174	MET
1	D	178	LEU
1	D	183	LEU
1	D	190	LEU
1	D	195	ASP

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Mol	Chain	Res	Type
1	D	196[A]	SER
1	D	196[B]	SER
1	D	224	LYS
1	D	248	THR
1	D	255	SER
1	D	276	MET
1	D	295	LEU
1	D	319	SER
1	D	323	LEU
1	D	328	LYS
1	D	330	LEU
1	E	13	LEU
1	E	14	LYS
1	E	15	GLU
1	E	54	ILE
1	E	84	ASN
1	E	100	GLN
1	E	101	GLN
1	E	107[A]	LEU
1	E	107[B]	LEU
1	E	134	LEU
1	E	178	LEU
1	E	183	LEU
1	E	190	LEU
1	E	209	VAL
1	E	211	LEU
1	E	224	LYS
1	E	248	THR
1	E	310	SER
1	E	328	LYS
1	E	330	LEU
1	E	331	GLN
1	E	332	PHE
1	F	3	THR
1	F	13	LEU
1	F	17	GLN
1	F	20	GLN
1	F	41	MET
1	F	54	ILE
1	F	73	ARG
1	F	84	ASN
1	F	106	ARG

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Mol	Chain	Res	Type
1	F	107	LEU
1	F	134	LEU
1	F	178	LEU
1	F	183	LEU
1	F	190	LEU
1	F	195	ASP
1	F	213	THR
1	F	217	ASP
1	F	255	SER
1	F	295	LEU
1	F	316	LEU
1	F	317	LYS
1	F	330	LEU
1	F	331	GLN
1	G	13	LEU
1	G	18	THR
1	G	20	GLN
1	G	54	ILE
1	G	84	ASN
1	G	107	LEU
1	G	134	LEU
1	G	149	LYS
1	G	178	LEU
1	G	183	LEU
1	G	190	LEU
1	G	196	SER
1	G	209	VAL
1	G	226	GLN
1	G	233	GLN
1	G	237[A]	SER
1	G	237[B]	SER
1	G	248	THR
1	G	255	SER
1	G	323	LEU
1	G	328	LYS
1	H	17	GLN
1	H	54	ILE
1	H	73	ARG
1	H	84	ASN
1	H	99	ARG
1	H	107	LEU
1	H	132	LYS

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Mol	Chain	Res	Type
1	H	134	LEU
1	H	178	LEU
1	H	183	LEU
1	H	209	VAL
1	H	210	SER
1	H	222	LYS
1	H	224	LYS
1	H	248	THR
1	H	276	MET
1	H	285	ASP
1	H	291	VAL
1	H	323	LEU
1	H	330	LEU
1	H	331	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	84	ASN
1	A	108	ASN
1	A	111	GLN
1	A	113	ASN
1	A	164	ASN
1	A	205	ASN
1	A	298	ASN
1	B	11	ASN
1	B	84	ASN
1	B	108	ASN
1	B	113	ASN
1	B	205	ASN
1	B	231	HIS
1	C	84	ASN
1	C	111	GLN
1	C	113	ASN
1	C	205	ASN
1	C	231	HIS
1	C	298	ASN
1	D	20	GLN
1	D	84	ASN
1	D	100	GLN
1	D	108	ASN

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Mol	Chain	Res	Type
1	D	111	GLN
1	D	113	ASN
1	D	123	ASN
1	D	205	ASN
1	D	231	HIS
1	E	11	ASN
1	E	84	ASN
1	E	113	ASN
1	E	205	ASN
1	E	231	HIS
1	E	298	ASN
1	E	331	GLN
1	F	7	GLN
1	F	84	ASN
1	F	100	GLN
1	F	111	GLN
1	F	113	ASN
1	F	205	ASN
1	F	331	GLN
1	G	20	GLN
1	G	84	ASN
1	G	100	GLN
1	G	111	GLN
1	G	113	ASN
1	G	205	ASN
1	G	231	HIS
1	H	84	ASN
1	H	100	GLN
1	H	111	GLN
1	H	113	ASN
1	H	205	ASN
1	H	231	HIS
1	H	298	ASN
1	H	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	38K	A	501	-	34,37,37	2.42	7 (20%)	43,54,54	3.21	16 (37%)
