



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:04 PM GMT

PDB ID : 2F2S
Title : Human mitochondrial acetoacetyl-CoA thiolase
Authors : Min, J.R.; Dombrowski, L.; Antoshenko, T.; Wu, H.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2005-11-17
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

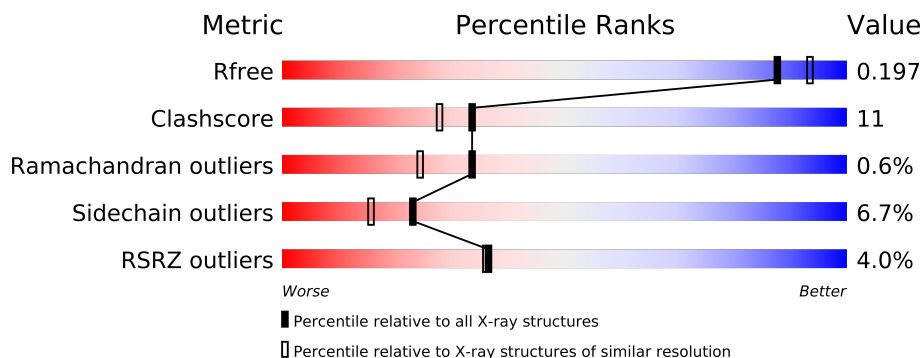
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	
1	D	406	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12020 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Acetyl-CoA acetyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2834	1783	486	544	21			
1	B	386	Total	C	N	O	S	0	0	0
			2818	1773	484	540	21			
1	C	388	Total	C	N	O	S	0	0	0
			2841	1789	487	544	21			
1	D	382	Total	C	N	O	S	0	0	0
			2801	1765	478	537	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	CLONING ARTIFACT	UNP P24752
A	23	GLY	-	CLONING ARTIFACT	UNP P24752
A	24	SER	-	CLONING ARTIFACT	UNP P24752
A	25	SER	-	CLONING ARTIFACT	UNP P24752
A	26	HIS	-	EXPRESSION TAG	UNP P24752
A	27	HIS	-	EXPRESSION TAG	UNP P24752
A	28	HIS	-	EXPRESSION TAG	UNP P24752
A	29	HIS	-	EXPRESSION TAG	UNP P24752
A	30	HIS	-	EXPRESSION TAG	UNP P24752
A	31	HIS	-	EXPRESSION TAG	UNP P24752
A	32	SER	-	CLONING ARTIFACT	UNP P24752
A	33	SER	-	CLONING ARTIFACT	UNP P24752
A	34	GLY	-	CLONING ARTIFACT	UNP P24752
A	35	LEU	-	CLONING ARTIFACT	UNP P24752
A	36	VAL	-	CLONING ARTIFACT	UNP P24752
A	37	PRO	-	CLONING ARTIFACT	UNP P24752
A	38	ARG	-	CLONING ARTIFACT	UNP P24752
A	39	GLY	-	CLONING ARTIFACT	UNP P24752
A	40	SER	-	CLONING ARTIFACT	UNP P24752
A	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752
B	22	MET	-	CLONING ARTIFACT	UNP P24752

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	GLY	-	CLONING ARTIFACT	UNP P24752
B	24	SER	-	CLONING ARTIFACT	UNP P24752
B	25	SER	-	CLONING ARTIFACT	UNP P24752
B	26	HIS	-	EXPRESSION TAG	UNP P24752
B	27	HIS	-	EXPRESSION TAG	UNP P24752
B	28	HIS	-	EXPRESSION TAG	UNP P24752
B	29	HIS	-	EXPRESSION TAG	UNP P24752
B	30	HIS	-	EXPRESSION TAG	UNP P24752
B	31	HIS	-	EXPRESSION TAG	UNP P24752
B	32	SER	-	CLONING ARTIFACT	UNP P24752
B	33	SER	-	CLONING ARTIFACT	UNP P24752
B	34	GLY	-	CLONING ARTIFACT	UNP P24752
B	35	LEU	-	CLONING ARTIFACT	UNP P24752
B	36	VAL	-	CLONING ARTIFACT	UNP P24752
B	37	PRO	-	CLONING ARTIFACT	UNP P24752
B	38	ARG	-	CLONING ARTIFACT	UNP P24752
B	39	GLY	-	CLONING ARTIFACT	UNP P24752
B	40	SER	-	CLONING ARTIFACT	UNP P24752
B	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752
C	22	MET	-	CLONING ARTIFACT	UNP P24752
C	23	GLY	-	CLONING ARTIFACT	UNP P24752
C	24	SER	-	CLONING ARTIFACT	UNP P24752
C	25	SER	-	CLONING ARTIFACT	UNP P24752
C	26	HIS	-	EXPRESSION TAG	UNP P24752
C	27	HIS	-	EXPRESSION TAG	UNP P24752
C	28	HIS	-	EXPRESSION TAG	UNP P24752
C	29	HIS	-	EXPRESSION TAG	UNP P24752
C	30	HIS	-	EXPRESSION TAG	UNP P24752
C	31	HIS	-	EXPRESSION TAG	UNP P24752
C	32	SER	-	CLONING ARTIFACT	UNP P24752
C	33	SER	-	CLONING ARTIFACT	UNP P24752
C	34	GLY	-	CLONING ARTIFACT	UNP P24752
C	35	LEU	-	CLONING ARTIFACT	UNP P24752
C	36	VAL	-	CLONING ARTIFACT	UNP P24752
C	37	PRO	-	CLONING ARTIFACT	UNP P24752
C	38	ARG	-	CLONING ARTIFACT	UNP P24752
C	39	GLY	-	CLONING ARTIFACT	UNP P24752
C	40	SER	-	CLONING ARTIFACT	UNP P24752
C	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752
D	22	MET	-	CLONING ARTIFACT	UNP P24752
D	23	GLY	-	CLONING ARTIFACT	UNP P24752
D	24	SER	-	CLONING ARTIFACT	UNP P24752

