



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:30 PM GMT

PDB ID : 1TXT
Title : Staphylococcus aureus 3-hydroxy-3-methylglutaryl-CoA synthase
Authors : Campobasso, N.; Patel, M.; Wilding, I.E.; Kallender, H.; Rosenberg, M.; Gwynn, M.
Deposited on : 2004-07-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

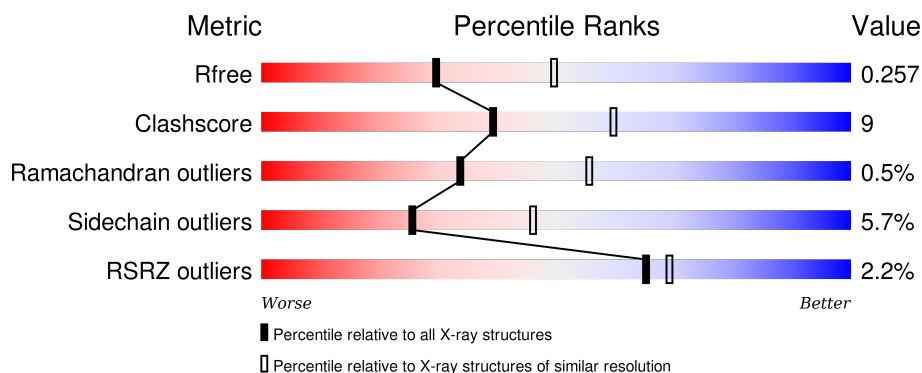
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	388	<div> <div>4%</div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	B	388	<div> <div>%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	C	388	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
1	D	388	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CAA	A	5866	X	-	-	-
2	CAA	B	6866	X	-	-	-
2	CAA	C	7866	X	-	-	-
2	CAA	D	8866	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12750 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.

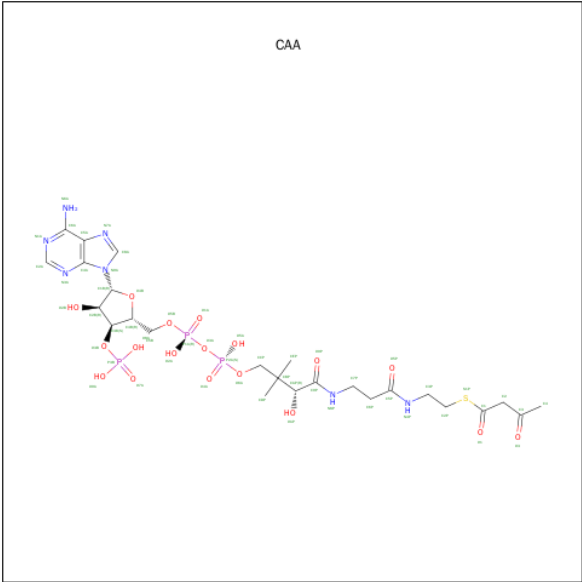
- Molecule 1 is a protein called 3-hydroxy-3-methylglutaryl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3040	1921	510	599	10			
1	B	387	Total	C	N	O	S	0	0	0
			3040	1921	510	599	10			
1	C	387	Total	C	N	O	S	0	0	0
			3040	1921	510	599	10			
1	D	387	Total	C	N	O	S	0	0	0
			3040	1921	510	599	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	CSD	CYS	MODIFIED RESIDUE	UNP Q9FD87
A	320	GLU	VAL	CONFLICT	UNP Q9FD87
B	111	CSD	CYS	MODIFIED RESIDUE	UNP Q9FD87
B	320	GLU	VAL	CONFLICT	UNP Q9FD87
C	111	CSD	CYS	MODIFIED RESIDUE	UNP Q9FD87
C	320	GLU	VAL	CONFLICT	UNP Q9FD87
D	111	CSD	CYS	MODIFIED RESIDUE	UNP Q9FD87
D	320	GLU	VAL	CONFLICT	UNP Q9FD87

- Molecule 2 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: C₂₅H₄₀N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

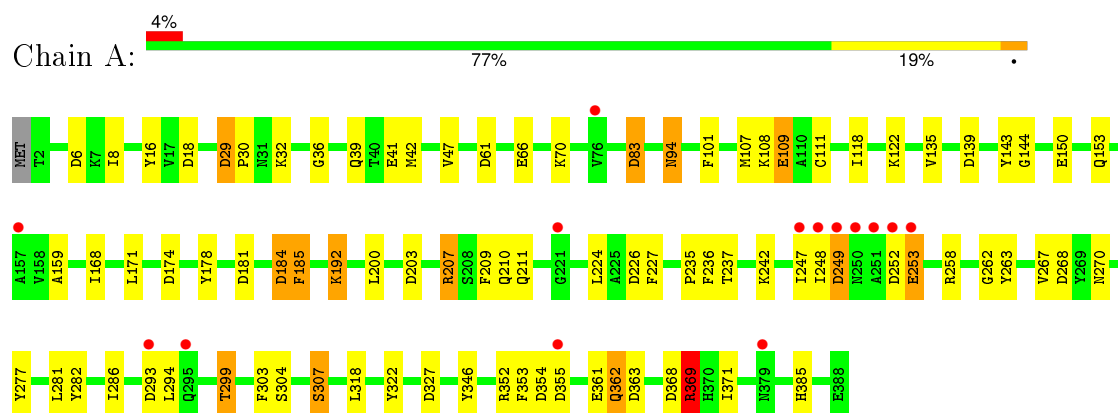
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	93	Total	O	0	0
			93	93		
3	C	102	Total	O	0	0
			102	102		
3	D	90	Total	O	0	0
			90	90		

