



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 07:43 PM GMT

PDB ID : 3K6M
Title : Dynamic domains of Succinyl-CoA:3-ketoacid-coenzymeA transferase from pig heart.
Authors : Coker, S.; Lloyd, A.; Mitchell, E.; Lewis, G.R.; Shoolingin-Jordan, P.; Coker, A.R.
Deposited on : 2009-10-09
Resolution : 1.50 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>

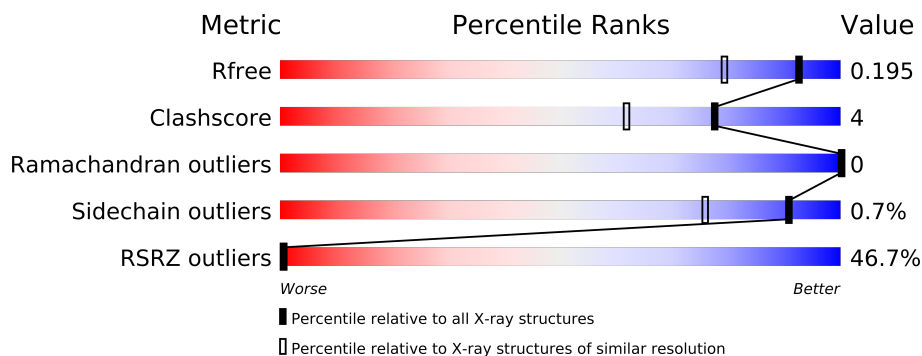
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 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}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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. 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	481	
1	B	481	
1	C	481	
1	D	481	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	C	5000	-	X
3	GOL	C	5001	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16054 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 Succinyl-CoA:3-ketoacid-coenzymeA transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	3	11	0
			3601	2292	610	678	21			
1	D	462	Total	C	N	O	S	2	19	0
			3623	2313	610	680	20			
1	C	466	Total	C	N	O	S	0	16	0
			3627	2311	613	680	23			
1	B	461	Total	C	N	O	S	16	17	0
			3608	2296	609	681	22			

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

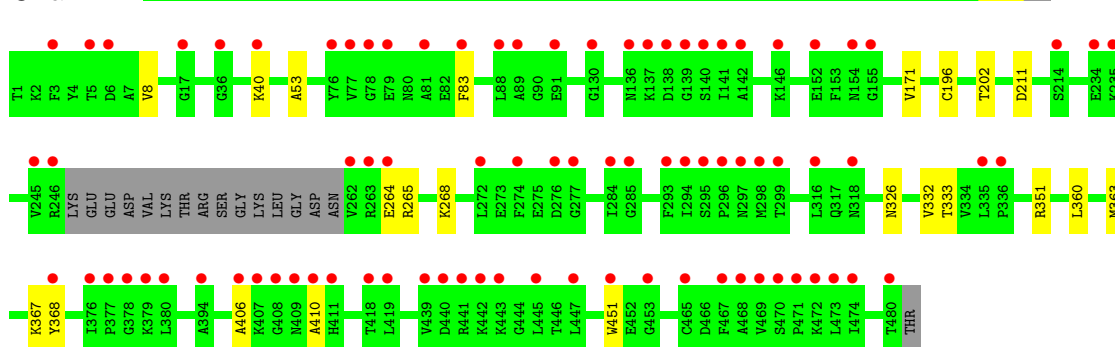
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	353	Total	O	0	0
			353	353		
4	D	352	Total	O	0	0
			352	352		
4	C	474	Total	O	0	0
			474	474		
4	B	402	Total	O	0	0
			402	402		

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.

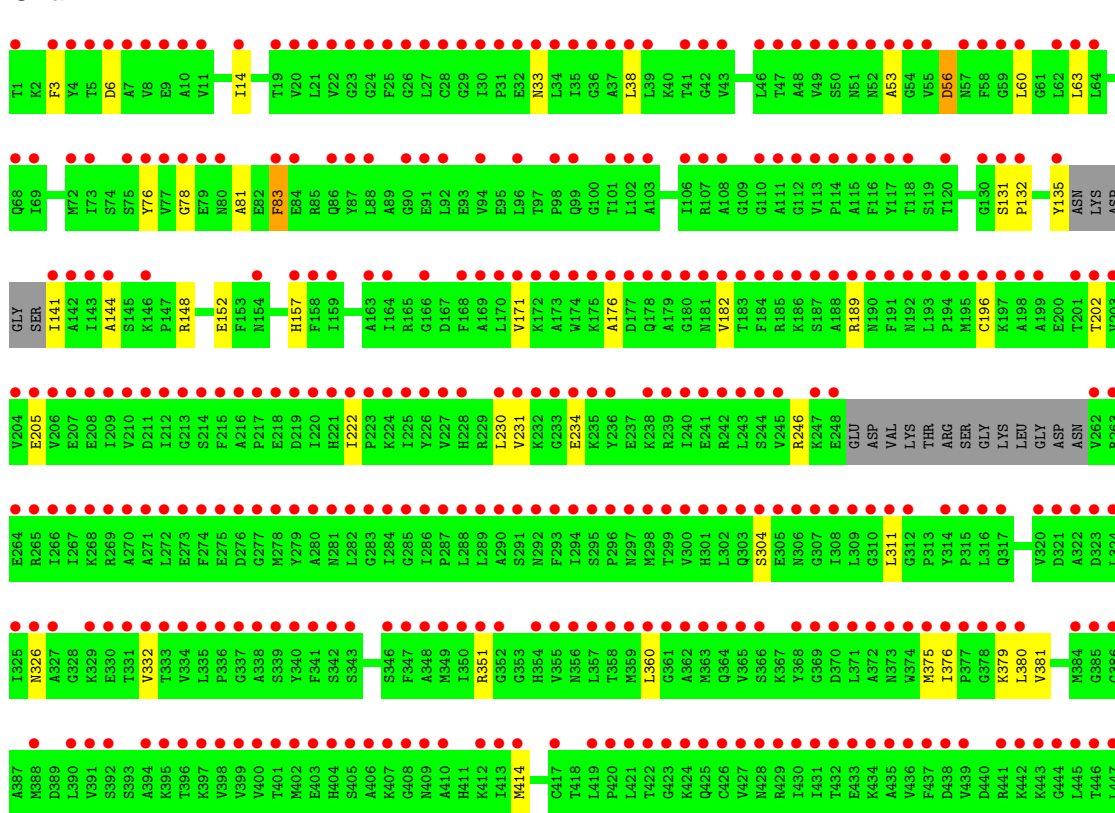
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzymeA transferase 1, mitochondrial

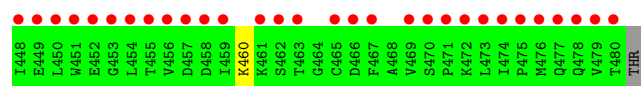
Chain A:



- Molecule 1: Succinyl-CoA:3-ketoacid-coenzymeA transferase 1, mitochondrial

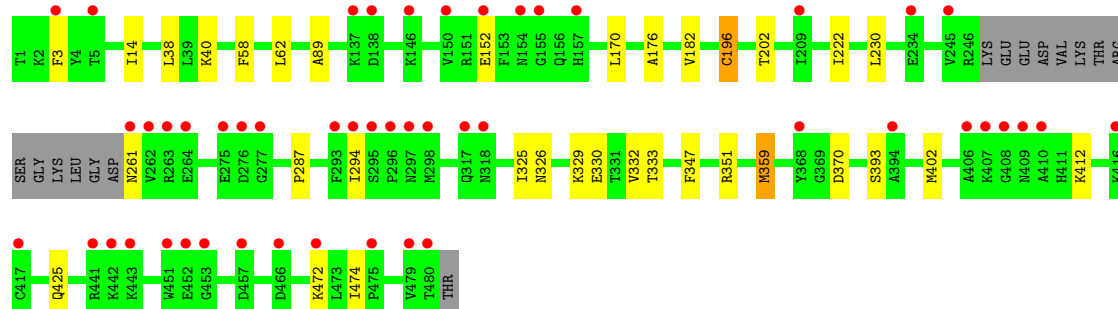
Chain D:





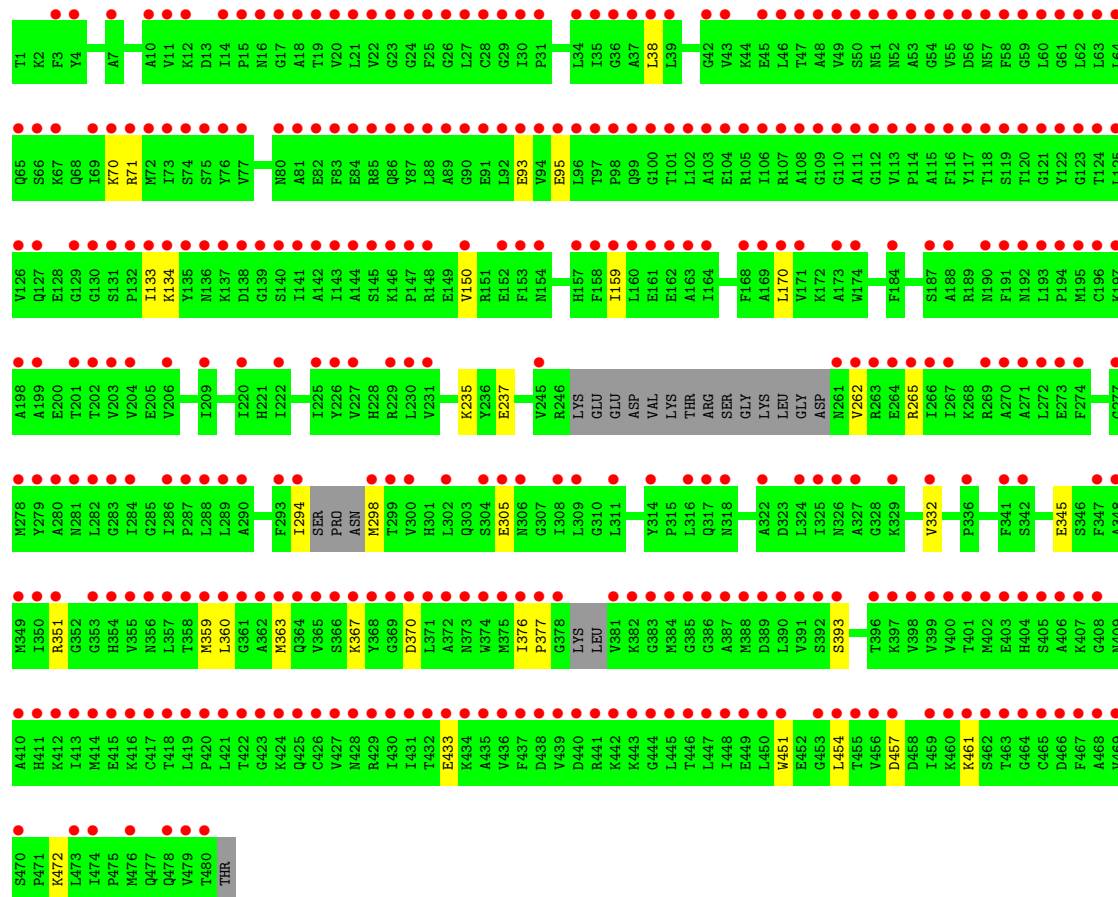
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzymeA transferase 1, mitochondrial

Chain C:



- Molecule 1: Succinyl-CoA:3-ketoacid-coenzymeA transferase 1, mitochondrial

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.72Å 133.57Å 102.23Å 90.00° 104.98° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 19.79 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.50) 97.6 (19.79-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.185 0.177 , 0.195	Depositor DCC
R_{free} test set	14899 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 296782 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16054	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: GOL, 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	0.70	2/3689 (0.1%)	0.74	0/4976
1	B	0.71	4/3705 (0.1%)	0.76	3/4995 (0.1%)
1	C	0.84	5/3733 (0.1%)	0.83	1/5036 (0.0%)
1	D	0.74	0/3728	0.82	6/5030 (0.1%)
All	All	0.75	11/14855 (0.1%)	0.79	10/20037 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196[A]	CYS	CB-SG	-5.76	1.72	1.81
1	C	196[B]	CYS	CB-SG	-5.76	1.72	1.81
1	C	393[A]	SER	N-CA	5.59	1.57	1.46
1	C	393[B]	SER	N-CA	5.59	1.57	1.46
1	B	305[A]	GLU	CD-OE1	5.57	1.31	1.25
1	B	305[B]	GLU	CD-OE1	5.57	1.31	1.25
1	B	305[A]	GLU	CB-CG	-5.29	1.42	1.52
1	B	305[B]	GLU	CB-CG	-5.29	1.42	1.52
1	A	363[A]	MET	CG-SD	-5.14	1.67	1.81
1	A	363[B]	MET	CG-SD	-5.14	1.67	1.81
1	C	425	GLN	CD-NE2	-5.05	1.20	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	359[A]	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	359[B]	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	370	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	189	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	6	ASP	CB-CG-OD2	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	246	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	135	TYR	CB-CA-C	-5.15	100.09	110.40
1	C	370	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3601	0	3704	19	0
1	B	3608	0	3705	27	0
1	C	3627	0	3748	31	0
1	D	3623	0	3734	32	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	C	12	0	16	0	0
4	A	353	0	0	1	0
4	B	402	0	0	6	0
4	C	474	0	0	5	0
4	D	352	0	0	2	0
All	All	16054	0	14907	108	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 4.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:196[B]:CYS:SG	1:C:202[B]:THR:HG21	2.03	0.97
1:D:76[B]:TYR:CE2	1:D:78:GLY:HA2	2.01	0.95
1:C:3:PHE:CE2	1:C:230[B]:LEU:HD23	2.01	0.95
1:D:3:PHE:CE2	1:D:230[A]:LEU:HD23	2.01	0.94
1:D:196[B]:CYS:SG	1:D:202[B]:THR:HG21	2.13	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196[B]:CYS:SG	1:A:202[B]:THR:HG21	2.19	0.82
1:B:93[B]:GLU:HG3	1:B:133:ILE:HG22	1.68	0.76
1:C:326:ASN:HB3	1:C:332[B]:VAL:HG21	1.69	0.75
1:A:196[A]:CYS:O	1:A:202[A]:THR:HG21	1.90	0.71
1:D:76[B]:TYR:CE2	1:D:78:GLY:CA	2.76	0.68
1:C:332[A]:VAL:HG22	1:C:333:THR:H	1.59	0.68
1:C:332[A]:VAL:HG22	1:C:333:THR:N	2.09	0.66
1:A:326:ASN:HB3	1:A:332[B]:VAL:HG21	1.77	0.66
1:B:345[B]:GLU:HA	1:B:345[B]:GLU:OE1	1.95	0.66
1:A:332[B]:VAL:HG12	1:A:333:THR:N	2.11	0.65
1:B:472:LYS:HG2	1:B:472:LYS:O	1.96	0.65
1:D:53:ALA:HB3	1:D:83:PHE:CD1	2.31	0.65
1:B:95:GLU:HG3	4:B:820:HOH:O	1.97	0.64
1:D:414:MET:HE2	4:D:794:HOH:O	1.97	0.64
1:D:375[A]:MET:SD	1:D:380:LEU:O	2.56	0.63
1:B:93[B]:GLU:HG2	1:B:133:ILE:CG2	2.29	0.63
1:C:402[A]:MET:CE	1:C:412:LYS:HE2	2.30	0.61
1:A:332[B]:VAL:HG12	1:A:333:THR:O	2.00	0.61
1:B:93[B]:GLU:CG	1:B:133:ILE:HG22	2.31	0.60
1:C:402[A]:MET:HE2	1:C:412:LYS:HE2	1.84	0.60
1:B:93[B]:GLU:CG	1:B:133:ILE:CG2	2.79	0.60
1:D:132[A]:PRO:HD3	1:D:141:ILE:HD12	1.82	0.59
1:D:152:GLU:HB2	1:D:157[B]:HIS:CD2	2.37	0.59
1:B:351:ARG:HD3	4:B:545:HOH:O	2.04	0.58
1:C:196[B]:CYS:HG	1:C:202[B]:THR:HG21	1.70	0.57
1:D:131[A]:SER:O	1:D:144:ALA:HA	2.05	0.57
1:D:132[A]:PRO:CD	1:D:141:ILE:HD12	2.35	0.56
1:B:70:LYS:NZ	4:B:891:HOH:O	2.39	0.55
1:C:182:VAL:HG22	1:C:222:ILE:HB	1.87	0.55
1:B:265:ARG:HD3	1:B:451:TRP:CZ2	2.42	0.54
1:D:14:ILE:HD12	1:D:38[A]:LEU:HD21	1.89	0.54
1:C:3:PHE:CZ	1:C:230[B]:LEU:HD23	2.42	0.53
1:D:152:GLU:HB2	1:D:157[B]:HIS:NE2	2.24	0.53
1:C:38[A]:LEU:HD11	1:C:170:LEU:HD11	1.91	0.53
1:A:211:ASP:HB2	1:D:157[B]:HIS:CD2	2.44	0.52
1:A:332[B]:VAL:CG1	1:A:333:THR:N	2.74	0.52
1:C:196[B]:CYS:SG	1:C:202[B]:THR:CG2	2.89	0.51
1:B:451:TRP:HB3	1:B:454:LEU:HD12	1.93	0.51
1:B:150[A]:VAL:HG22	1:B:159:ILE:HG22	1.94	0.50
1:A:351:ARG:HD3	4:A:7042:HOH:O	2.11	0.50
1:B:294:ILE:HG23	1:B:298:MET:HE3	1.94	0.50
1:B:294:ILE:HG23	1:B:298:MET:CE	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:56:ASP:OD1	1:D:81:ALA:HB3	2.12	0.49
1:D:326:ASN:HB3	1:D:332[A]:VAL:HG11	1.93	0.49
1:D:176:ALA:CB	1:D:230[B]:LEU:HD11	2.42	0.49
1:C:152:GLU:HG2	4:C:5565:HOH:O	2.12	0.49
1:C:472:LYS:O	1:C:474:ILE:HG23	2.13	0.49
1:B:265:ARG:HD3	1:B:451:TRP:CE2	2.48	0.48
1:C:14:ILE:HD12	1:C:38[A]:LEU:HD21	1.94	0.48
1:D:176:ALA:HB1	1:D:230[B]:LEU:HD11	1.95	0.48
1:C:330:GLU:O	1:C:332[B]:VAL:HG23	2.13	0.48
1:B:457:ASP:O	1:B:461:LYS:HG3	2.13	0.48
1:C:332[A]:VAL:CG2	1:C:333:THR:N	2.77	0.48
1:D:196[B]:CYS:SG	1:D:202[B]:THR:CG2	2.96	0.47
1:B:93[B]:GLU:HG3	1:B:133:ILE:CG2	2.41	0.46
1:C:332[A]:VAL:CG2	1:C:333:THR:H	2.28	0.46
1:B:367:LYS:NZ	4:B:847:HOH:O	2.48	0.46
1:A:332[B]:VAL:HG12	1:A:333:THR:H	1.79	0.46
1:B:70:LYS:NZ	1:B:93[A]:GLU:OE1	2.47	0.46
1:C:3:PHE:CE2	1:C:230[B]:LEU:CD2	2.89	0.46
1:A:171:VAL:HG11	1:A:196[A]:CYS:SG	2.56	0.46
1:D:351:ARG:HD3	4:D:549:HOH:O	2.16	0.46
1:C:294:ILE:HD12	4:C:5472:HOH:O	2.17	0.45
1:C:176:ALA:CB	1:C:230[B]:LEU:HD21	2.47	0.45
1:C:325:ILE:HD12	1:C:329:LYS:HA	1.98	0.45
1:B:38[B]:LEU:HD11	1:B:170:LEU:HD11	1.99	0.45
1:A:196[B]:CYS:SG	1:A:202[B]:THR:CG2	3.00	0.45
1:A:265:ARG:HD3	1:A:451:TRP:CD2	2.52	0.45
1:C:287:PRO:HB3	1:C:359[A]:MET:HB3	1.98	0.44
1:D:182:VAL:HG22	1:D:222:ILE:HB	1.99	0.44
1:D:176:ALA:CB	1:D:230[A]:LEU:HD21	2.47	0.44
1:A:406:ALA:HB3	1:A:410:ALA:HB3	2.00	0.44
1:A:8:VAL:HG21	1:A:40[B]:LYS:HD3	1.99	0.43
1:A:53:ALA:HB3	1:A:83:PHE:CD1	2.54	0.43
1:D:205:GLU:HA	1:D:231:VAL:O	2.19	0.43
1:C:261:ASN:N	4:C:5515:HOH:O	2.51	0.43
1:B:363[A]:MET:SD	1:B:376:ILE:HG23	2.58	0.43
1:D:33:ASN:OD1	1:D:234[A]:GLU:HG2	2.18	0.43
1:D:60:LEU:CD2	1:D:63:LEU:HD12	2.48	0.43
1:C:332[A]:VAL:HG22	1:C:333:THR:O	2.19	0.43
1:A:332[B]:VAL:CG1	1:A:333:THR:H	2.32	0.42
1:D:3:PHE:CZ	1:D:230[A]:LEU:HD23	2.51	0.42
1:C:40:LYS:HE3	4:C:5379:HOH:O	2.18	0.42
1:D:171:VAL:HG11	1:D:196[A]:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:235:LYS:HE2	1:B:237:GLU:HG2	2.02	0.42
1:B:71[A]:ARG:CD	4:B:820:HOH:O	2.66	0.42
1:A:367:LYS:HD2	1:A:368:TYR:CE1	2.55	0.42
1:C:347:PHE:O	1:C:351[B]:ARG:HB2	2.20	0.42
1:D:375[A]:MET:HE1	1:D:381:VAL:HA	2.01	0.41
1:D:141:ILE:O	1:D:141:ILE:HG23	2.20	0.41
1:D:376:ILE:HG21	1:D:379:LYS:HD2	2.01	0.41
1:A:264[A]:GLU:OE2	1:A:268:LYS:HE3	2.19	0.41
1:D:304:SER:HB2	1:D:311:LEU:HD11	2.01	0.41
1:B:472:LYS:O	1:B:472:LYS:CG	2.66	0.41
1:A:265:ARG:HD3	1:A:451:TRP:CE3	2.56	0.41
1:B:71[A]:ARG:HD3	4:B:820:HOH:O	2.21	0.40
1:C:89:ALA:HB2	4:C:5448:HOH:O	2.21	0.40
1:B:93[A]:GLU:HG2	1:B:134:LYS:HD2	2.03	0.40
1:B:262:VAL:HG13	1:B:433:GLU:HB3	2.03	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	472/481 (98%)	464 (98%)	8 (2%)	0	100	100
1	B	470/481 (98%)	463 (98%)	7 (2%)	0	100	100
1	C	478/481 (99%)	469 (98%)	9 (2%)	0	100	100
1	D	475/481 (99%)	464 (98%)	11 (2%)	0	100	100
All	All	1895/1924 (98%)	1860 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/393 (99%)	389 (100%)	1 (0%)	96	88
1	B	392/393 (100%)	386 (98%)	6 (2%)	76	47
1	C	396/393 (101%)	393 (99%)	3 (1%)	89	73
1	D	394/393 (100%)	390 (99%)	4 (1%)	85	65
All	All	1572/1572 (100%)	1558 (99%)	14 (1%)	91	69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	LEU
1	D	56	ASP
1	D	83	PHE
1	D	360	LEU
1	D	460	LYS
1	C	58	PHE
1	C	359[A]	MET
1	C	359[B]	MET
1	B	332[A]	VAL
1	B	332[B]	VAL
1	B	360	LEU
1	B	377	PRO
1	B	393[A]	SER
1	B	393[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	301	HIS
1	B	99	GLN
1	B	154	ASN
1	B	411	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GOL	C	5000	-	5,5,5	0.17	0	5,5,5	0.26	0
3	GOL	C	5001	-	5,5,5	0.64	0	5,5,5	0.64	0