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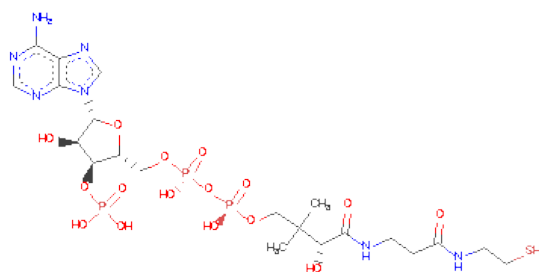
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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	SER	-	CLONING ARTIFACT	UNP P24752
D	26	HIS	-	EXPRESSION TAG	UNP P24752
D	27	HIS	-	EXPRESSION TAG	UNP P24752
D	28	HIS	-	EXPRESSION TAG	UNP P24752
D	29	HIS	-	EXPRESSION TAG	UNP P24752
D	30	HIS	-	EXPRESSION TAG	UNP P24752
D	31	HIS	-	EXPRESSION TAG	UNP P24752
D	32	SER	-	CLONING ARTIFACT	UNP P24752
D	33	SER	-	CLONING ARTIFACT	UNP P24752
D	34	GLY	-	CLONING ARTIFACT	UNP P24752
D	35	LEU	-	CLONING ARTIFACT	UNP P24752
D	36	VAL	-	CLONING ARTIFACT	UNP P24752
D	37	PRO	-	CLONING ARTIFACT	UNP P24752
D	38	ARG	-	CLONING ARTIFACT	UNP P24752
D	39	GLY	-	CLONING ARTIFACT	UNP P24752
D	40	SER	-	CLONING ARTIFACT	UNP P24752
D	126	SCY	CYS	MODIFIED RESIDUE	UNP P24752

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 4 is water.

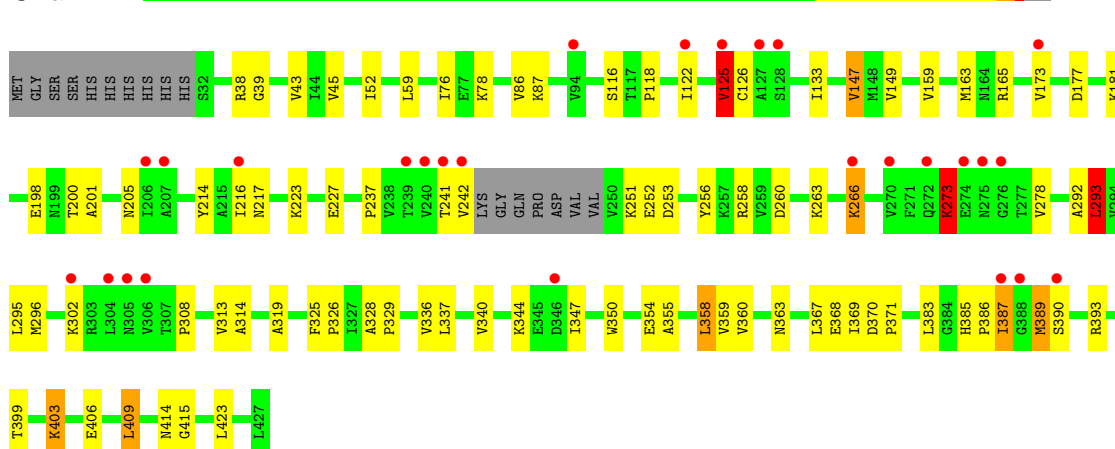
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total 99	O 99	0	0
4	B	172	Total 172	O 172	0	0
4	C	137	Total 137	O 137	0	0
4	D	123	Total 123	O 123	0	0

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.

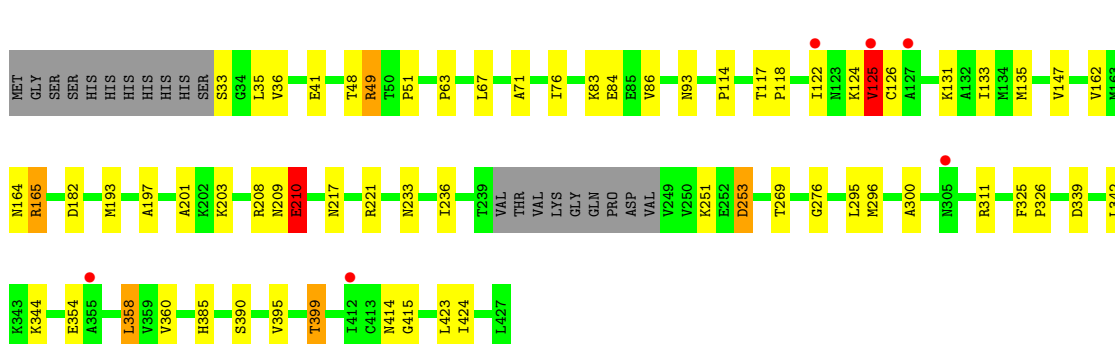
- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial

Chain A:



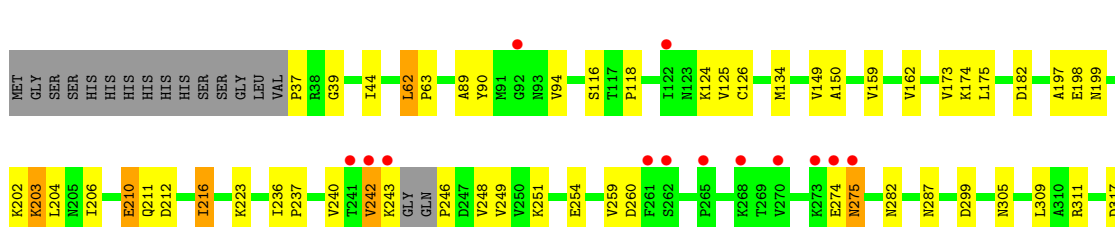
- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial

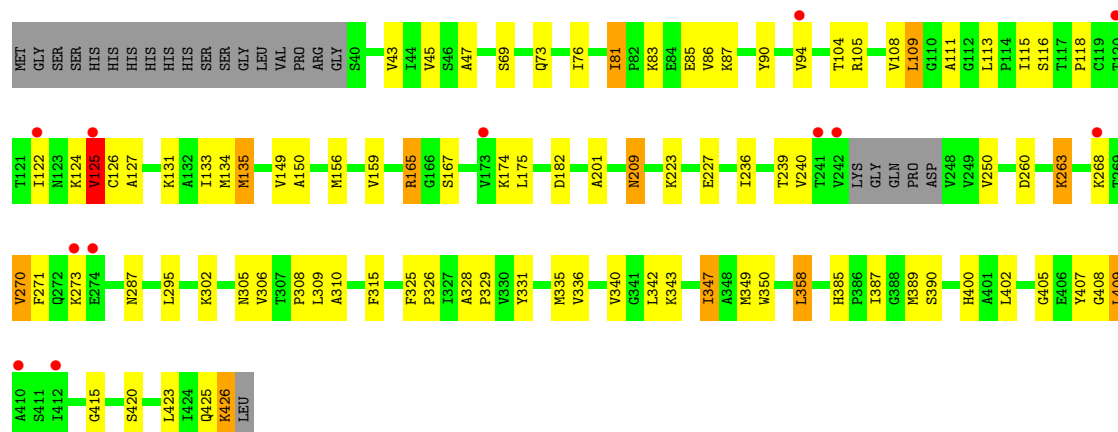
Chain B:



- Molecule 1: Acetyl-CoA acetyltransferase, mitochondrial

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.99Å 126.64Å 111.86Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	33.80 – 2.00 33.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.80-2.00) 99.0 (33.78-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.257 0.203 , 0.197	Depositor DCC
R_{free} test set	5269 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 104558 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SCY, CL

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	0.78	0/2864	0.87	5/3876 (0.1%)
1	B	0.98	3/2848 (0.1%)	0.95	8/3851 (0.2%)
1	C	0.90	0/2871	0.87	3/3883 (0.1%)
1	D	0.82	0/2830	0.84	5/3828 (0.1%)
All	All	0.87	3/11413 (0.0%)	0.88	21/15438 (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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CG-CD	7.71	1.63	1.51
1	B	210	GLU	CB-CG	6.04	1.63	1.52
1	B	71	ALA	CA-CB	5.93	1.64	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	A	165	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	B	49	ARG	NE-CZ-NH1	12.89	126.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	D	165	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	182	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	182	ASP	CB-CG-OD1	6.70	124.33	118.30
1	D	165	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	409	LEU	CA-CB-CG	6.25	129.69	115.30
1	C	246	PRO	N-CA-CB	6.23	110.78	103.30
1	B	165	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	49	ARG	CD-NE-CZ	6.19	132.26	123.60
1	D	409	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	165	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	358	LEU	CA-CB-CG	-5.40	102.89	115.30
1	A	165	ARG	CD-NE-CZ	5.21	130.89	123.60
1	B	253	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	293	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	409	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	358	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	C	182	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	PRO	Peptide
1	B	125	VAL	Mainchain
1	D	425	GLN	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2834	0	2887	59	0
1	B	2818	0	2882	61	0
1	C	2841	0	2910	62	0
1	D	2801	0	2869	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	5	0
3	C	48	0	32	2	0
3	D	48	0	32	0	0
4	A	99	0	0	0	0
4	B	172	0	0	7	0
4	C	137	0	0	5	0
4	D	123	0	0	6	0
All	All	12020	0	11676	252	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (252) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:VAL:C	1:A:126:SCY:H2	1.21	1.44
1:B:131:LYS:HG3	1:B:135:MET:HE2	1.08	1.07
1:B:131:LYS:HG3	1:B:135:MET:CE	1.86	1.06
1:D:426:LYS:O	1:D:426:LYS:HD3	1.58	1.03
1:D:309:LEU:O	1:D:426:LYS:HG2	1.66	0.96
1:A:38:ARG:HB3	1:B:36:VAL:HG13	1.46	0.94
1:A:133:ILE:HG23	1:A:295:LEU:HD11	1.49	0.93
1:C:94:VAL:HG21	1:C:387:ILE:HG22	1.51	0.92
1:D:309:LEU:O	1:D:426:LYS:CG	2.22	0.87
1:D:126:SCY:HE1	1:D:415:GLY:H	1.45	0.82
1:C:202:LYS:O	1:C:203:LYS:HB2	1.77	0.81
1:D:223:LYS:O	1:D:227:GLU:HG2	1.81	0.81
1:D:122:ILE:HG13	1:D:135:MET:HE1	1.62	0.80
1:D:125:VAL:CG1	1:D:126:SCY:HE2	2.13	0.79
1:D:347:ILE:HD11	1:D:350:TRP:CZ2	2.18	0.79
1:D:125:VAL:HG12	1:D:126:SCY:HE2	1.64	0.78
1:C:126:SCY:CE	1:C:415:GLY:H	1.97	0.77
1:B:126:SCY:HE1	1:B:415:GLY:H	1.48	0.77
1:C:126:SCY:HE1	1:C:415:GLY:H	1.49	0.76
1:A:125:VAL:C	1:A:126:SCY:H	1.86	0.75
1:A:201:ALA:HB2	1:A:358:LEU:CD1	2.18	0.74
1:B:48:THR:HG22	4:B:2104:HOH:O	1.86	0.74