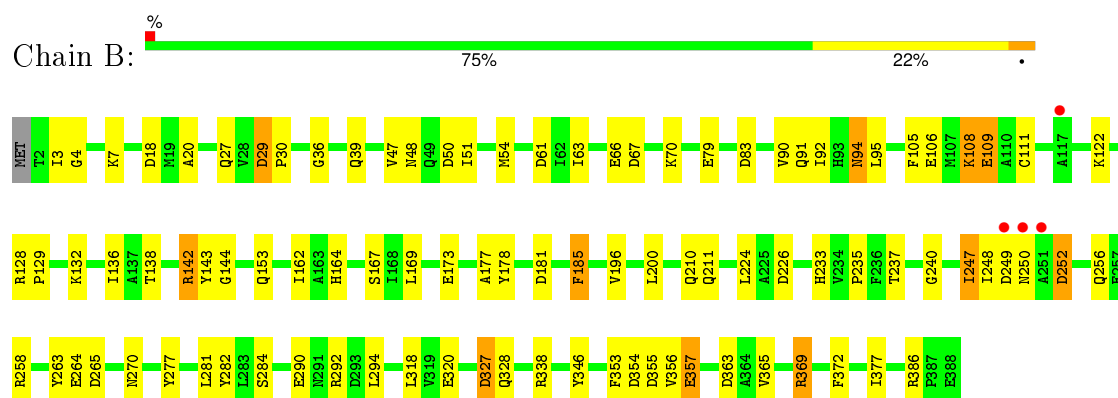
3 Residue-property plots

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.

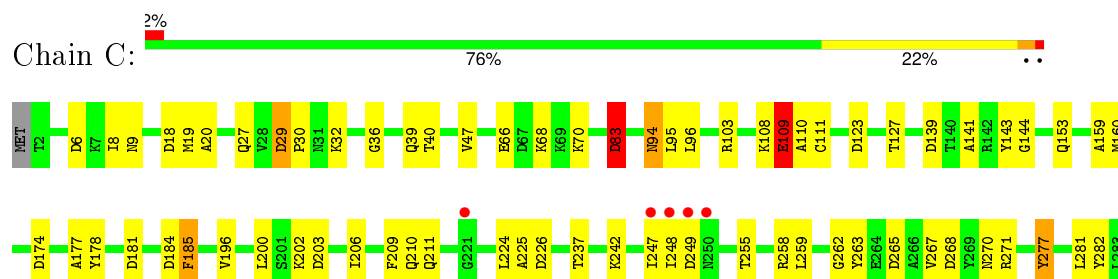
- Molecule 1: 3-hydroxy-3-methylglutaryl-CoA synthase



- Molecule 1: 3-hydroxy-3-methylglutaryl-CoA synthase

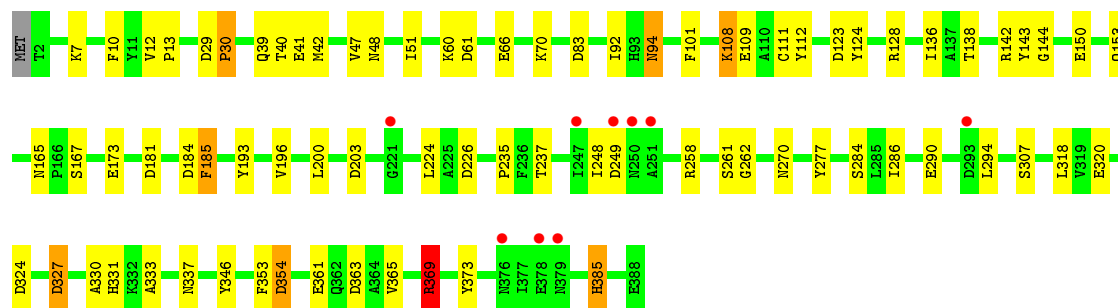
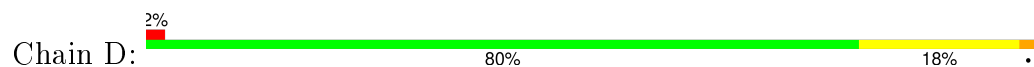


- Molecule 1: 3-hydroxy-3-methylglutaryl-CoA synthase





- Molecule 1: 3-hydroxy-3-methylglutaryl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.95Å 64.48Å 121.91Å 90.00° 97.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 44.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (20.00-2.50) 85.5 (44.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.187 , 0.255 0.191 , 0.257	Depositor DCC
R_{free} test set	2991 reflections (5.72%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.0	EDS
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	17 of 59617 reflections (0.029%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12750	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1190e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CSD, CAA

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	0.95	0/3094	1.03	19/4193 (0.5%)
1	B	0.95	0/3094	1.02	14/4193 (0.3%)
1	C	0.96	2/3094 (0.1%)	1.06	20/4193 (0.5%)
1	D	0.94	0/3094	1.01	13/4193 (0.3%)
All	All	0.95	2/12376 (0.0%)	1.03	66/16772 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	320	GLU	CD-OE2	6.07	1.32	1.25
1	C	277	TYR	CE2-CZ	5.35	1.45	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ASP	CB-CG-OD2	10.44	127.69	118.30
1	C	258	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	D	181	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	327	ASP	CB-CG-OD2	8.03	125.53	118.30
1	C	327	ASP	CB-CG-OD2	7.99	125.49	118.30
1	C	265	ASP	CB-CG-OD2	7.80	125.32	118.30
1	B	354	ASP	CB-CG-OD2	7.59	125.14	118.30
1	C	271	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	D	258	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	D	354	ASP	CB-CG-OD2	7.54	125.09	118.30
1	C	6	ASP	CB-CG-OD2	7.34	124.91	118.30
1	D	61	ASP	CB-CG-OD2	7.05	124.64	118.30
1	C	258	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	C	268	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	258	ARG	NE-CZ-NH1	6.95	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	226	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	203	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	184	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	258	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	363	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	226	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	67	ASP	CB-CG-OD2	6.42	124.07	118.30
1	C	181	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	258	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	C	293	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	139	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	268	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	258	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	354	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	142	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	29	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	352	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	29	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	324	ASP	CB-CG-OD2	5.88	123.60	118.30
1	A	181	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	252	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	252	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	226	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	174	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	83	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	368	ASP	CB-CG-OD2	5.75	123.47	118.30
1	D	142	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	293	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	265	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	61	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	203	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	369	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	174	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	355	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	268	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	6	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	123	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	369	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	184	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	369	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	184	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	123	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	83	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	128	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	226	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	61	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	18	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	363	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	271	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3040	0	2938	59	0
1	B	3040	0	2938	62	0
1	C	3040	0	2938	55	0
1	D	3040	0	2938	46	0
2	A	54	0	36	10	0
2	B	54	0	36	3	0
2	C	54	0	36	8	0
2	D	54	0	36	2	0
3	A	89	0	0	0	0
3	B	93	0	0	6	0
3	C	102	0	0	1	0
3	D	90	0	0	1	0
All	All	12750	0	11896	216	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 9.