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	GOL	C	5000	-	-	0/4/4/4	0/0/0/0
3	GOL	C	5001	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	465/481 (96%)	1.14	86 (18%) 2 2	18, 25, 31, 37	1 (0%)
1	B	461/481 (95%)	4.46	352 (76%) 0 0	18, 24, 32, 43	2 (0%)
1	C	466/481 (96%)	0.70	49 (10%) 7 7	20, 24, 32, 39	0
1	D	462/481 (96%)	4.46	380 (82%) 0 0	17, 25, 34, 42	1 (0%)
All	All	1854/1924 (96%)	2.68	867 (46%) 1 0	17, 25, 32, 43	4 (0%)

All (867) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	413	ILE	20.5
1	D	279	TYR	18.2
1	B	430	ILE	17.6
1	D	266	ILE	17.6
1	D	430	ILE	17.2
1	B	368	TYR	17.0
1	B	437	PHE	17.0
1	D	431	ILE	16.7
1	B	365	VAL	16.6
1	B	431	ILE	16.6
1	B	445	LEU	16.1
1	B	421	LEU	16.0
1	B	436	VAL	14.3
1	D	288	LEU	13.6
1	B	371	LEU	13.5
1	B	459	ILE	13.4
1	D	271	ALA	12.9
1	D	325	ILE	12.9
1	B	374	TRP	12.9
1	D	282	LEU	12.7
1	D	400	VAL	12.7

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Mol	Chain	Res	Type	RSRZ
1	B	417	CYS	12.3
1	D	206	VAL	12.2
1	B	158	PHE	11.8
1	D	324	LEU	11.7
1	D	332[A]	VAL	11.6
1	B	444	GLY	11.5
1	B	447	LEU	11.4
1	D	294	ILE	11.4
1	D	280	ALA	11.3
1	D	278	MET	11.3
1	B	426	CYS	11.3
1	B	439	VAL	11.2
1	B	465	CYS	11.0
1	B	400	VAL	10.9
1	B	402	MET	10.9
1	D	311	LEU	10.9
1	D	220	ILE	10.9
1	D	432	THR	10.8
1	D	204	VAL	10.8
1	B	369	GLY	10.8
1	B	159	ILE	10.7
1	B	422	THR	10.7
1	D	141	ILE	10.6
1	B	117	TYR	10.5
1	D	308	ILE	10.5
1	D	290	ALA	10.5
1	B	366	SER	10.4
1	D	374	TRP	10.4
1	B	367	LYS	10.3
1	D	240	ILE	10.3
1	B	122	TYR	10.2
1	D	436	VAL	10.1
1	D	270	ALA	10.1
1	D	171	VAL	10.0
1	D	230[A]	LEU	10.0
1	B	126	VAL	10.0
1	D	359	MET	9.9
1	D	360	LEU	9.9
1	D	272	LEU	9.8
1	B	69	ILE	9.8
1	B	266	ILE	9.7
1	B	113	VAL	9.6