1:A:252:GLU:OE2	1:A:256:TYR:OH	2.05	0.74
1:B:197:ALA:O	1:B:358:LEU:HD21	1.89	0.73
1:D:126:SCY:C	1:D:127:ALA:CA	2.67	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:274:GLU:HG2	1:C:275:ASN:ND2	2.03	0.73
1:B:131:LYS:CG	1:B:135:MET:HE2	2.04	0.72
1:A:125:VAL:HG22	1:A:126:SCY:CE	2.19	0.72
1:A:223:LYS:O	1:A:227:GLU:HG2	1.90	0.72
1:D:122:ILE:HG13	1:D:135:MET:CE	2.19	0.72
1:D:426:LYS:O	1:D:426:LYS:CD	2.37	0.71
1:D:125:VAL:HG12	1:D:126:SCY:CE	2.21	0.70
1:B:126:SCY:HE1	1:B:415:GLY:N	2.06	0.70
1:C:116:SER:O	1:C:118:PRO:HD3	1.92	0.70
1:C:197:ALA:O	1:C:358:LEU:HD11	1.90	0.70
1:D:125:VAL:CG1	1:D:126:SCY:CE	2.69	0.69
1:A:201:ALA:HB2	1:A:358:LEU:HD13	1.74	0.69
1:B:126:SCY:CE	1:B:415:GLY:H	2.05	0.69
1:D:385:HIS:HD2	1:D:390:SER:OG	1.74	0.69
1:B:49:ARG:NH2	1:B:253:ASP:OD1	2.25	0.68
1:B:122:ILE:CG2	1:B:135:MET:HE1	2.24	0.67
1:A:126:SCY:HE1	1:A:415:GLY:H	1.59	0.67
1:C:212:ASP:O	1:C:216:ILE:HG23	1.93	0.67
1:B:67:LEU:HD12	1:B:67:LEU:H	1.59	0.66
1:B:124:LYS:NZ	1:B:414:ASN:HD21	1.94	0.66
1:C:210:GLU:HB3	4:C:1137:HOH:O	1.95	0.66
1:D:209:ASN:H	1:D:209:ASN:HD22	1.41	0.66
1:C:274:GLU:HG2	1:C:275:ASN:HD22	1.60	0.66
1:B:122:ILE:HG21	1:B:135:MET:CE	2.26	0.65
1:B:197:ALA:HB1	1:B:358:LEU:HD23	1.77	0.65
1:A:125:VAL:HG22	1:A:126:SCY:HE2	1.77	0.65
1:C:259:VAL:HG22	1:C:260:ASP:H	1.60	0.65
1:D:131:LYS:O	1:D:135:MET:HE2	1.97	0.64
1:B:126:SCY:HE2	1:B:126:SCY:H	1.62	0.64
1:C:287:ASN:ND2	1:C:385:HIS:H	1.96	0.64
1:D:94:VAL:HG21	1:D:387:ILE:HG22	1.79	0.64
1:D:47:ALA:O	1:D:400:HIS:HE1	1.79	0.64
1:B:233:ASN:HB2	4:B:2062:HOH:O	1.97	0.64
1:C:126:SCY:HE1	1:C:415:GLY:N	2.12	0.63
1:B:164:ASN:ND2	4:B:2149:HOH:O	2.29	0.63
1:C:344:LYS:HB2	1:C:369:ILE:HD11	1.80	0.63
1:C:330:VAL:HG22	1:C:367:LEU:CD2	2.29	0.62
1:D:385:HIS:CD2	1:D:390:SER:OG	2.53	0.62
1:D:309:LEU:O	1:D:426:LYS:HG3	1.99	0.61
1:D:76:ILE:HD13	1:D:113:LEU:HD11	1.81	0.61
1:D:86:VAL:HG11	1:D:149:VAL:HG12	1.81	0.61
1:B:122:ILE:HG23	1:B:135:MET:HE1	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:ARG:HB3	1:B:36:VAL:CG1	2.28	0.61
1:A:163:MET:CE	1:D:175:LEU:HD21	2.31	0.61
1:C:354:GLU:HB3	1:C:381:VAL:HG23	1.82	0.60
3:B:1002:COA:H52A	4:B:2111:HOH:O	2.00	0.60
1:C:199:ASN:HB3	4:C:1065:HOH:O	2.01	0.60
1:D:402:LEU:HD11	1:D:408:GLY:HA3	1.83	0.60
1:C:124:LYS:HE2	1:C:317:ASP:OD1	2.02	0.60
1:D:126:SCY:H	1:D:126:SCY:HE2	1.65	0.60
1:C:39:GLY:HA2	1:C:299:ASP:OD2	2.00	0.59
1:B:395:VAL:O	1:B:399:THR:HG23	2.03	0.59
1:D:426:LYS:CB	4:D:1126:HOH:O	2.51	0.59
1:D:125:VAL:CB	1:D:126:SCY:HE2	2.34	0.58
1:A:314:ALA:HB3	1:A:336:VAL:HG13	1.85	0.57
1:A:253:ASP:OD2	1:A:383:LEU:HD22	2.04	0.57
1:A:403:LYS:N	1:A:406:GLU:OE1	2.33	0.57
1:A:86:VAL:HG11	1:A:149:VAL:HG23	1.86	0.57
1:B:114:PRO:HG2	1:B:117:THR:HG23	1.87	0.57
1:C:204:LEU:HD12	1:C:365:LYS:HD2	1.86	0.56
1:D:81:ILE:HG22	1:D:306:VAL:HG21	1.87	0.56
1:D:328:ALA:N	1:D:329:PRO:CD	2.69	0.56
1:B:217:ASN:O	1:B:221:ARG:HG3	2.04	0.56
1:A:337:LEU:HD21	1:A:347:ILE:HD11	1.87	0.56
1:C:259:VAL:HG22	1:C:260:ASP:N	2.21	0.56
1:C:44:ILE:HD12	1:C:424:ILE:HD12	1.86	0.56
1:C:259:VAL:HG23	3:C:1003:COA:H61A	1.71	0.55
1:C:287:ASN:HD22	1:C:385:HIS:H	1.54	0.55
1:A:163:MET:HE1	1:D:175:LEU:HD21	1.89	0.55
1:C:309:LEU:O	1:C:426:LYS:HD2	2.06	0.55
1:A:198:GLU:OE2	1:A:278:VAL:HG12	2.06	0.55
1:A:147:VAL:HB	1:A:296:MET:HG3	1.89	0.55
1:C:326:PRO:HB3	1:C:359:VAL:HG22	1.89	0.55
1:B:83:LYS:HE2	4:B:2088:HOH:O	2.07	0.54
1:B:124:LYS:HZ2	1:B:414:ASN:ND2	2.04	0.54
1:A:126:SCY:CE	1:A:415:GLY:H	2.19	0.54