All (216) 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:A:143:TYR:H	1:A:153:GLN:HE21	1.08	0.96
1:B:143:TYR:H	1:B:153:GLN:HE21	1.12	0.94
1:D:143:TYR:H	1:D:153:GLN:HE21	0.94	0.93
1:C:143:TYR:H	1:C:153:GLN:HE21	1.02	0.92
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.36	0.90
1:B:91:GLN:HG3	3:B:6939:HOH:O	1.71	0.89
1:D:143:TYR:N	1:D:153:GLN:HE21	1.71	0.88
1:D:143:TYR:H	1:D:153:GLN:NE2	1.75	0.84
1:D:94:ASN:C	1:D:94:ASN:HD22	1.81	0.81
1:C:143:TYR:H	1:C:153:GLN:NE2	1.78	0.81
1:D:39:GLN:NE2	1:D:237:THR:HG23	1.97	0.80
1:C:143:TYR:N	1:C:153:GLN:HE21	1.81	0.79
1:A:143:TYR:H	1:A:153:GLN:NE2	1.81	0.79
1:D:369:ARG:HB2	1:D:369:ARG:HH11	1.49	0.78
1:A:224:LEU:HD13	1:A:248:ILE:HG22	1.65	0.76
1:C:39:GLN:NE2	1:C:237:THR:H	1.83	0.76
1:B:143:TYR:H	1:B:153:GLN:NE2	1.84	0.76
1:C:290:GLU:HB3	1:C:328:GLN:HG3	1.67	0.74
1:C:224:LEU:HD13	1:C:248:ILE:HG22	1.69	0.74
1:C:39:GLN:HE21	1:C:237:THR:H	1.36	0.73
1:B:143:TYR:N	1:B:153:GLN:HE21	1.84	0.73
1:B:320:GLU:HB2	1:D:165:ASN:OD1	1.87	0.73
1:B:94:ASN:C	1:B:94:ASN:HD22	1.92	0.73
1:A:207:ARG:CG	1:A:207:ARG:HH11	2.02	0.72
1:B:320:GLU:HG3	3:B:6952:HOH:O	1.90	0.72
1:D:39:GLN:HE21	1:D:237:THR:H	1.39	0.70
1:A:143:TYR:N	1:A:153:GLN:HE21	1.87	0.69
1:A:369:ARG:HH11	1:A:369:ARG:HB2	1.57	0.69
1:A:39:GLN:HE21	1:A:237:THR:H	1.38	0.69
1:B:39:GLN:NE2	1:B:237:THR:HG23	2.09	0.68
1:A:94:ASN:C	1:A:94:ASN:HD22	1.98	0.67
1:B:143:TYR:OH	2:B:6866:CAA:C4	2.44	0.66
1:A:242:LYS:NZ	2:A:5866:CAA:O8A	2.25	0.66
1:C:83:ASP:O	1:D:108:LYS:HE3	1.96	0.66
1:C:210:GLN:HG2	1:C:247:ILE:HD13	1.78	0.65
1:D:39:GLN:HE22	1:D:237:THR:HG23	1.62	0.65
1:B:143:TYR:OH	2:B:6866:CAA:H4'2	1.96	0.64
1:A:144:GLY:H	1:A:153:GLN:NE2	1.95	0.64
1:A:270:ASN:H	1:A:270:ASN:HD22	1.45	0.64
1:C:8:ILE:HA	1:C:159:ALA:O	1.97	0.64
1:B:290:GLU:HB3	1:B:328:GLN:HG3	1.78	0.63
1:C:270:ASN:H	1:C:270:ASN:HD22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HD3	1:A:362:GLN:HE22	1.65	0.62
1:C:94:ASN:HD22	1:C:94:ASN:C	2.03	0.62
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.64	0.61
1:D:327:ASP:HB3	1:D:330:ALA:HB3	1.83	0.61
1:D:94:ASN:C	1:D:94:ASN:ND2	2.54	0.60
1:B:210:GLN:HG2	1:B:247:ILE:HD13	1.83	0.60
1:D:224:LEU:HD13	1:D:248:ILE:HG22	1.84	0.60
1:C:185:PHE:HB3	1:C:307:SER:OG	2.03	0.59
1:A:144:GLY:H	1:A:153:GLN:HE22	1.48	0.59
1:D:40:THR:HG22	1:D:41:GLU:HG3	1.85	0.59
1:B:320:GLU:CG	3:B:6952:HOH:O	2.50	0.59
1:D:47:VAL:HG22	1:D:353:PHE:HA	1.84	0.58
1:D:193:TYR:OH	1:D:354:ASP:OD1	2.22	0.58
1:B:39:GLN:HE21	1:B:237:THR:H	1.52	0.58
1:A:270:ASN:H	1:A:270:ASN:ND2	2.02	0.57
1:A:282:TYR:O	1:A:286:ILE:HG13	2.05	0.57
1:B:122:LYS:NZ	1:B:173:GLU:OE2	2.38	0.57
1:C:32:LYS:HE2	2:C:7866:CAA:O2A	2.05	0.56
2:C:7866:CAA:O7A	2:C:7866:CAA:C2B	2.53	0.56
2:A:5866:CAA:O7A	2:A:5866:CAA:C2B	2.53	0.56
1:C:39:GLN:HE22	1:C:237:THR:HG23	1.70	0.56
1:A:249:ASP:N	1:A:249:ASP:OD1	2.38	0.56
1:D:144:GLY:H	1:D:153:GLN:NE2	2.03	0.56
1:B:338:ARG:HD2	3:B:6879:HOH:O	2.06	0.55
1:C:103:ARG:HG2	1:D:112:TYR:OH	2.06	0.55
1:C:281:LEU:HD23	1:C:282:TYR:CZ	2.42	0.54
1:D:39:GLN:NE2	1:D:237:THR:H	2.05	0.54
1:B:70:LYS:HB2	1:B:132:LYS:HD2	1.90	0.54
1:D:12:VAL:HB	1:D:13:PRO:HD2	1.90	0.54
1:B:224:LEU:HD13	1:B:248:ILE:HG22	1.90	0.54
1:B:39:GLN:HE22	1:B:237:THR:HG23	1.72	0.54
1:A:352:ARG:HD3	1:A:362:GLN:NE2	2.23	0.53