2	38K	B	501	-	34,37,37	2.59	8 (23%)	43,54,54	3.52	15 (34%)
2	38K	C	501	-	34,37,37	2.23	9 (26%)	43,54,54	3.46	21 (48%)
2	38K	D	501	-	34,37,37	2.73	9 (26%)	43,54,54	3.47	16 (37%)
2	38K	E	501	-	34,37,37	2.46	11 (32%)	43,54,54	3.63	20 (46%)
2	38K	F	501	-	34,37,37	2.46	4 (11%)	43,54,54	3.63	19 (44%)
2	38K	G	501	-	34,37,37	2.42	7 (20%)	43,54,54	3.47	20 (46%)
2	38K	H	501	-	34,37,37	2.31	9 (26%)	43,54,54	4.14	24 (55%)

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	38K	A	501	-	-	0/18/22/22	0/4/4/4
2	38K	B	501	-	-	0/18/22/22	0/4/4/4
2	38K	C	501	-	-	1/18/22/22	0/4/4/4
2	38K	D	501	-	-	0/18/22/22	0/4/4/4
2	38K	E	501	-	-	0/18/22/22	0/4/4/4
2	38K	F	501	-	-	0/18/22/22	0/4/4/4
2	38K	G	501	-	-	0/18/22/22	0/4/4/4
2	38K	H	501	-	-	0/18/22/22	0/4/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	38K	C10-S28	-12.51	1.61	1.77
2	D	501	38K	C10-S28	-12.37	1.61	1.77
2	F	501	38K	C10-S28	-11.81	1.62	1.77
2	G	501	38K	C10-S28	-11.08	1.63	1.77
2	A	501	38K	C10-S28	-10.76	1.63	1.77
2	E	501	38K	C10-S28	-10.51	1.63	1.77
2	H	501	38K	C10-S28	-9.56	1.65	1.77
2	C	501	38K	C10-S28	-8.75	1.66	1.77
2	G	501	38K	S28-N31	-4.36	1.51	1.60
2	A	501	38K	S28-N31	-4.17	1.51	1.60
2	F	501	38K	S28-N31	-4.03	1.51	1.60
2	B	501	38K	S28-N31	-3.85	1.52	1.60
2	H	501	38K	S28-N31	-3.76	1.52	1.60
2	C	501	38K	S28-N31	-3.65	1.52	1.60
2	D	501	38K	S28-N31	-3.47	1.52	1.60
2	E	501	38K	S28-N31	-3.37	1.53	1.60
2	C	501	38K	C19-C20	-2.48	1.39	1.41
2	G	501	38K	C19-C20	-2.41	1.39	1.41
2	B	501	38K	C14-C13	-2.34	1.39	1.42
2	C	501	38K	C9-C14	-2.34	1.39	1.43
2	F	501	38K	C19-C20	-2.26	1.39	1.41
2	G	501	38K	C4-N8	-2.20	1.36	1.40
2	C	501	38K	C15-C14	-2.13	1.37	1.42
2	B	501	38K	C21-N22	2.01	1.35	1.33
2	E	501	38K	C15-C16	2.03	1.40	1.36
2	B	501	38K	O29-S28	2.06	1.47	1.43
2	D	501	38K	O29-S28	2.07	1.47	1.43
2	E	501	38K	O26-C21	2.07	1.39	1.33
2	A	501	38K	O24-C20	2.08	1.38	1.35
2	H	501	38K	O24-C20	2.09	1.38	1.35
2	G	501	38K	C21-N25	2.12	1.36	1.33
2	D	501	38K	O24-C20	2.12	1.38	1.35
2	A	501	38K	O26-C21	2.14	1.39	1.33
2	E	501	38K	O24-C20	2.27	1.38	1.35
2	G	501	38K	C9-C10	2.28	1.42	1.40
2	H	501	38K	C21-N25	2.30	1.36	1.33
2	H	501	38K	C20-N25	2.39	1.35	1.32
2	B	501	38K	C21-N25	2.43	1.36	1.33
2	D	501	38K	O30-S28	2.54	1.48	1.43
2	B	501	38K	C20-N25	2.54	1.36	1.32