1:A:326:PRO:HB3	1:A:359:VAL:HG22	1.89	0.54
1:B:122:ILE:HG21	1:B:135:MET:HE1	1.89	0.54
1:C:94:VAL:HG21	1:C:387:ILE:CG2	2.32	0.54
1:A:389:MET:HE3	1:A:390:SER:HA	1.88	0.54
1:C:358:LEU:C	1:C:358:LEU:HD23	2.28	0.53
1:B:122:ILE:CG2	1:B:135:MET:CE	2.86	0.53
1:D:45:VAL:CG1	1:D:306:VAL:HG11	2.38	0.53
1:C:126:SCY:HE2	1:C:126:SCY:H	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:193:MET:HE3	3:B:1002:COA:S1P	2.48	0.53
1:D:69:SER:O	1:D:73:GLN:HG3	2.07	0.53
1:A:214:TYR:O	1:A:217:ASN:HB3	2.09	0.53
1:A:86:VAL:CG1	1:A:149:VAL:HG23	2.39	0.52
1:B:67:LEU:HD12	1:B:67:LEU:N	2.23	0.52
1:A:329:PRO:HG2	1:A:363:ASN:HD21	1.75	0.52
1:D:405:GLY:H	1:D:426:LYS:C	2.12	0.52
1:C:89:ALA:CB	1:C:149:VAL:HG23	2.40	0.52
1:C:249:VAL:HG12	1:C:251:LYS:HG2	1.91	0.52
1:C:126:SCY:OCD	3:C:1003:COA:S1P	2.67	0.51
1:B:125:VAL:HG12	1:B:126:SCY:CE	2.39	0.51
1:D:125:VAL:HB	1:D:126:SCY:HE2	1.91	0.51
1:D:260:ASP:OD2	1:D:263:LYS:HB2	2.10	0.51
1:C:426:LYS:C	4:C:1128:HOH:O	2.47	0.51
1:D:94:VAL:HG21	1:D:387:ILE:CG2	2.41	0.51
1:C:212:ASP:HB3	1:C:282:ASN:HB3	1.93	0.51
1:B:342:LEU:HD12	1:B:423:LEU:HD21	1.93	0.50
1:B:51:PRO:HD3	1:B:236:ILE:O	2.12	0.50
1:A:125:VAL:HG22	1:A:126:SCY:HE3	1.93	0.50
1:C:197:ALA:O	1:C:358:LEU:CD1	2.58	0.50
1:C:44:ILE:CD1	1:C:424:ILE:HD12	2.41	0.50
1:C:349:MET:HG2	1:C:376:ILE:HD12	1.92	0.50
1:A:126:SCY:OCD	3:A:1001:COA:S1P	2.69	0.49
1:B:41:GLU:OE2	1:B:311:ARG:NH2	2.37	0.49
1:A:39:GLY:O	1:B:36:VAL:HG11	2.12	0.49
1:C:331:TYR:O	1:C:335:MET:HG3	2.13	0.49
1:A:116:SER:O	1:A:118:PRO:HD3	2.12	0.49
1:A:87:LYS:O	1:A:118:PRO:HD2	2.12	0.49
1:D:209:ASN:H	1:D:209:ASN:ND2	2.09	0.49
1:D:45:VAL:HG11	1:D:306:VAL:HG11	1.94	0.49
1:A:126:SCY:SG	1:A:387:ILE:HG12	2.53	0.48
1:A:358:LEU:HG	1:A:358:LEU:O	2.13	0.48
1:B:210:GLU:HG3	4:B:2051:HOH:O	2.13	0.48
1:D:325:PHE:N	1:D:326:PRO:CD	2.76	0.48
1:B:385:HIS:HD2	1:B:390:SER:OG	1.96	0.48
1:D:126:SCY:HA	1:D:387:ILE:HG23	1.95	0.48
1:B:296:MET:HG2	1:B:300:ALA:HB3	1.96	0.48
1:A:313:VAL:HG11	1:A:423:LEU:HD23	1.95	0.48
1:D:43:VAL:HB	1:D:308:PRO:HB3	1.96	0.48
1:D:124:LYS:HE2	1:D:420:SER:OG	2.14	0.48
1:D:358:LEU:O	1:D:358:LEU:HG	2.04	0.47
1:B:399:THR:HG22	1:B:424:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:197:ALA:HB1	1:C:358:LEU:HD13	1.96	0.47
1:A:266:LYS:HE3	1:A:266:LYS:HB2	1.52	0.47
1:C:37:PRO:HG3	1:C:311:ARG:HD2	1.96	0.47
1:B:354:GLU:HG2	1:B:360:VAL:HG21	1.97	0.47
1:A:52:ILE:HD11	1:A:393:ARG:HD3	1.96	0.47
1:A:177:ASP:OD2	1:D:165:ARG:NH2	2.47	0.47
1:A:163:MET:HE2	1:D:175:LEU:HD21	1.96	0.47
1:A:43:VAL:HB	1:A:308:PRO:HB3	1.96	0.47
1:C:242:VAL:O	1:C:243:LYS:HB2	2.15	0.47
1:B:165:ARG:HD2	1:C:159:VAL:O	2.14	0.47
1:A:354:GLU:HG2	1:A:360:VAL:HG21	1.97	0.46
1:B:114:PRO:HG2	1:B:117:THR:CG2	2.45	0.46
1:B:122:ILE:HG21	1:B:135:MET:HE3	1.97	0.46
1:A:355:ALA:HB1	3:A:1001:COA:C2P	2.45	0.46
1:D:310:ALA:HA	1:D:426:LYS:HG2	1.97	0.46
1:D:347:ILE:HG22	1:D:407:TYR:HB3	1.98	0.46
1:D:76:ILE:CD1	1:D:113:LEU:HD11	2.46	0.46
1:C:134:MET:HG3	1:C:422:MET:HE3	1.97	0.46
1:A:260:ASP:CG	1:A:263:LYS:HG3	2.35	0.46
1:B:63:PRO:O	1:B:67:LEU:CD1	2.64	0.46
1:C:243:LYS:N	4:C:1104:HOH:O	2.48	0.46
1:C:126:SCY:SG	1:C:387:ILE:HD12	2.56	0.45
1:B:125:VAL:CG1	1:B:126:SCY:CE	2.94	0.45
1:B:193:MET:HG3	3:B:1002:COA:H22	1.98	0.45
1:D:201:ALA:HB2	1:D:358:LEU:HD13	1.97	0.45
1:C:126:SCY:HE2	1:C:415:GLY:H	1.79	0.45
1:B:162:VAL:HG12	1:C:162:VAL:HG12	1.98	0.45
1:B:126:SCY:OCD	3:B:1002:COA:S1P	2.70	0.45
1:A:328:ALA:N	1:A:329:PRO:HD2	2.32	0.45