1:A:39:GLN:NE2	1:A:237:THR:H	2.05	0.53
1:A:108:LYS:HE2	1:B:106:GLU:OE1	2.08	0.53
1:C:18:ASP:OD2	1:C:20:ALA:HB3	2.08	0.53
1:B:355:ASP:HB2	1:B:357:GLU:HG2	1.91	0.53
1:C:36:GLY:HA3	2:C:7866:CAA:H1B	1.91	0.53
1:B:94:ASN:C	1:B:94:ASN:ND2	2.61	0.52
1:D:369:ARG:HG2	3:D:8927:HOH:O	2.09	0.52
1:B:129:PRO:HA	1:B:164:HIS:CD2	2.45	0.52
1:C:185:PHE:CD1	2:C:7866:CAA:H4'3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HD3	1:B:294:LEU:HD21	1.92	0.52
1:A:307:SER:OG	2:A:5866:CAA:H2'2	2.10	0.52
1:B:111:CSD:OD1	1:B:277:TYR:CD2	2.63	0.52
1:B:143:TYR:HE2	1:B:196:VAL:HG21	1.74	0.52
1:A:122:LYS:HE3	1:A:171:LEU:O	2.10	0.52
1:C:177:ALA:O	1:D:101:PHE:HA	2.09	0.52
1:D:369:ARG:NH1	1:D:369:ARG:HB2	2.21	0.51
2:A:5866:CAA:O7A	2:A:5866:CAA:H2B	2.10	0.51
1:A:224:LEU:HD11	1:A:247:ILE:HG23	1.92	0.51
1:B:90:VAL:HB	3:B:6939:HOH:O	2.11	0.51
1:B:292:ARG:HG3	1:B:292:ARG:NH1	2.26	0.51
1:A:32:LYS:HE2	2:A:5866:CAA:O2A	2.10	0.51
1:C:224:LEU:HD11	1:C:247:ILE:HG23	1.92	0.51
1:A:236:PHE:HE2	2:A:5866:CAA:H32	1.76	0.51
1:C:270:ASN:H	1:C:270:ASN:ND2	2.09	0.51
1:A:8:ILE:HA	1:A:159:ALA:O	2.11	0.50
1:A:83:ASP:O	1:B:108:LYS:HE3	2.11	0.50
1:D:48:ASN:ND2	1:D:365:VAL:HG12	2.27	0.50
1:D:270:ASN:HD21	1:D:284:SER:HA	1.76	0.50
1:C:19:MET:HB2	1:C:40:THR:O	2.11	0.50
1:B:51:ILE:HB	1:B:138:THR:HG23	1.93	0.50
1:C:262:GLY:O	1:C:263:TYR:C	2.51	0.50
1:C:178:TYR:CZ	1:C:211:GLN:HG3	2.47	0.49
1:C:255:THR:O	1:C:259:LEU:HG	2.13	0.49
1:A:184:ASP:OD1	1:A:185:PHE:N	2.46	0.49
1:D:185:PHE:HB3	1:D:307:SER:OG	2.13	0.49
1:D:290:GLU:OE2	1:D:331:HIS:CE1	2.66	0.49
1:B:252:ASP:O	1:B:256:GLN:HG3	2.12	0.49
1:D:143:TYR:OH	2:D:8866:CAA:H4'2	2.13	0.49
1:C:185:PHE:HB3	1:C:307:SER:CB	2.43	0.48
1:A:185:PHE:HB3	1:A:307:SER:OG	2.13	0.48
1:B:48:ASN:ND2	1:B:365:VAL:HG12	2.29	0.48
1:C:143:TYR:OH	2:C:7866:CAA:C4	2.62	0.48
1:C:242:LYS:NZ	2:C:7866:CAA:O8A	2.41	0.48
1:A:207:ARG:CG	1:A:207:ARG:NH1	2.72	0.48
1:C:143:TYR:HE2	1:C:196:VAL:HG21	1.79	0.48
2:C:7866:CAA:H2B	2:C:7866:CAA:O7A	2.13	0.48
1:C:308:GLY:N	1:C:309:SER:HA	2.28	0.48
1:C:289:LEU:HD22	1:C:318:LEU:HD21	1.96	0.48
1:B:356:VAL:HG11	1:B:377:ILE:HD11	1.95	0.48
1:D:143:TYR:HE2	1:D:196:VAL:HG21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLY:H	1:D:153:GLN:HE22	1.61	0.47
1:D:261:SER:O	1:D:262:GLY:C	2.52	0.47
1:D:10:PHE:HD2	1:D:286:ILE:HD13	1.79	0.47
1:C:202:LYS:NZ	1:C:242:LYS:HZ2	2.12	0.47
1:A:101:PHE:HA	1:B:177:ALA:O	2.15	0.47
1:A:281:LEU:HD22	1:A:304:SER:HB2	1.97	0.47
1:B:270:ASN:HD21	1:B:284:SER:HA	1.79	0.47
1:B:355:ASP:HB2	1:B:357:GLU:CG	2.45	0.47
1:B:270:ASN:HD22	1:B:270:ASN:H	1.62	0.47
1:C:209:PHE:HB2	1:C:303:PHE:CE2	2.50	0.47
1:A:94:ASN:C	1:A:94:ASN:ND2	2.67	0.47
1:C:111:CSD:OD1	1:C:277:TYR:CD2	2.68	0.47
1:B:169:LEU:HD23	1:B:318:LEU:HA	1.98	0.46
1:C:144:GLY:H	1:C:153:GLN:NE2	2.13	0.46
1:C:68:LYS:HE2	1:C:96:LEU:O	2.15	0.46
1:B:281:LEU:HD23	1:B:282:TYR:CZ	2.51	0.46
1:A:227:PHE:CD2	1:A:299:THR:HG22	2.51	0.46
1:B:129:PRO:HG3	1:C:127:THR:HA	1.96	0.46
1:C:39:GLN:NE2	1:C:237:THR:HG23	2.30	0.46
1:D:29:ASP:HA	1:D:30:PRO:HD2	1.79	0.46
1:D:51:ILE:HB	1:D:138:THR:HG23	1.98	0.45
1:A:369:ARG:NH1	1:A:369:ARG:HB2	2.28	0.45
1:A:209:PHE:HB2	1:A:303:PHE:CE2	2.51	0.45
1:D:92:ILE:HG21	1:D:136:ILE:HD12	1.99	0.45
1:B:144:GLY:H	1:B:153:GLN:NE2	2.15	0.45