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Mol	Chain	Res	Type	RSRZ
1	D	209	ILE	9.6
1	B	404	HIS	9.6
1	D	291	SER	9.6
1	D	340	TYR	9.6
1	B	73	ILE	9.6
1	B	121	GLY	9.6
1	D	286	ILE	9.4
1	D	203	VAL	9.4
1	D	479	VAL	9.4
1	B	427	VAL	9.3
1	D	413	ILE	9.3
1	D	27	LEU	9.3
1	D	402	MET	9.3
1	D	267	ILE	9.3
1	B	448	ILE	9.3
1	D	28	CYS	9.2
1	B	399	VAL	9.1
1	D	34	LEU	9.1
1	B	160	LEU	9.1
1	B	398	VAL	9.0
1	B	467	PHE	9.0
1	D	398	VAL	9.0
1	B	424	LYS	8.9
1	D	287	PRO	8.9
1	D	274	PHE	8.8
1	D	174	TRP	8.8
1	B	466	ASP	8.7
1	D	459	ILE	8.7
1	D	334	VAL	8.7
1	D	399	VAL	8.7
1	D	341	PHE	8.7
1	B	435	ALA	8.7
1	D	231	VAL	8.6
1	B	92	LEU	8.6
1	D	182	VAL	8.5
1	D	243	LEU	8.5
1	B	432	THR	8.5
1	B	282	LEU	8.5
1	D	281	ASN	8.4
1	B	118	THR	8.4
1	B	60	LEU	8.4
1	D	38[A]	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
1	B	120	THR	8.3
1	B	143	ILE	8.3
1	B	362	ALA	8.3
1	D	227	VAL	8.3
1	D	401	THR	8.3
1	D	170	LEU	8.3
1	D	371	LEU	8.3
1	B	463	THR	8.2
1	B	96	LEU	8.1
1	D	30	ILE	8.1
1	B	94	VAL	8.1
1	B	414	MET	8.1
1	B	401	THR	8.0
1	B	22	VAL	8.0
1	D	365	VAL	8.0
1	D	222	ILE	8.0
1	B	423	GLY	7.9
1	D	322	ALA	7.9
1	D	404	HIS	7.8
1	B	49	VAL	7.8
1	B	372	ALA	7.8
1	B	446	THR	7.8
1	B	20	VAL	7.7
1	D	173	ALA	7.7
1	D	196[A]	CYS	7.7
1	D	309	LEU	7.7
1	D	225	ILE	7.7
1	D	302	LEU	7.6
1	D	362	ALA	7.6
1	B	370	ASP	7.5
1	D	320	VAL	7.5
1	D	277	GLY	7.5
1	B	325	ILE	7.5
1	B	450	LEU	7.5
1	B	116	PHE	7.4
1	D	262	VAL	7.4
1	B	98	PRO	7.4
1	D	58	PHE	7.4
1	B	21	LEU	7.3
1	D	426	CYS	7.3
1	B	204	VAL	7.3
1	D	176	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	7.2
1	B	171	VAL	7.2
1	B	360	LEU	7.2
1	B	388	MET	7.2
1	B	138	ASP	7.1
1	B	64	LEU	7.1
1	B	14	ILE	7.1
1	A	284	ILE	7.1
1	D	476	MET	7.0
1	B	468	ALA	7.0
1	B	38[A]	LEU	7.0
1	C	407	LYS	7.0
1	D	339	SER	6.9
1	D	184	PHE	6.9
1	B	391	VAL	6.9
1	B	62	LEU	6.8
1	D	422	THR	6.8
1	B	425	GLN	6.8
1	D	169	ALA	6.8
1	B	135	TYR	6.8
1	B	124	THR	6.8
1	B	350	ILE	6.8
1	C	297	ASN	6.7
1	D	331	THR	6.7
1	B	441	ARG	6.7
1	D	437	PHE	6.7
1	B	363[A]	MET	6.7
1	A	296	PRO	6.7
1	B	101	THR	6.7
1	B	63	LEU	6.7
1	A	408	GLY	6.6
1	B	106	ILE	6.6
1	D	187	SER	6.6
1	D	268	LYS	6.6
1	B	440	ASP	6.6
1	B	196[A]	CYS	6.6
1	D	11	VAL	6.6
1	B	203	VAL	6.6
1	B	140	SER	6.6
1	B	97	THR	6.5
1	B	164	ILE	6.5
1	B	279	TYR	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	280	ALA	6.5
1	B	412	LYS	6.5
1	B	34	LEU	6.5
1	D	439	VAL	6.5
1	B	419	LEU	6.4
1	B	114	PRO	6.4
1	B	361	GLY	6.4
1	D	21	LEU	6.4
1	D	180	GLY	6.4
1	B	46	LEU	6.4
1	B	170	LEU	6.4
1	B	462[A]	SER	6.4
1	D	450	LEU	6.3
1	D	202[A]	THR	6.3
1	D	338	ALA	6.3
1	B	53	ALA	6.3
1	A	407	LYS	6.3
1	D	20	VAL	6.3
1	D	333	THR	6.3
1	A	297	ASN	6.3
1	D	215	PHE	6.3
1	B	141	ILE	6.3
1	A	453	GLY	6.3
1	B	225	ILE	6.2
1	D	210	VAL	6.2
1	D	480	THR	6.2
1	D	248	GLU	6.2
1	B	443	LYS	6.2
1	B	168	PHE	6.1
1	B	87	TYR	6.1
1	B	434	LYS	6.1
1	B	390	LEU	6.1
1	A	378	GLY	6.1
1	D	435	ALA	6.1
1	B	108	ALA	6.1
1	B	442	LYS	6.1
1	D	427	VAL	6.1
1	B	261	ASN	6.0
1	D	407	LYS	6.0
1	B	112	GLY	6.0
1	D	25	PHE	6.0
1	D	193	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	296	PRO	6.0
1	B	453	GLY	5.9
1	B	83	PHE	5.9
1	D	284	ILE	5.9
1	C	294	ILE	5.9
1	C	408	GLY	5.9
1	B	150[A]	VAL	5.9
1	D	372	ALA	5.9
1	D	448	ILE	5.9
1	D	451	TRP	5.9
1	B	286	ILE	5.9
1	B	364	GLN	5.8
1	B	125	LEU	5.8
1	D	226	TYR	5.8
1	B	373	ASN	5.8
1	D	421	LEU	5.8
1	B	420	PRO	5.8
1	D	113	VAL	5.8
1	B	27	LEU	5.8
1	B	102	LEU	5.8
1	D	378	GLY	5.8
1	D	168	PHE	5.8
1	D	293	PHE	5.8
1	B	72	MET	5.8
1	D	380	LEU	5.7
1	B	136	ASN	5.7
1	D	361	GLY	5.7
1	B	123	GLY	5.7
1	D	296	PRO	5.7
1	B	133	ILE	5.7
1	C	261	ASN	5.7
1	B	411	HIS	5.7
1	D	350	ILE	5.6
1	A	409	ASN	5.6
1	B	39	LEU	5.6
1	D	35	ILE	5.6
1	B	115	ALA	5.6