1:B:125:VAL:HG12	1:B:126:SCY:HE3	1.98	0.45
1:C:242:VAL:HG12	1:C:243:LYS:N	2.32	0.44
1:D:116:SER:O	1:D:118:PRO:HD3	2.16	0.44
1:D:133:ILE:HG23	1:D:295:LEU:HD11	1.99	0.44
1:D:331:TYR:O	1:D:335:MET:HG3	2.18	0.44
1:A:313:VAL:CG1	1:A:423:LEU:HD23	2.48	0.44
1:D:426:LYS:HB2	4:D:1126:HOH:O	2.15	0.44
1:B:193:MET:CE	3:B:1002:COA:S1P	3.06	0.44
1:B:84:GLU:HA	1:B:114:PRO:HG3	1.99	0.44
1:A:76:ILE:CD1	1:A:86:VAL:HG21	2.48	0.43
1:A:159:VAL:O	1:D:165:ARG:NH1	2.50	0.43
1:A:125:VAL:HG13	1:A:414:ASN:HB2	1.99	0.43
1:D:306:VAL:HG13	4:D:1112:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:83:LYS:HG2	1:D:113:LEU:HD12	1.98	0.43
1:C:89:ALA:HB2	1:C:149:VAL:HG23	1.99	0.43
1:B:133:ILE:HG23	1:B:295:LEU:HD11	1.99	0.43
1:D:270:VAL:HG23	1:D:271:PHE:CD2	2.54	0.43
1:D:135:MET:HE2	1:D:135:MET:HB2	1.60	0.43
1:D:268:LYS:HG2	4:D:1099:HOH:O	2.17	0.43
1:C:340:VAL:HG12	1:C:342:LEU:HB2	2.00	0.43
1:B:33:SER:N	4:B:2076:HOH:O	2.51	0.43
1:C:327:ILE:O	1:C:330:VAL:HB	2.19	0.43
1:B:325:PHE:N	1:B:326:PRO:CD	2.82	0.42
1:C:325:PHE:HD1	1:C:413:CYS:HG	1.67	0.42
1:D:126:SCY:CA	1:D:127:ALA:N	2.71	0.42
1:D:105:ARG:HG3	1:D:109:LEU:HD22	2.01	0.42
1:C:330:VAL:HG22	1:C:367:LEU:HD22	2.01	0.42
1:B:201:ALA:HB2	1:B:358:LEU:CD2	2.49	0.42
1:D:349:MET:HE3	4:D:1045:HOH:O	2.20	0.42
1:C:134:MET:HG3	1:C:422:MET:CE	2.49	0.42
1:D:287:ASN:ND2	1:D:385:HIS:H	2.18	0.42
1:A:385:HIS:HD2	1:A:390:SER:OG	2.03	0.41
1:D:73:GLN:HG2	1:D:111:ALA:HB1	2.01	0.41
1:C:275:ASN:HD22	1:C:275:ASN:N	2.17	0.41
1:D:86:VAL:CG1	1:D:149:VAL:HG12	2.48	0.41
1:A:214:TYR:OH	1:A:360:VAL:HG11	2.20	0.41
1:A:126:SCY:HE1	1:A:415:GLY:N	2.31	0.41
1:B:147:VAL:HG22	1:B:296:MET:HG3	2.02	0.41
1:D:45:VAL:HG13	1:D:306:VAL:CG1	2.50	0.41
1:A:325:PHE:N	1:A:326:PRO:CD	2.83	0.41
1:A:370:ASP:HA	1:A:371:PRO:HD2	1.93	0.41
1:D:122:ILE:HG21	1:D:135:MET:HE1	2.03	0.41
1:B:125:VAL:HG12	1:B:126:SCY:HE2	2.01	0.41
1:B:124:LYS:HZ3	1:B:414:ASN:HD21	1.66	0.41
1:A:273:LYS:HD2	1:A:273:LYS:H	1.86	0.41
1:C:236:ILE:HA	1:C:237:PRO:HD3	1.94	0.41
1:B:117:THR:HA	1:B:118:PRO:HD3	1.84	0.41
1:A:319:ALA:O	1:D:116:SER:HA	2.21	0.41
1:D:90:TYR:O	1:D:150:ALA:HA	2.20	0.41
1:D:340:VAL:HG23	1:D:342:LEU:HG	2.02	0.41
1:D:156:MET:HA	1:D:159:VAL:HG23	2.02	0.41
1:D:104:THR:O	1:D:108:VAL:HG23	2.20	0.41
1:D:328:ALA:N	1:D:329:PRO:HD3	2.36	0.41
1:C:62:LEU:HA	1:C:63:PRO:HD2	1.87	0.41
1:B:76:ILE:HD11	1:B:86:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:269:THR:HG21	1:B:276:GLY:C	2.41	0.41
1:C:370:ASP:HA	1:C:371:PRO:HD3	1.82	0.41
1:A:237:PRO:HG3	1:A:251:LYS:HD3	2.03	0.41
1:C:90:TYR:O	1:C:150:ALA:HA	2.21	0.41
1:D:122:ILE:HG13	1:D:135:MET:HE3	2.01	0.41
1:D:134:MET:HE3	1:D:315:PHE:CD1	2.56	0.41
1:D:426:LYS:HB3	4:D:1126:HOH:O	2.19	0.40
1:B:67:LEU:H	1:B:67:LEU:CD1	2.32	0.40
1:C:210:GLU:CB	4:C:1137:HOH:O	2.64	0.40
1:A:350:TRP:CZ2	1:A:369:ILE:HG21	2.55	0.40
1:A:251:LYS:HD2	1:A:251:LYS:O	2.20	0.40
1:C:89:ALA:HB2	1:C:149:VAL:CG2	2.51	0.40
1:D:347:ILE:HG23	1:D:347:ILE:HD13	1.79	0.40
1:C:206:ILE:HG22	1:C:211:GLN:HG3	2.04	0.40
1:D:85:GLU:O	1:D:87:LYS:HD3	2.22	0.40
1:A:292:ALA:C	1:A:293:LEU:HD23	2.42	0.40
1:D:336:VAL:HG11	1:D:423:LEU:HB2	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	384/406 (95%)	370 (96%)	11 (3%)	3 (1%)	27	17
1	B	381/406 (94%)	369 (97%)	10 (3%)	2 (0%)	38	29
1	C	383/406 (94%)	362 (94%)	18 (5%)	3 (1%)	27	17
1	D	377/406 (93%)	367 (97%)	9 (2%)	1 (0%)	50	44
All	All	1525/1624 (94%)	1468 (96%)	48 (3%)	9 (1%)	33	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	VAL