1:B:224:LEU:HD11	1:B:247:ILE:HG23	1.98	0.45
1:B:92:ILE:HG21	1:B:136:ILE:HD12	1.98	0.45
1:D:294:LEU:HB3	1:D:318:LEU:CD1	2.47	0.45
1:B:47:VAL:HG22	1:B:353:PHE:HA	1.99	0.45
1:B:250:ASN:N	3:B:6912:HOH:O	2.49	0.45
1:A:352:ARG:HH22	1:A:363:ASP:CG	2.19	0.45
1:A:237:THR:HG22	1:A:267:VAL:HB	1.99	0.44
1:C:270:ASN:HD21	1:C:284:SER:HA	1.83	0.44
1:D:373:TYR:CD2	1:D:385:HIS:CD2	3.06	0.44
1:B:327:ASP:N	1:B:327:ASP:OD2	2.50	0.44
1:A:47:VAL:HG22	1:A:353:PHE:HA	1.98	0.44
1:A:39:GLN:NE2	1:A:237:THR:HG23	2.32	0.44
1:C:237:THR:HG22	1:C:267:VAL:HB	2.00	0.44
1:D:111:CSD:OD1	1:D:277:TYR:CD2	2.71	0.43
1:A:29:ASP:HA	1:A:30:PRO:HD2	1.79	0.43
1:A:210:GLN:HG2	1:A:247:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:CZ	1:B:211:GLN:HG3	2.53	0.43
1:A:262:GLY:O	1:A:263:TYR:C	2.56	0.43
1:B:36:GLY:HA3	2:B:6866:CAA:H1B	2.00	0.43
1:D:235:PRO:HG3	2:D:8866:CAA:H22	2.01	0.43
1:A:42:MET:HE1	1:A:150:GLU:O	2.18	0.43
1:C:95:LEU:HB3	1:C:372:PHE:CE2	2.54	0.43
1:A:185:PHE:CD1	2:A:5866:CAA:H4'3	2.54	0.43
1:A:185:PHE:HB3	1:A:307:SER:CB	2.49	0.43
1:A:178:TYR:CZ	1:A:211:GLN:HG3	2.54	0.43
1:A:118:ILE:HG22	1:A:135:VAL:HG21	2.01	0.43
1:C:29:ASP:O	1:C:30:PRO:C	2.58	0.43
1:C:143:TYR:CE2	1:C:196:VAL:HG21	2.53	0.42
1:C:109:GLU:O	1:C:110:ALA:C	2.57	0.42
1:C:202:LYS:NZ	1:C:242:LYS:NZ	2.67	0.42
1:A:36:GLY:HA3	2:A:5866:CAA:H1B	2.01	0.42
1:C:83:ASP:O	1:D:108:LYS:CE	2.64	0.42
1:B:210:GLN:HG2	1:B:247:ILE:CD1	2.49	0.42
1:A:111:CSD:OD1	1:A:277:TYR:CD2	2.73	0.42
1:D:290:GLU:OE1	1:D:331:HIS:ND1	2.52	0.42
1:A:294:LEU:HB3	1:A:318:LEU:CD1	2.50	0.42
1:D:42:MET:HE1	1:D:150:GLU:O	2.20	0.42
1:C:371:ILE:O	1:C:385:HIS:HD2	2.02	0.42
1:C:9:ASN:ND2	3:C:7938:HOH:O	2.50	0.41
1:A:107:MET:HE2	1:B:105:PHE:CE1	2.55	0.41
1:B:185:PHE:CD2	1:B:185:PHE:C	2.93	0.41
1:B:233:HIS:CD2	1:B:235:PRO:HD3	2.55	0.41
1:B:240:GLY:HA3	1:B:263:TYR:OH	2.20	0.41
1:C:141:ALA:O	1:C:153:GLN:HG2	2.21	0.41
1:B:4:GLY:O	1:B:162:ILE:HA	2.21	0.41
1:A:371:ILE:O	1:A:385:HIS:HD2	2.03	0.41
1:C:143:TYR:OH	2:C:7866:CAA:H4'1	2.20	0.41
1:C:47:VAL:HG22	1:C:353:PHE:HA	2.02	0.41
1:B:95:LEU:HB3	1:B:372:PHE:CE2	2.56	0.41
1:D:270:ASN:H	1:D:270:ASN:ND2	2.18	0.41
1:A:207:ARG:HG3	1:A:207:ARG:NH1	2.16	0.41
1:C:290:GLU:OE1	1:C:331:HIS:ND1	2.53	0.41
1:B:3:ILE:HG21	1:B:122:LYS:HA	2.03	0.41
1:D:124:TYR:CZ	1:D:128:ARG:HD2	2.55	0.41
1:D:333:ALA:O	1:D:337:ASN:HB2	2.20	0.41
1:A:235:PRO:HG3	2:A:5866:CAA:H22	2.03	0.41
1:A:168:ILE:HA	1:A:322:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:OD2	1:B:20:ALA:HB3	2.21	0.40
1:B:270:ASN:ND2	1:B:270:ASN:H	2.19	0.40
1:B:29:ASP:O	1:B:30:PRO:C	2.59	0.40
1:A:143:TYR:OH	2:A:5866:CAA:H4'2	2.21	0.40
1:C:8:ILE:HD12	1:C:160:MET:HG2	2.04	0.40
1:B:142:ARG:CZ	1:B:353:PHE:CD2	3.05	0.40
1:A:192:LYS:HB3	1:A:192:LYS:HE3	1.90	0.40
1:D:143:TYR:N	1:D:153:GLN:NE2	2.50	0.40
1:B:50:ASP:O	1:B:54:MET:HG3	2.20	0.40
1:A:16:TYR:CE1	1:A:41:GLU:OE2	2.74	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	384/388 (99%)	361 (94%)	20 (5%)	3 (1%)	24	41
1	B	384/388 (99%)	366 (95%)	17 (4%)	1 (0%)	46	68
1	C	384/388 (99%)	364 (95%)	17 (4%)	3 (1%)	24	41
1	D	384/388 (99%)	363 (94%)	20 (5%)	1 (0%)	46	68
All	All	1536/1552 (99%)	1454 (95%)	74 (5%)	8 (0%)	34	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	225	ALA
1	A	109	GLU
1	A	307	SER
1	A	253	GLU
1	B	109	GLU