1	D	307	GLY	5.6
1	A	262	VAL	5.6
1	D	22	VAL	5.6
1	B	77	VAL	5.6
1	D	273	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	5.5
1	D	183	THR	5.5
1	D	269	ARG	5.5
1	B	111	ALA	5.5
1	B	359[A]	MET	5.5
1	D	7	ALA	5.5
1	D	191	PHE	5.5
1	D	46	LEU	5.5
1	D	63	LEU	5.5
1	D	299	THR	5.5
1	B	74	SER	5.5
1	D	236	TYR	5.5
1	D	300	VAL	5.5
1	B	454	LEU	5.4
1	B	392	SER	5.4
1	D	310	GLY	5.4
1	D	245	VAL	5.4
1	B	47	THR	5.4
1	B	103	ALA	5.4
1	D	312	GLY	5.4
1	B	35	ILE	5.4
1	B	267	ILE	5.4
1	A	451	TRP	5.4
1	D	60	LEU	5.4
1	B	377	PRO	5.3
1	B	384	MET	5.3
1	D	327	ALA	5.2
1	B	81	ALA	5.2
1	B	270	ALA	5.2
1	B	415	GLU	5.2
1	D	355	VAL	5.2
1	D	298	MET	5.2
1	D	175	LYS	5.2
1	A	441	ARG	5.2
1	D	390	LEU	5.2
1	B	332[A]	VAL	5.1
1	D	337	GLY	5.1
1	B	163	ALA	5.1
1	D	198	ALA	5.1
1	D	447	LEU	5.1
1	A	471	PRO	5.1
1	B	405	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	408	GLY	5.1
1	B	473	LEU	5.1
1	D	14	ILE	5.1
1	B	464	GLY	5.1
1	D	217	PRO	5.1
1	A	410	ALA	5.0
1	B	451	TRP	5.0
1	D	315	PRO	5.0
1	B	355	VAL	5.0
1	B	28	CYS	5.0
1	B	169	ALA	5.0
1	B	23	GLY	5.0
1	B	396	THR	5.0
1	D	349	MET	5.0
1	D	181	ASN	5.0
1	D	106	ILE	5.0
1	D	314	TYR	4.9
1	D	62	LEU	4.9
1	D	473	LEU	4.9
1	D	172	LYS	4.9
1	B	119	SER	4.9
1	D	92	LEU	4.9
1	D	289	LEU	4.9
1	D	347	PHE	4.9
1	B	347	PHE	4.9
1	A	472	LYS	4.9
1	A	480	THR	4.9
1	D	29	GLY	4.9
1	D	31	PRO	4.8
1	B	202[A]	THR	4.8
1	B	357	LEU	4.8
1	D	186	LYS	4.8
1	B	88	LEU	4.8
1	D	188	ALA	4.8
1	D	369	GLY	4.8
1	C	409	ASN	4.8
1	D	189	ARG	4.8
1	A	469	VAL	4.8
1	B	191	PHE	4.8
1	D	232	LYS	4.7
1	B	288	LEU	4.7
1	B	438	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	262	VAL	4.7
1	D	26	GLY	4.7
1	D	304	SER	4.7
1	B	105	ARG	4.7
1	B	11	VAL	4.7
1	B	227	VAL	4.7
1	D	478	GLN	4.7
1	B	50	SER	4.7
1	B	89	ALA	4.7
1	B	85	ARG	4.6
1	B	262	VAL	4.6
1	B	317	GLN	4.6
1	D	179	ALA	4.6
1	A	141	ILE	4.6
1	B	30	ILE	4.6
1	B	222	ILE	4.6
1	D	55	VAL	4.6
1	D	233	GLY	4.6
1	B	476	MET	4.6
1	D	306	ASN	4.6
1	B	281	ASN	4.6
1	D	208	GLU	4.6
1	D	373	ASN	4.6
1	D	224	LYS	4.6
1	D	423	GLY	4.6
1	D	221	HIS	4.6
1	B	145	SER	4.6
1	B	386	GLY	4.6
1	D	33	ASN	4.5
1	D	363	MET	4.5
1	B	19	THR	4.5
1	D	264	GLU	4.5
1	D	49	VAL	4.5
1	D	456	VAL	4.5
1	D	463	THR	4.5
1	D	469	VAL	4.5
1	B	139	GLY	4.5
1	D	410	ALA	4.5
1	D	342	SER	4.5
1	B	381	VAL	4.5
1	B	349	MET	4.5
1	B	416	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	5	THR	4.4
1	B	25	PHE	4.4
1	B	153	PHE	4.4
1	D	445	LEU	4.4
1	D	467	PHE	4.4
1	B	324	LEU	4.4
1	A	406	ALA	4.4
1	D	379	LYS	4.4
1	D	461	LYS	4.4
1	D	142	ALA	4.4
1	D	292	ASN	4.4
1	B	290	ALA	4.4
1	B	318	ASN	4.4
1	B	470	SER	4.4
1	D	474	ILE	4.4
1	D	223	PRO	4.4
1	B	134	LYS	4.4
1	B	193	LEU	4.3
1	D	69	ILE	4.3
1	D	441	ARG	4.3
1	B	375[A]	MET	4.3
1	D	10	ALA	4.3
1	B	383	GLY	4.3
1	D	216	ALA	4.3
1	B	61	GLY	4.3
1	D	326	ASN	4.3
1	D	357	LEU	4.2
1	B	127	GLN	4.2
1	B	75	SER	4.2
1	D	59[A]	GLY	4.2
1	D	77	VAL	4.2
1	B	309	LEU	4.2
1	B	198	ALA	4.2
1	A	418	THR	4.2
1	B	308	ILE	4.2
1	B	429	ARG	4.2
1	D	453	GLY	4.2
1	B	55	VAL	4.2
1	D	241[A]	GLU	4.1
1	D	323	ASP	4.1
1	B	348	ALA	4.1
1	D	396	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	205	GLU	4.1
1	D	335	LEU	4.1
1	B	226	TYR	4.1
1	D	376	ILE	4.1
1	D	88	LEU	4.1
1	B	272	LEU	4.1
1	D	83	PHE	4.0
1	D	190	ASN	4.0
1	A	368	TYR	4.0
1	D	228	HIS	4.0
1	B	418	THR	4.0
1	A	299	THR	4.0
1	B	70	LYS	4.0
1	D	87	TYR	4.0
1	C	295	SER	4.0
1	C	480	THR	4.0
1	B	144	ALA	4.0
1	D	316	LEU	3.9
1	D	455	THR	3.9
1	B	327	ALA	3.9
1	B	341	PHE	3.9
1	B	148	ARG	3.9
1	D	321	ASP	3.9
1	B	294	ILE	3.9
1	D	37	ALA	3.9
1	B	184	PHE	3.9
1	D	244	SER	3.9
1	D	283	GLY	3.9
1	D	265	ARG	3.9
1	D	4	TYR	3.9
1	D	303	GLN	3.9
1	A	470	SER	3.9
1	D	8	VAL	3.8
1	A	5	THR	3.8
1	B	480	THR	3.8