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Mol	Chain	Res	Type
1	A	340	VAL
1	C	203	LYS
1	A	273	LYS
1	C	242	VAL
1	D	125	VAL
1	B	125	VAL
1	C	125	VAL
1	B	93	ASN

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	296/317 (93%)	269 (91%)	27 (9%)	14	8
1	B	296/317 (93%)	287 (97%)	9 (3%)	53	50
1	C	299/317 (94%)	277 (93%)	22 (7%)	20	12
1	D	295/317 (93%)	273 (92%)	22 (8%)	19	12
All	All	1186/1268 (94%)	1106 (93%)	80 (7%)	23	16

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	59	LEU
1	A	78	LYS
1	A	122	ILE
1	A	125	VAL
1	A	147	VAL
1	A	173	VAL
1	A	181	LYS
1	A	200	THR
1	A	205	ASN
1	A	216	ILE
1	A	241	THR
1	A	242	VAL
1	A	258	ARG

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Mol	Chain	Res	Type
1	A	266	LYS
1	A	273	LYS
1	A	293	LEU
1	A	302	LYS
1	A	344	LYS
1	A	358	LEU
1	A	367	LEU
1	A	368	GLU
1	A	387	ILE
1	A	389	MET
1	A	399	THR
1	A	403	LYS
1	A	409	LEU
1	B	35	LEU
1	B	203	LYS
1	B	208	ARG
1	B	209	ASN
1	B	210	GLU
1	B	251	LYS
1	B	339	ASP
1	B	344	LYS
1	B	399	THR
1	C	62	LEU
1	C	173	VAL
1	C	174	LYS
1	C	175	LEU
1	C	198	GLU
1	C	210	GLU
1	C	216	ILE
1	C	223	LYS
1	C	240	VAL
1	C	248	VAL
1	C	254	GLU
1	C	275	ASN
1	C	305	ASN
1	C	334	SER
1	C	336	VAL
1	C	338	LYS
1	C	340	VAL
1	C	344	LYS
1	C	369	ILE
1	C	383	LEU

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Mol	Chain	Res	Type
1	C	389	MET
1	C	409	LEU
1	D	81	ILE
1	D	109	LEU
1	D	115	ILE
1	D	125	VAL
1	D	135	MET
1	D	167	SER
1	D	174	LYS
1	D	209	ASN
1	D	236	ILE
1	D	239	THR
1	D	240	VAL
1	D	250	VAL
1	D	263	LYS
1	D	270	VAL
1	D	273	LYS
1	D	302	LYS
1	D	305	ASN
1	D	343	LYS
1	D	347	ILE
1	D	389	MET
1	D	409	LEU
1	D	426	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	287	ASN
1	A	363	ASN
1	A	377	ASN
1	A	385	HIS
1	B	164	ASN
1	B	209	ASN
1	B	211	GLN
1	B	377	ASN
1	B	385	HIS
1	B	414	ASN
1	C	275	ASN
1	C	287	ASN
1	C	305	ASN

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Mol	Chain	Res	Type
1	C	353	ASN
1	C	425	GLN
1	D	209	ASN
1	D	287	ASN
1	D	377	ASN
1	D	385	HIS
1	D	400	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	SCY	A	126	1	8,8,9	5.00	2 (25%)	7,9,11	4.64	3 (42%)
1	SCY	B	126	1	8,8,9	6.08	3 (37%)	7,9,11	7.40	2 (28%)
1	SCY	C	126	1	8,8,9	4.67	2 (25%)	7,9,11	5.39	3 (42%)
1	SCY	D	126	1	8,8,9	5.61	3 (37%)	7,9,11	4.11	3 (42%)

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	SCY	A	126	1	-	2/5/7/9	0/0/0/0
1	SCY	B	126	1	-	0/5/7/9	0/0/0/0
1	SCY	C	126	1	-	0/5/7/9	0/0/0/0
1	SCY	D	126	1	-	0/5/7/9	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	SCY	O-C	16.57	1.22	1.11
1	D	126	SCY	O-C	15.21	1.21	1.11
1	A	126	SCY	O-C	13.13	1.20	1.11
1	C	126	SCY	O-C	12.48	1.19	1.11
1	A	126	SCY	CB-SG	-4.59	1.76	1.81
1	C	126	SCY	CB-SG	-3.74	1.77	1.81
1	D	126	SCY	CB-SG	-3.59	1.77	1.81
1	B	126	SCY	CB-SG	-3.51	1.77	1.81
1	D	126	SCY	CA-C	2.09	1.52	1.48
1	B	126	SCY	CA-C	2.09	1.52	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	SCY	CB-SG-CD	-18.92	87.56	100.97
1	C	126	SCY	CB-SG-CD	-12.14	92.36	100.97
1	D	126	SCY	CB-SG-CD	-8.78	94.74	100.97
1	A	126	SCY	CB-SG-CD	-8.31	95.08	100.97
1	A	126	SCY	C-CA-N	-8.22	105.62	113.83
1	C	126	SCY	C-CA-N	-5.78	108.06	113.83
1	D	126	SCY	CA-CB-SG	-4.87	103.04	112.94
1	B	126	SCY	CA-CB-SG	-4.53	103.74	112.94
1	C	126	SCY	CA-CB-SG	-4.20	104.40	112.94
1	A	126	SCY	CA-CB-SG	-3.71	105.41	112.94
1	D	126	SCY	C-CA-N	-3.17	110.67	113.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	126	SCY	CE-CD-SG-CB
1	A	126	SCY	OCD-CD-SG-CB

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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$
3	COA	A	1001	-	50,50,50	1.52	3 (6%)	75,75,75	1.80	10 (13%)
3	COA	B	1002	-	50,50,50	1.56	5 (10%)	75,75,75	1.72	11 (14%)
3	COA	C	1003	-	50,50,50	1.54	4 (8%)	75,75,75	1.75	9 (12%)
3	COA	D	1004	-	50,50,50	1.54	3 (6%)	75,75,75	1.76	9 (12%)

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
3	COA	A	1001	-	-	0/48/64/64	0/1/3/3
3	COA	B	1002	-	-	0/48/64/64	0/1/3/3
3	COA	C	1003	-	-	0/48/64/64	0/1/3/3
3	COA	D	1004	-	-	0/48/64/64	0/1/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	COA	O9P-C9P	9.02	1.41	1.23
3	C	1003	COA	O9P-C9P	8.82	1.40	1.23
3	B	1002	COA	O9P-C9P	8.72	1.40	1.23
3	D	1004	COA	O9P-C9P	8.70	1.40	1.23
3	D	1004	COA	C2A-N3A	3.53	1.39	1.32
3	C	1003	COA	C2A-N3A	3.28	1.38	1.32
3	B	1002	COA	C2A-N3A	3.20	1.38	1.32
3	A	1001	COA	C2A-N3A	3.16	1.38	1.32
3	C	1003	COA	C2A-N1A	2.68	1.39	1.33
3	D	1004	COA	C2A-N1A	2.51	1.38	1.33
3	B	1002	COA	P1A-O3A	2.43	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	COA	C2A-N1A	2.41	1.38	1.33
3	A	1001	COA	C2A-N1A	2.31	1.38	1.33
3	C	1003	COA	P2A-O3A	2.30	1.64	1.59
3	B	1002	COA	P2A-O3A	2.09	1.63	1.59