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Mol	Chain	Res	Type
1	C	109	GLU
1	C	307	SER
1	D	30	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/319 (99%)	300 (95%)	17 (5%)	27	49
1	B	317/319 (99%)	297 (94%)	20 (6%)	22	40
1	C	317/319 (99%)	301 (95%)	16 (5%)	30	53
1	D	317/319 (99%)	298 (94%)	19 (6%)	24	43
All	All	1268/1276 (99%)	1196 (94%)	72 (6%)	25	46

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	66	GLU
1	A	70	LYS
1	A	94	ASN
1	A	109	GLU
1	A	139	ASP
1	A	185	PHE
1	A	192	LYS
1	A	200	LEU
1	A	207	ARG
1	A	249	ASP
1	A	253	GLU
1	A	299	THR
1	A	346	TYR
1	A	361	GLU
1	A	362	GLN
1	A	369	ARG
1	B	7	LYS

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Mol	Chain	Res	Type
1	B	27	GLN
1	B	63	ILE
1	B	66	GLU
1	B	79	GLU
1	B	83	ASP
1	B	94	ASN
1	B	108	LYS
1	B	109	GLU
1	B	167	SER
1	B	185	PHE
1	B	200	LEU
1	B	247	ILE
1	B	249	ASP
1	B	264	GLU
1	B	327	ASP
1	B	346	TYR
1	B	357	GLU
1	B	369	ARG
1	B	386	ARG
1	C	27	GLN
1	C	66	GLU
1	C	70	LYS
1	C	83	ASP
1	C	94	ASN
1	C	108	LYS
1	C	109	GLU
1	C	185	PHE
1	C	200	LEU
1	C	206	ILE
1	C	249	ASP
1	C	302	LEU
1	C	327	ASP
1	C	346	TYR
1	C	369	ARG
1	C	386	ARG
1	D	7	LYS
1	D	60	LYS
1	D	66	GLU
1	D	70	LYS
1	D	83	ASP
1	D	94	ASN
1	D	108	LYS

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Mol	Chain	Res	Type
1	D	109	GLU
1	D	167	SER
1	D	173	GLU
1	D	185	PHE
1	D	200	LEU
1	D	249	ASP
1	D	320	GLU
1	D	327	ASP
1	D	346	TYR
1	D	361	GLU
1	D	369	ARG
1	D	385	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	94	ASN
1	A	153	GLN
1	A	211	GLN
1	A	270	ASN
1	A	362	GLN
1	A	385	HIS
1	B	27	GLN
1	B	39	GLN
1	B	94	ASN
1	B	130	ASN
1	B	153	GLN
1	B	270	ASN
1	B	385	HIS
1	C	39	GLN
1	C	94	ASN
1	C	153	GLN
1	C	270	ASN
1	C	325	HIS
1	D	39	GLN
1	D	94	ASN
1	D	153	GLN
1	D	270	ASN
1	D	385	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	CSD	A	111	1	3,7,8	0.96	0	3,8,10	3.71	3 (100%)
1	CSD	B	111	1	3,7,8	0.78	0	3,8,10	3.09	1 (33%)
1	CSD	C	111	1	3,7,8	1.11	0	3,8,10	2.54	1 (33%)
1	CSD	D	111	1	3,7,8	0.88	0	3,8,10	3.88	1 (33%)