2	H	501	38K	C11-C10	2.57	1.42	1.39
2	D	501	38K	C15-C16	2.58	1.42	1.36
2	E	501	38K	O29-S28	2.58	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	38K	C21-N22	2.60	1.35	1.33
2	C	501	38K	C9-C10	2.61	1.43	1.40
2	A	501	38K	O29-S28	2.63	1.48	1.43
2	C	501	38K	C21-N22	2.69	1.36	1.33
2	G	501	38K	C21-N22	2.81	1.36	1.33
2	A	501	38K	O30-S28	2.82	1.48	1.43
2	E	501	38K	C9-C10	2.87	1.43	1.40
2	B	501	38K	O30-S28	2.93	1.48	1.43
2	C	501	38K	O30-S28	2.98	1.48	1.43
2	E	501	38K	O30-S28	3.01	1.49	1.43
2	H	501	38K	O30-S28	3.03	1.49	1.43
2	H	501	38K	C21-N22	3.14	1.36	1.33
2	E	501	38K	C21-N25	3.22	1.37	1.33
2	C	501	38K	O29-S28	3.37	1.49	1.43
2	D	501	38K	C21-N22	3.37	1.36	1.33
2	F	501	38K	C21-N22	3.42	1.36	1.33
2	A	501	38K	C21-N22	3.50	1.36	1.33
2	E	501	38K	C20-N25	3.51	1.37	1.32
2	H	501	38K	C9-C10	3.84	1.44	1.40
2	D	501	38K	C21-N25	4.02	1.38	1.33
2	D	501	38K	C20-N25	4.19	1.38	1.32

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	38K	N22-C21-N25	-13.97	119.42	128.33
2	B	501	38K	N22-C21-N25	-13.90	119.47	128.33
2	H	501	38K	N22-C21-N25	-13.33	119.83	128.33
2	A	501	38K	N22-C21-N25	-13.30	119.85	128.33
2	F	501	38K	N22-C21-N25	-12.38	120.44	128.33
2	F	501	38K	O29-S28-O30	-11.75	102.28	118.80
2	D	501	38K	N22-C21-N25	-10.95	121.35	128.33
2	G	501	38K	O29-S28-O30	-10.89	103.50	118.80
2	C	501	38K	N22-C21-N25	-10.88	121.39	128.33
2	H	501	38K	O29-S28-O30	-10.84	103.56	118.80
2	B	501	38K	O29-S28-O30	-10.41	104.17	118.80
2	G	501	38K	N22-C21-N25	-10.23	121.81	128.33
2	D	501	38K	O29-S28-O30	-9.89	104.90	118.80
2	C	501	38K	O29-S28-O30	-9.11	105.99	118.80
2	E	501	38K	O29-S28-O30	-6.52	109.63	118.80
2	E	501	38K	C19-C20-N25	-5.96	118.42	124.53
2	H	501	38K	C5-C4-C3	-5.84	112.71	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	38K	C19-C20-N25	-5.45	118.94	124.53
2	F	501	38K	C19-C20-N25	-5.37	119.03	124.53
2	C	501	38K	C19-C20-N25	-5.37	119.03	124.53
2	A	501	38K	O29-S28-N31	-4.98	100.83	107.28
2	G	501	38K	C19-C23-N22	-4.95	119.26	125.06
2	A	501	38K	C19-C20-N25	-4.56	119.86	124.53
2	G	501	38K	C19-C20-N25	-4.40	120.02	124.53
2	H	501	38K	C15-C14-C13	-4.35	113.89	118.33
2	D	501	38K	C19-C20-N25	-4.34	120.08	124.53
2	E	501	38K	C15-C14-C13	-4.27	113.97	118.33
2	B	501	38K	C19-C20-N25	-4.18	120.24	124.53
2	A	501	38K	C19-C23-N22	-3.98	120.39	125.06
2	H	501	38K	C19-C23-N22	-3.96	120.42	125.06