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	COA	N3A-C2A-N1A	-11.07	119.46	128.71
3	D	1004	COA	N3A-C2A-N1A	-10.08	120.29	128.71
3	A	1001	COA	N3A-C2A-N1A	-9.91	120.43	128.71
3	B	1002	COA	N3A-C2A-N1A	-9.67	120.62	128.71
3	A	1001	COA	O4B-C1B-N9A	6.43	114.42	108.44
3	D	1004	COA	O4B-C1B-N9A	5.82	113.86	108.44
3	C	1003	COA	O4B-C1B-N9A	4.39	112.52	108.44
3	B	1002	COA	C7P-C6P-C5P	-3.86	105.68	112.25
3	A	1001	COA	N3A-C4A-N9A	3.81	132.30	125.43
3	D	1004	COA	CBP-CAP-C9P	3.74	116.36	112.73
3	D	1004	COA	N3A-C4A-N9A	3.73	132.17	125.43
3	A	1001	COA	P2A-O3A-P1A	-3.59	121.15	131.68
3	B	1002	COA	N3A-C4A-N9A	3.55	131.84	125.43
3	B	1002	COA	O4B-C1B-N9A	3.54	111.74	108.44
3	C	1003	COA	C1B-N9A-C4A	-3.28	120.98	126.64
3	C	1003	COA	N3A-C4A-N9A	3.25	131.29	125.43
3	A	1001	COA	C4A-C5A-N7A	-2.97	106.98	109.52
3	D	1004	COA	P2A-O3A-P1A	-2.77	123.56	131.68
3	B	1002	COA	O5P-C5P-C6P	-2.66	116.63	121.92
3	A	1001	COA	C5A-C4A-N3A	-2.63	119.97	125.70
3	C	1003	COA	CBP-CAP-C9P	2.53	115.18	112.73
3	B	1002	COA	C1B-N9A-C4A	-2.46	122.39	126.64
3	B	1002	COA	N7A-C8A-N9A	-2.34	107.73	114.36
3	A	1001	COA	CBP-CAP-C9P	2.28	114.94	112.73
3	D	1004	COA	C1B-N9A-C4A	-2.24	122.76	126.64
3	D	1004	COA	C5A-C4A-N3A	-2.23	120.83	125.70
3	C	1003	COA	P2A-O3A-P1A	-2.22	125.17	131.68
3	C	1003	COA	C2A-N3A-C4A	2.21	120.31	114.01
3	B	1002	COA	C4A-C5A-N7A	-2.21	107.63	109.52
3	D	1004	COA	C2A-N3A-C4A	2.20	120.28	114.01
3	B	1002	COA	CBP-CAP-C9P	2.20	114.87	112.73
3	A	1001	COA	C2A-N3A-C4A	2.20	120.28	114.01
3	B	1002	COA	C5A-C4A-N3A	-2.18	120.96	125.70
3	B	1002	COA	C2B-C3B-C4B	2.14	107.33	103.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	COA	N7A-C8A-N9A	-2.10	108.42	114.36
3	A	1001	COA	O6A-CCP-CBP	2.05	113.99	110.57
3	D	1004	COA	N7A-C8A-N9A	-2.03	108.62	114.36
3	C	1003	COA	C5A-C4A-N3A	-2.02	121.29	125.70
3	C	1003	COA	N7A-C8A-N9A	-2.00	108.69	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	389/406 (95%)	0.38	27 (6%) 17 16	30, 48, 69, 80	0
1	B	386/406 (95%)	-0.02	6 (1%) 68 69	21, 34, 49, 55	0
1	C	388/406 (95%)	0.17	17 (4%) 33 32	23, 38, 60, 71	0
1	D	382/406 (94%)	0.03	12 (3%) 47 46	30, 41, 58, 67	0
All	All	1545/1624 (95%)	0.14	62 (4%) 36 36	21, 41, 63, 80	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	VAL	5.5
1	A	242	VAL	4.9
1	A	387	ILE	4.1
1	C	241	THR	3.9
1	A	305	ASN	3.9
1	D	242	VAL	3.7
1	D	273	LYS	3.5
1	A	275	ASN	3.4
1	A	272	GLN	3.4
1	A	239	THR	3.3
1	A	240	VAL	3.3
1	D	268	LYS	3.2
1	A	127	ALA	3.1
1	A	274	GLU	3.1
1	B	355	ALA	3.0
1	C	122	ILE	3.0
1	A	241	THR	3.0
1	A	304	LEU	3.0
1	C	275	ASN	2.9
1	D	274	GLU	2.9
1	B	122	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	346	ASP	2.7
1	D	94	VAL	2.7
1	B	412	ILE	2.7
1	A	207	ALA	2.6
1	C	273	LYS	2.6
1	D	122	ILE	2.5
1	B	305	ASN	2.5
1	A	206	ILE	2.5
1	B	125	VAL	2.5
1	A	122	ILE	2.5
1	D	173	VAL	2.5
1	D	412	ILE	2.5
1	A	216	ILE	2.5
1	A	125	VAL	2.4
1	C	270	VAL	2.4
1	A	266	LYS	2.4
1	C	243	LYS	2.4
1	A	388	GLY	2.3
1	C	268	LYS	2.3
1	A	390	SER	2.3
1	D	241	THR	2.3
1	A	270	VAL	2.3
1	D	125	VAL	2.3
1	C	274	GLU	2.3
1	A	306	VAL	2.3
1	C	262	SER	2.2
1	A	173	VAL	2.2
1	A	302	LYS	2.2
1	C	387	ILE	2.2
1	D	410	ALA	2.2
1	C	92	GLY	2.1
1	B	127	ALA	2.1
1	A	94	VAL	2.1
1	C	341	GLY	2.1
1	C	353	ASN	2.1
1	C	265	PRO	2.1
1	C	261	PHE	2.1
1	C	412	ILE	2.0
1	D	120	THR	2.0
1	A	276	GLY	2.0
1	A	128	SER	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SCY	C	126	9/10	0.23	1.24	31,33,48,56	0
1	SCY	A	126	9/10	0.28	1.24	43,46,53,54	0
1	SCY	B	126	9/10	0.21	0.42	25,28,42,51	0
1	SCY	D	126	9/10	0.20	0.30	32,34,48,50	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	COA	C	1003	48/48	0.23	1.14	69,81,93,93	0
3	COA	D	1004	48/48	0.17	0.98	57,67,78,79	0
3	COA	B	1002	48/48	0.16	0.62	44,62,71,73	0
3	COA	A	1001	48/48	0.20	0.61	71,98,105,106	0
2	CL	B	2001	1/1	0.14	0.17	29,29,29,29	0
2	CL	A	2003	1/1	0.11	-0.57	42,42,42,42	0
2	CL	B	2002	1/1	0.11	-0.68	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.