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
1	CSD	A	111	1	-	0/2/6/8	0/0/0/0
1	CSD	B	111	1	-	0/2/6/8	0/0/0/0
1	CSD	C	111	1	-	0/2/6/8	0/0/0/0
1	CSD	D	111	1	-	0/2/6/8	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	111	CSD	OD1-SG-CB	-6.30	94.90	105.40
1	A	111	CSD	OD1-SG-CB	-5.21	96.72	105.40
1	B	111	CSD	OD1-SG-CB	-4.91	97.22	105.40
1	C	111	CSD	OD1-SG-CB	-3.79	99.08	105.40
1	A	111	CSD	CB-CA-C	-3.02	103.18	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	CSD	O-C-CA	-2.23	119.67	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	111	CSD	1	0
1	B	111	CSD	1	0
1	C	111	CSD	1	0
1	D	111	CSD	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CAA	A	5866	-	45,56,56	1.47	7 (15%)	58,83,83	2.94	21 (36%)
2	CAA	B	6866	-	45,56,56	1.44	4 (8%)	58,83,83	2.47	14 (24%)
2	CAA	C	7866	-	45,56,56	1.47	4 (8%)	58,83,83	2.79	16 (27%)
2	CAA	D	8866	-	45,56,56	1.39	3 (6%)	58,83,83	2.99	17 (29%)

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	CAA	A	5866	-	1/1/13/15	0/50/71/71	0/3/3/3
2	CAA	B	6866	-	1/1/13/15	0/50/71/71	0/3/3/3
2	CAA	C	7866	-	1/1/13/15	0/50/71/71	0/3/3/3
2	CAA	D	8866	-	1/1/13/15	0/50/71/71	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6866	CAA	C1-S1P	-5.40	1.65	1.76
2	C	7866	CAA	C1-S1P	-5.19	1.65	1.76
2	A	5866	CAA	C1-S1P	-4.93	1.66	1.76
2	C	7866	CAA	C4-C3	-4.72	1.31	1.49
2	D	8866	CAA	C1-S1P	-4.59	1.66	1.76
2	B	6866	CAA	C4-C3	-4.54	1.32	1.49
2	A	5866	CAA	C4-C3	-4.46	1.32	1.49
2	D	8866	CAA	C4-C3	-4.39	1.33	1.49
2	A	5866	CAA	C2B-C3B	-2.02	1.48	1.53
2	A	5866	CAA	C2A-N1A	2.06	1.37	1.33
2	A	5866	CAA	C2A-N3A	2.09	1.35	1.32
2	B	6866	CAA	C5A-C4A	2.10	1.45	1.40
2	A	5866	CAA	C5A-C4A	2.17	1.45	1.40
2	C	7866	CAA	C5A-C4A	2.43	1.46	1.40
2	B	6866	CAA	O3-C3	3.08	1.32	1.21
2	D	8866	CAA	O3-C3	3.18	1.32	1.21
2	C	7866	CAA	O3-C3	3.30	1.33	1.21
2	A	5866	CAA	O3-C3	3.54	1.34	1.21