2	E	501	38K	C23-C19-C17	-3.94	114.98	120.06
2	H	501	38K	C7-C2-C1	-3.71	115.46	120.45
2	C	501	38K	C3-C4-N8	-3.69	108.77	120.31
2	G	501	38K	C3-C4-N8	-3.61	109.04	120.31
2	F	501	38K	C19-C23-N22	-3.47	120.99	125.06
2	C	501	38K	O30-S28-N31	-3.44	102.83	107.28
2	D	501	38K	C19-C23-N22	-3.37	121.11	125.06
2	C	501	38K	C19-C23-N22	-3.28	121.21	125.06
2	H	501	38K	C23-C19-C17	-3.22	115.91	120.06
2	H	501	38K	C6-C7-C2	-3.11	116.45	120.56
2	C	501	38K	C5-C4-C3	-3.10	115.98	119.69
2	G	501	38K	C5-C4-C3	-3.02	116.07	119.69
2	G	501	38K	C10-C11-N12	-2.90	120.88	123.40
2	D	501	38K	C15-C14-C13	-2.83	115.44	118.33
2	B	501	38K	C19-C23-N22	-2.65	121.95	125.06
2	E	501	38K	C7-C2-C1	-2.62	116.93	120.45
2	B	501	38K	C14-C13-N12	-2.61	120.10	122.88
2	A	501	38K	C15-C14-C13	-2.50	115.77	118.33
2	D	501	38K	C5-C4-C3	-2.49	116.71	119.69
2	F	501	38K	C5-C4-C3	-2.46	116.75	119.69
2	B	501	38K	C10-C11-N12	-2.42	121.29	123.40
2	A	501	38K	C14-C13-N12	-2.33	120.40	122.88
2	H	501	38K	C14-C13-N12	-2.30	120.43	122.88
2	A	501	38K	O29-S28-O30	-2.22	115.68	118.80
2	F	501	38K	C15-C14-C13	-2.22	116.07	118.33
2	E	501	38K	C14-C13-N12	-2.20	120.54	122.88
2	E	501	38K	C19-C23-N22	-2.16	122.53	125.06
2	F	501	38K	C14-C13-N12	-2.11	120.63	122.88
2	F	501	38K	C10-C11-N12	-2.10	121.58	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	38K	C23-C19-C17	-2.10	117.36	120.06
2	G	501	38K	O29-S28-N31	-2.08	104.59	107.28
2	C	501	38K	C11-N12-C13	2.00	119.23	116.95
2	C	501	38K	O30-S28-C10	2.01	110.13	107.28
2	F	501	38K	C14-C9-N8	2.04	124.74	120.56
2	D	501	38K	C2-C3-C4	2.09	123.47	121.52
2	D	501	38K	C14-C9-N8	2.10	124.84	120.56
2	F	501	38K	O26-C21-N22	2.12	123.40	116.28
2	H	501	38K	C11-N12-C13	2.14	119.38	116.95
2	C	501	38K	C6-C5-C4	2.15	122.45	119.72
2	E	501	38K	C7-C2-C3	2.17	121.04	118.17
2	F	501	38K	C5-C4-N8	2.22	127.90	120.66
2	G	501	38K	C9-C14-C13	2.23	119.68	117.25
2	B	501	38K	C17-C18-C13	2.26	123.13	120.80
2	E	501	38K	C18-C13-C14	2.39	122.64	119.61
2	A	501	38K	C10-S28-N31	2.39	112.51	108.41
2	E	501	38K	C9-C14-C13	2.47	119.94	117.25
2	D	501	38K	C9-C14-C13	2.48	119.95	117.25
2	B	501	38K	C9-C14-C13	2.53	120.00	117.25
2	C	501	38K	C27-O26-C21	2.54	122.37	117.63
2	E	501	38K	O29-S28-N31	2.60	110.65	107.28
2	F	501	38K	O30-S28-C10	2.66	111.04	107.28
2	B	501	38K	O29-S28-N31	2.71	110.79	107.28
2	H	501	38K	C5-C4-N8	2.71	129.52	120.66