1	D	449	GLU	3.8
1	D	54	GLY	3.8
1	B	230	LEU	3.8
1	A	264[A]	GLU	3.8
1	D	412	LYS	3.8
1	C	154	ASN	3.8
1	B	428	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	302	LEU	3.8
1	B	316	LEU	3.8
1	B	59	GLY	3.8
1	D	343	SER	3.8
1	B	76	TYR	3.8
1	D	219	ASP	3.8
1	A	394	ALA	3.8
1	D	48	ALA	3.8
1	B	31	PRO	3.7
1	B	245	VAL	3.7
1	D	53	ALA	3.7
1	D	466	ASP	3.7
1	B	278	MET	3.7
1	A	295	SER	3.7
1	B	110	GLY	3.7
1	B	351	ARG	3.7
1	A	139	GLY	3.7
1	B	173	ALA	3.7
1	B	387	ALA	3.7
1	D	417	CYS	3.7
1	D	94	VAL	3.7
1	D	110	GLY	3.7
1	D	108	ALA	3.7
1	D	132[A]	PRO	3.7
1	A	88	LEU	3.7
1	D	102	LEU	3.7
1	D	218	GLU	3.7
1	B	91[A]	GLU	3.7
1	A	154	ASN	3.7
1	D	185	ARG	3.7
1	B	385	GLY	3.7
1	C	466	ASP	3.7
1	D	406	ALA	3.6
1	A	376	ILE	3.6
1	D	212	ILE	3.6
1	B	287	PRO	3.6
1	D	348	ALA	3.6
1	B	157	HIS	3.6
1	B	36	GLY	3.6
1	D	195	MET	3.6
1	D	301	HIS	3.6
1	D	103	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	207	GLU	3.6
1	C	155	GLY	3.6
1	B	456	VAL	3.6
1	D	41	THR	3.5
1	B	65[A]	GLN	3.5
1	C	137	LYS	3.5
1	B	403[A]	GLU	3.5
1	D	24	GLY	3.5
1	D	275	GLU	3.5
1	B	263	ARG	3.5
1	B	269	ARG	3.5
1	D	73	ILE	3.5
1	B	26	GLY	3.5
1	D	295	SER	3.5
1	B	188	ALA	3.5
1	A	83	PHE	3.5
1	B	271	ALA	3.5
1	D	177	ASP	3.5
1	D	64	LEU	3.5
1	B	201	THR	3.5
1	A	293	PHE	3.5
1	B	58	PHE	3.5
1	D	199	ALA	3.4
1	A	137	LYS	3.4
1	B	265	ARG	3.4
1	B	99	GLN	3.4
1	D	76[A]	TYR	3.4
1	D	135	TYR	3.4
1	D	23	GLY	3.4
1	A	316	LEU	3.4
1	B	474	ILE	3.4
1	B	206	VAL	3.4
1	D	285	GLY	3.4
1	B	129	GLY	3.4
1	C	293	PHE	3.4
1	D	154	ASN	3.4
1	B	406	ALA	3.4
1	B	24	GLY	3.4
1	B	100	GLY	3.4
1	D	366	SER	3.4
1	B	80	ASN	3.4
1	A	336	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	429	ARG	3.4
1	D	118	THR	3.4
1	A	276	ASP	3.4
1	A	294	ILE	3.3
1	C	317	GLN	3.3
1	C	3	PHE	3.3
1	A	298	MET	3.3
1	B	71[A]	ARG	3.3
1	B	378	GLY	3.3
1	D	397	LYS	3.3
1	C	406	ALA	3.3
1	B	18	ALA	3.3
1	B	455	THR	3.3
1	D	234[A]	GLU	3.3
1	D	42	GLY	3.3
1	D	112	GLY	3.3
1	B	393[A]	SER	3.3
1	D	472	LYS	3.3
1	D	433	GLU	3.2
1	D	201	THR	3.2
1	B	93[A]	GLU	3.2
1	B	162	GLU	3.2
1	D	329	LYS	3.2
1	A	140	SER	3.2
1	D	471	PRO	3.2
1	D	242	ARG	3.2
1	B	199	ALA	3.2
1	A	442	LYS	3.2
1	D	434	LYS	3.2
1	D	164	ILE	3.2
1	B	376	ILE	3.2
1	B	82	GLU	3.2
1	C	442	LYS	3.2
1	D	43	VAL	3.2
1	D	458	ASP	3.2
1	B	264	GLU	3.2
1	A	335	LEU	3.2
1	D	391	VAL	3.2
1	B	469	VAL	3.2
1	B	479	VAL	3.2
1	C	441	ARG	3.1
1	D	247	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	86	GLN	3.1
1	B	274	PHE	3.1
1	D	235	LYS	3.1
1	B	195	MET	3.1
1	B	358	THR	3.1
1	A	447	LEU	3.1
1	B	131	SER	3.1
1	D	194	PRO	3.1
1	B	109	GLY	3.1
1	B	408	GLY	3.1
1	C	443	LYS	3.1
1	D	96	LEU	3.1
1	B	51	ASN	3.1
1	B	90	GLY	3.1
1	B	130	GLY	3.1
1	B	460	LYS	3.1
1	D	462[A]	SER	3.1
1	B	52	ASN	3.0
1	A	40[A]	LYS	3.0
1	D	146	LYS	3.0
1	D	214	SER	3.0
1	D	111	ALA	3.0
1	D	477	GLN	3.0
1	D	72	MET	3.0
1	D	57	ASN	3.0
1	B	147	PRO	3.0
1	A	136	ASN	3.0
1	B	298	MET	3.0
1	A	419	LEU	3.0
1	A	155	GLY	3.0
1	D	1	THR	3.0
1	B	457	ASP	3.0
1	B	197	LYS	3.0
1	B	161	GLU	3.0
1	B	29	GLY	2.9
1	B	389	ASP	2.9
1	B	273	GLU	2.9
1	B	449	GLU	2.9
1	A	245	VAL	2.9
1	B	382	LYS	2.9
1	A	138	ASP	2.9
1	B	433	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	3	PHE	2.9
1	C	234	GLU	2.9
1	B	43	VAL	2.9
1	D	6	ASP	2.9
1	D	211	ASP	2.9
1	D	428	ASN	2.9
1	D	446	THR	2.9
1	B	194	PRO	2.9
1	B	353	GLY	2.9
1	A	379	LYS	2.9
1	D	403	GLU	2.9
1	D	405	SER	2.9
1	A	473	LEU	2.9
1	D	159	ILE	2.9
1	B	17	GLY	2.9
1	D	368	TYR	2.9
1	D	98	PRO	2.8
1	A	263	ARG	2.8
1	B	174	TRP	2.8
1	B	220	ILE	2.8
1	D	192	ASN	2.8
1	C	452	GLU	2.8
1	C	277	GLY	2.8
1	D	419	LEU	2.8
1	D	454	LEU	2.8
1	C	472	LYS	2.8
1	B	37	ALA	2.8
1	D	475	PRO	2.8
1	A	440	ASP	2.8
1	D	143	ILE	2.8
1	C	263	ARG	2.8
1	D	117	TYR	2.8