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	8866	CAA	N3A-C2A-N1A	-11.96	119.74	128.89
2	C	7866	CAA	N3A-C2A-N1A	-11.89	119.79	128.89
2	A	5866	CAA	C1B-N9A-C4A	-9.89	112.02	126.94
2	C	7866	CAA	C1B-N9A-C4A	-9.82	112.12	126.94
2	A	5866	CAA	N3A-C2A-N1A	-9.07	121.95	128.89
2	B	6866	CAA	N3A-C2A-N1A	-8.83	122.13	128.89
2	D	8866	CAA	C1B-N9A-C4A	-8.70	113.81	126.94
2	B	6866	CAA	C1B-N9A-C4A	-8.06	114.78	126.94
2	D	8866	CAA	C4B-O4B-C1B	-7.85	101.09	109.72
2	A	5866	CAA	C4B-O4B-C1B	-7.29	101.71	109.72
2	A	5866	CAA	O3A-P2A-O6A	-5.62	88.02	102.94
2	B	6866	CAA	C2B-C1B-N9A	-5.62	105.70	114.29
2	B	6866	CAA	C4B-O4B-C1B	-5.26	103.94	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6866	CAA	P2A-O3A-P1A	-4.57	119.88	132.73
2	C	7866	CAA	C4B-O4B-C1B	-4.54	104.73	109.72
2	C	7866	CAA	P2A-O3A-P1A	-4.41	120.35	132.73
2	B	6866	CAA	O1-C1-S1P	-4.36	119.37	122.83
2	D	8866	CAA	O3A-P2A-O6A	-4.34	91.42	102.94
2	A	5866	CAA	O5P-C5P-C6P	-4.22	114.71	121.98
2	C	7866	CAA	C2B-C1B-N9A	-4.21	107.86	114.29
2	A	5866	CAA	C2B-C1B-N9A	-4.20	107.87	114.29
2	A	5866	CAA	P2A-O3A-P1A	-3.98	121.56	132.73
2	D	8866	CAA	O1-C1-S1P	-3.94	119.71	122.83
2	A	5866	CAA	C7P-N8P-C9P	-3.85	114.91	122.53
2	D	8866	CAA	C2B-C1B-N9A	-3.39	109.11	114.29
2	D	8866	CAA	P2A-O3A-P1A	-3.26	123.58	132.73
2	C	7866	CAA	O3B-C3B-C2B	-3.22	98.99	111.51
2	A	5866	CAA	C4A-C5A-N7A	-2.64	107.05	109.48
2	D	8866	CAA	C4A-C5A-N7A	-2.60	107.09	109.48
2	D	8866	CAA	O3B-C3B-C2B	-2.53	101.68	111.51
2	D	8866	CAA	O5B-P1A-O1A	-2.50	99.90	109.62
2	B	6866	CAA	O3B-C3B-C2B	-2.35	102.38	111.51
2	A	5866	CAA	O1-C1-S1P	-2.34	120.97	122.83
2	A	5866	CAA	C2P-S1P-C1	-2.24	94.10	102.09
2	A	5866	CAA	O3B-C3B-C2B	-2.04	103.58	111.51
2	B	6866	CAA	O5B-P1A-O1A	-2.01	101.81	109.62
2	C	7866	CAA	CEP-CBP-CCP	-2.00	105.91	108.50
2	A	5866	CAA	C2A-N1A-C6A	2.00	122.35	118.77
2	A	5866	CAA	P3B-O3B-C3B	2.11	126.63	121.56
2	A	5866	CAA	CEP-CBP-CDP	2.11	113.52	109.28
2	C	7866	CAA	C7P-N8P-C9P	2.17	126.83	122.53
2	D	8866	CAA	CAP-C9P-N8P	2.18	121.30	116.47
2	B	6866	CAA	O9A-P3B-O8A	2.25	115.94	107.38
2	A	5866	CAA	O5A-P2A-O3A	2.27	115.37	105.09
2	D	8866	CAA	O2A-P1A-O1A	2.27	124.83	112.53
2	C	7866	CAA	O9A-P3B-O8A	2.31	116.18	107.38
2	B	6866	CAA	C2A-N1A-C6A	2.35	122.97	118.77
2	C	7866	CAA	CEP-CBP-CDP	2.42	114.13	109.28
2	B	6866	CAA	O2A-P1A-O1A	2.52	126.17	112.53
2	A	5866	CAA	N6A-C6A-N1A	2.61	124.81	119.20
2	C	7866	CAA	O5B-C5B-C4B	2.69	119.04	109.12
2	D	8866	CAA	N6A-C6A-N1A	2.78	125.17	119.20
2	D	8866	CAA	C2A-N1A-C6A	2.78	123.73	118.77
2	C	7866	CAA	N6A-C6A-N1A	2.83	125.27	119.20
2	A	5866	CAA	C2P-C3P-N4P	2.83	118.03	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6866	CAA	N6A-C6A-N1A	3.07	125.80	119.20
2	C	7866	CAA	C2P-C3P-N4P	3.16	118.68	112.36
2	C	7866	CAA	C3P-C2P-S1P	3.32	120.25	111.36
2	C	7866	CAA	C2A-N1A-C6A	3.42	124.87	118.77
2	A	5866	CAA	C6P-C5P-N4P	3.55	122.63	116.46
2	B	6866	CAA	O4B-C1B-N9A	3.84	116.14	108.10
2	A	5866	CAA	O4B-C1B-N9A	3.87	116.21	108.10
2	D	8866	CAA	C2P-C3P-N4P	3.95	120.25	112.36
2	B	6866	CAA	C2-C1-S1P	5.11	118.60	113.50
2	C	7866	CAA	O4B-C1B-N9A	5.17	118.93	108.10
2	D	8866	CAA	O4B-C1B-N9A	5.45	119.51	108.10
2	A	5866	CAA	C2-C1-S1P	6.14	119.62	113.50
2	D	8866	CAA	C2-C1-S1P	6.27	119.75	113.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	8866	CAA	C2B
2	B	6866	CAA	C2B
2	C	7866	CAA	C2B
2	A	5866	CAA	C2B

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5866	CAA	10	0
2	B	6866	CAA	3	0
2	C	7866	CAA	8	0
2	D	8866	CAA	2	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	386/388 (99%)	-0.10	14 (3%) 46 51	13, 23, 36, 50	0
1	B	386/388 (99%)	-0.10	4 (1%) 84 86	13, 23, 36, 49	0
1	C	386/388 (99%)	-0.12	7 (1%) 71 75	12, 23, 37, 48	0
1	D	386/388 (99%)	-0.14	9 (2%) 64 67	12, 23, 35, 50	0
All	All	1544/1552 (99%)	-0.11	34 (2%) 65 69	12, 23, 37, 50	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ASN	6.7
1	B	250	ASN	4.9
1	C	250	ASN	4.8
1	D	250	ASN	4.4
1	A	249	ASP	3.2
1	A	221	GLY	3.0
1	A	251	ALA	2.9
1	D	376	ASN	2.9
1	D	247	ILE	2.8
1	C	248	ILE	2.7
1	C	247	ILE	2.6
1	C	249	ASP	2.6
1	A	247	ILE	2.6
1	A	355	ASP	2.5
1	D	249	ASP	2.5
1	A	252	ASP	2.5
1	C	355	ASP	2.4
1	D	379	ASN	2.4
1	C	379	ASN	2.4
1	B	117	ALA	2.2
1	A	76	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLY	2.2
1	D	251	ALA	2.2
1	A	293	ASP	2.2
1	B	249	ASP	2.1
1	A	157	ALA	2.1
1	A	295	GLN	2.1
1	A	253	GLU	2.1
1	B	251	ALA	2.1
1	D	378	GLU	2.1
1	D	293	ASP	2.0
1	A	379	ASN	2.0
1	C	221	GLY	2.0
1	A	248	ILE	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. 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
1	CSD	C	111	8/9	0.98	0.11	-	18,20,26,30	0
1	CSD	D	111	8/9	0.97	0.12	-	17,18,26,26	0
1	CSD	A	111	8/9	0.98	0.12	-	19,21,27,28	0
1	CSD	B	111	8/9	0.96	0.14	-	17,18,27,27	0

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	CAA	D	8866	54/54	0.94	0.14	0.57	25,38,48,50	0
2	CAA	B	6866	54/54	0.94	0.13	0.43	24,36,49,50	0
2	CAA	C	7866	54/54	0.95	0.13	0.13	24,34,45,48	0
2	CAA	A	5866	54/54	0.94	0.14	0.10	25,33,44,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.