2	C	501	38K	C9-N8-C4	2.72	134.56	124.89
2	C	501	38K	C9-C14-C13	2.75	120.24	117.25
2	E	501	38K	C14-C9-N8	2.79	126.26	120.56
2	G	501	38K	C2-C3-C4	2.84	124.17	121.52
2	D	501	38K	C11-N12-C13	2.94	120.29	116.95
2	A	501	38K	C9-C14-C13	2.96	120.47	117.25
2	H	501	38K	C18-C17-C19	2.97	125.15	121.25
2	F	501	38K	O29-S28-C10	2.99	111.51	107.28
2	A	501	38K	C27-O26-C21	3.00	123.23	117.63
2	C	501	38K	C23-N22-C21	3.12	118.51	115.06
2	C	501	38K	C7-C2-C1	3.21	124.77	120.45
2	H	501	38K	C16-C15-C14	3.27	125.43	121.13
2	A	501	38K	O24-C20-C19	3.29	121.57	117.75
2	A	501	38K	O30-S28-N31	3.30	111.56	107.28
2	G	501	38K	O30-S28-N31	3.43	111.72	107.28
2	G	501	38K	C11-N12-C13	3.47	120.90	116.95
2	C	501	38K	O29-S28-N31	3.49	111.80	107.28
2	B	501	38K	O24-C20-C19	3.60	121.94	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	38K	C9-N8-C4	3.62	137.77	124.89
2	F	501	38K	C23-N22-C21	3.69	119.15	115.06
2	F	501	38K	C11-N12-C13	3.70	121.16	116.95
2	D	501	38K	O30-S28-C10	3.70	112.53	107.28
2	A	501	38K	C11-N12-C13	3.72	121.19	116.95
2	G	501	38K	O30-S28-C10	3.76	112.60	107.28
2	E	501	38K	O24-C20-C19	3.81	122.19	117.75
2	G	501	38K	C14-C9-N8	3.84	128.40	120.56
2	F	501	38K	O30-S28-N31	3.92	112.36	107.28
2	H	501	38K	C7-C2-C3	3.94	123.39	118.17
2	E	501	38K	C11-N12-C13	3.96	121.46	116.95
2	D	501	38K	C10-S28-N31	4.05	115.36	108.41
2	G	501	38K	C7-C2-C1	4.07	125.92	120.45
2	G	501	38K	C5-C4-N8	4.08	133.98	120.66
2	B	501	38K	C25-O24-C20	4.13	121.41	117.31
2	C	501	38K	C14-C9-N8	4.18	129.10	120.56
2	B	501	38K	C11-N12-C13	4.21	121.74	116.95
2	H	501	38K	C14-C9-N8	4.28	129.31	120.56
2	C	501	38K	C5-C4-N8	4.33	134.78	120.66
2	H	501	38K	C6-C5-C4	4.36	125.25	119.72
2	F	501	38K	C25-O24-C20	4.39	121.68	117.31
2	G	501	38K	C25-O24-C20	4.42	121.71	117.31
2	H	501	38K	C25-O24-C20	4.47	121.76	117.31
2	E	501	38K	C23-N22-C21	4.51	120.06	115.06
2	E	501	38K	C27-O26-C21	4.54	126.10	117.63
2	D	501	38K	C21-N25-C20	4.60	119.22	115.25
2	B	501	38K	O30-S28-C10	4.68	113.91	107.28
2	G	501	38K	C23-N22-C21	4.69	120.26	115.06
2	C	501	38K	O24-C20-C19	4.69	123.21	117.75
2	D	501	38K	C23-N22-C21	4.72	120.28	115.06
2	G	501	38K	C21-N25-C20	4.74	119.34	115.25
2	A	501	38K	C25-O24-C20	4.76	122.04	117.31
2	E	501	38K	C25-O24-C20	4.76	122.04	117.31
2	B	501	38K	C23-N22-C21	4.85	120.43	115.06
2	H	501	38K	O24-C20-C19	4.87	123.42	117.75