1	A	274	PHE	2.8
1	D	465	CYS	2.8
1	D	395	LYS	2.8
1	D	163	ALA	2.7
1	D	452	GLU	2.7
1	B	329	LYS	2.7
1	A	130	GLY	2.7
1	A	443	LYS	2.7
1	C	451	TRP	2.7
1	A	380	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	465	CYS	2.7
1	D	84	GLU	2.7
1	B	304	SER	2.7
1	D	239	ARG	2.7
1	C	453	GLY	2.7
1	B	10	ALA	2.7
1	D	158	PHE	2.7
1	D	39	LEU	2.7
1	D	178	GLN	2.7
1	D	354	HIS	2.7
1	A	235	LYS	2.7
1	A	36	GLY	2.7
1	B	95	GLU	2.7
1	B	284	ILE	2.7
1	D	409	ASN	2.7
1	B	192	ASN	2.7
1	D	101	THR	2.7
1	C	5	THR	2.7
1	B	299	THR	2.7
1	A	3	PHE	2.7
1	B	229	ARG	2.6
1	D	276	ASP	2.6
1	D	377	PRO	2.6
1	D	420	PRO	2.6
1	B	146	LYS	2.6
1	D	388	MET	2.6
1	D	99	GLN	2.6
1	B	56	ASP	2.6
1	A	234	GLU	2.6
1	D	32	GLU	2.6
1	D	116	PHE	2.6
1	A	468	ALA	2.6
1	D	346	SER	2.6
1	D	9[A]	GLU	2.6
1	D	385	GLY	2.6
1	B	410	ALA	2.6
1	C	152	GLU	2.6
1	B	45	GLU	2.6
1	A	76	TYR	2.6
1	D	75	SER	2.6
1	C	394	ALA	2.6
1	D	351	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	443	LYS	2.5
1	B	66	SER	2.5
1	C	298[A]	MET	2.5
1	C	457	ASP	2.5
1	B	54	GLY	2.5
1	D	336	PRO	2.5
1	B	209	ILE	2.5
1	A	6	ASP	2.5
1	D	414	MET	2.5
1	B	461	LYS	2.5
1	D	358	THR	2.5
1	D	370	ASP	2.5
1	C	416	LYS	2.5
1	B	397	LYS	2.5
1	C	150	VAL	2.5
1	A	78	GLY	2.5
1	B	354	HIS	2.5
1	B	336	PRO	2.5
1	D	364	GLN	2.5
1	A	146	LYS	2.5
1	D	444	GLY	2.4
1	B	283	GLY	2.4
1	C	138	ASP	2.4
1	D	424	LYS	2.4
1	D	115	ALA	2.4
1	D	47	THR	2.4
1	D	79	GLU	2.4
1	D	392	SER	2.4
1	A	77	VAL	2.4
1	D	50	SER	2.4
1	A	467	PHE	2.4
1	B	3	PHE	2.4
1	B	84	GLU	2.4
1	A	17	GLY	2.4
1	D	297	ASN	2.4
1	D	375[A]	MET	2.4
1	B	342	SER	2.4
1	D	317	GLN	2.4
1	C	264	GLU	2.4
1	A	142	ALA	2.4
1	B	289	LEU	2.4
1	D	442	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	425	GLN	2.3
1	B	311	LEU	2.3
1	A	377	PRO	2.3
1	D	157[A]	HIS	2.3
1	D	263	ARG	2.3
1	B	107	ARG	2.3
1	A	81	ALA	2.3
1	A	79	GLU	2.3
1	D	384	MET	2.3
1	D	86	GLN	2.3
1	D	51	ASN	2.3
1	D	80	ASN	2.3
1	D	197	LYS	2.3
1	D	238	LYS	2.3
1	B	356	ASN	2.3
1	D	131[A]	SER	2.3
1	B	152	GLU	2.3
1	A	277	GLY	2.3
1	D	19	THR	2.3
1	D	352	GLY	2.3
1	B	277	GLY	2.3
1	C	410	ALA	2.3
1	B	7	ALA	2.3
1	D	438	ASP	2.3
1	C	318	ASN	2.3
1	D	91	GLU	2.3
1	B	305[A]	GLU	2.3
1	B	478	GLN	2.3
1	A	285	GLY	2.3
1	C	209	ILE	2.2
1	A	91	GLU	2.2
1	C	275	GLU	2.2
1	B	154	ASN	2.2
1	C	245	VAL	2.2
1	B	231	VAL	2.2
1	C	475	PRO	2.2
1	D	78	GLY	2.2
1	A	89	ALA	2.2
1	D	144	ALA	2.2
1	A	411	HIS	2.2
1	D	52	ASN	2.2
1	D	356	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	68	GLN	2.2
1	B	104	GLU	2.2
1	D	36	GLY	2.2
1	D	166	GLY	2.2
1	B	15	PRO	2.2
1	B	306	ASN	2.2
1	A	246	ARG	2.2
1	B	187	SER	2.2
1	C	157	HIS	2.2
1	B	293	PHE	2.2
1	D	213	GLY	2.2
1	B	132	PRO	2.2
1	D	330	GLU	2.2
1	D	394	ALA	2.2
1	B	322	ALA	2.2
1	B	190	ASN	2.1
1	D	386	GLY	2.1
1	B	42	GLY	2.1
1	A	152	GLU	2.1
1	C	146	LYS	2.1
1	C	368	TYR	2.1
1	A	445	LEU	2.1
1	D	114	PRO	2.1
1	A	318	ASN	2.1
1	B	57	ASN	2.1
1	B	67	LYS	2.1
1	C	479	VAL	2.1
1	A	214	SER	2.1
1	D	120	THR	2.1
1	D	470	SER	2.1
1	D	107	ARG	2.1
1	D	130[A]	GLY	2.1
1	B	4	TYR	2.1
1	A	272	LEU	2.1
1	A	474	ILE	2.1
1	C	417	CYS	2.1
1	B	16	ASN	2.1
1	D	457	ASP	2.1
1	C	276	ASP	2.1
1	B	407	LYS	2.1
1	B	326	ASN	2.1
1	A	439	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	12	LYS	2.0
1	D	90	GLY	2.0
1	B	314	TYR	2.0
1	B	137	LYS	2.0
1	B	300	VAL	2.0
1	D	305	GLU	2.0

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

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

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	GOL	C	5000	6/6	0.21	4.63	20,21,23,24	0
3	GOL	C	5001	6/6	0.23	2.20	25,28,29,30	0
2	CL	A	6000	1/1	0.11	0.23	19,19,19,19	1
2	CL	D	6001	1/1	0.14	-2.23	15,15,15,15	1

6.5 Other polymers ⓘ

There are no such residues in this entry.