2	A	501	38K	C23-N22-C21	5.04	120.64	115.06
2	E	501	38K	O30-S28-C10	5.06	114.44	107.28
2	H	501	38K	C9-C14-C13	5.09	122.78	117.25
2	H	501	38K	C23-N22-C21	5.10	120.71	115.06
2	F	501	38K	O24-C20-C19	5.14	123.73	117.75
2	G	501	38K	O29-S28-C10	5.47	115.02	107.28
2	H	501	38K	O29-S28-C10	5.70	115.36	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	38K	O29-S28-C10	5.90	115.63	107.28
2	B	501	38K	C21-N25-C20	7.09	121.38	115.25
2	A	501	38K	C21-N25-C20	7.24	121.50	115.25
2	C	501	38K	C21-N25-C20	7.40	121.64	115.25
2	H	501	38K	C21-N25-C20	7.49	121.72	115.25
2	F	501	38K	C21-N25-C20	8.17	122.31	115.25
2	E	501	38K	C21-N25-C20	8.40	122.50	115.25
2	D	501	38K	C25-O24-C20	10.53	127.78	117.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	38K	C25-O24-C20-C19

There are no ring outliers.

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	38K	4	0
2	C	501	38K	7	0
2	D	501	38K	1	0
2	E	501	38K	4	0
2	F	501	38K	2	0
2	G	501	38K	7	0
2	H	501	38K	4	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	332/337 (98%)	-0.60	0 100 100	42, 57, 87, 124	0
1	B	331/337 (98%)	-0.58	2 (0%) 90 73	41, 58, 92, 111	0
1	C	332/337 (98%)	-0.65	0 100 100	40, 55, 87, 124	0
1	D	332/337 (98%)	-0.62	0 100 100	40, 56, 86, 127	0
1	E	331/337 (98%)	-0.35	7 (2%) 67 36	52, 76, 118, 143	0
1	F	331/337 (98%)	-0.61	2 (0%) 90 73	40, 59, 98, 124	0
1	G	331/337 (98%)	-0.73	1 (0%) 94 84	40, 57, 86, 106	0
1	H	331/337 (98%)	-0.50	3 (0%) 85 64	47, 70, 104, 147	0
All	All	2651/2696 (98%)	-0.58	15 (0%) 90 73	40, 61, 98, 147	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	15	GLU	3.3
1	E	15	GLU	2.9
1	B	102	GLU	2.6
1	E	100	GLN	2.6
1	G	102	GLU	2.5
1	E	328	LYS	2.5
1	E	16	GLU	2.2
1	E	284	LYS	2.2
1	F	15	GLU	2.2
1	F	331	GLN	2.1
1	E	102	GLU	2.1
1	B	103	GLY	2.1
1	E	239	TYR	2.1
1	H	14	LYS	2.1
1	H	17	GLN	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(Å ²)	Q<0.9
2	38K	G	501	34/34	0.94	0.20	1.53	43,50,97,105	0
2	38K	H	501	34/34	0.93	0.28	1.14	55,77,143,155	0
2	38K	E	501	34/34	0.94	0.27	0.92	61,83,96,101	0
2	38K	A	501	34/34	0.97	0.21	0.81	47,60,68,72	0
2	38K	F	501	34/34	0.97	0.18	0.80	47,58,78,84	0
2	38K	C	501	34/34	0.92	0.21	0.56	43,50,109,114	0
2	38K	D	501	34/34	0.96	0.20	0.49	43,52,64,80	0
2	38K	B	501	34/34	0.97	0.19	0.21	46,57,76,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.