



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:08 PM UTC

PDB ID : 7W5U / pdb_00007w5u
Title : Acetyl-CoA Carboxylase-AccB
Authors : Ali, I.; Zheng, J.
Deposited on : 2021-11-30
Resolution : 2.34 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

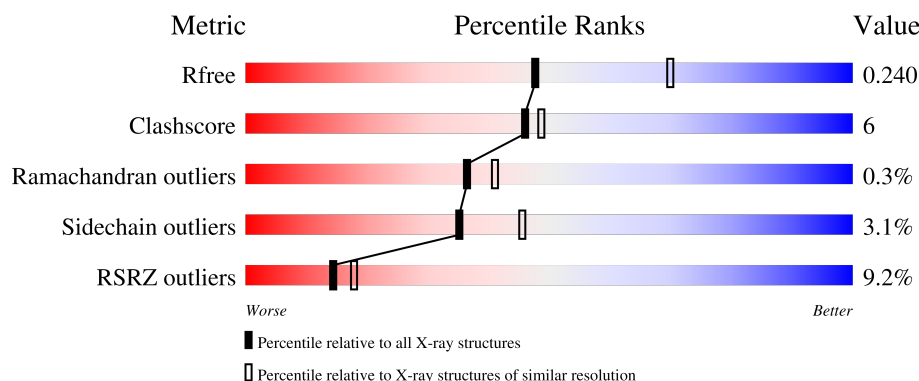
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	514	7% 89% 10%
1	B	514	9% 87% 11%
1	C	514	11% 85% 13%
1	D	514	8% 87% 12%
1	E	514	10% 87% 11%

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Mol	Chain	Length	Quality of chain
1	F	514	11% 85% 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23603 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 Acetyl-CoA carboxylase complex, beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3905	2440	708	739	18			
1	B	513	Total	C	N	O	S	0	0	0
			3905	2440	708	739	18			
1	C	513	Total	C	N	O	S	0	0	0
			3907	2442	709	738	18			
1	D	513	Total	C	N	O	S	0	0	0
			3911	2444	709	740	18			
1	E	513	Total	C	N	O	S	0	0	0
			3911	2444	709	740	18			
1	F	513	Total	C	N	O	S	0	0	0
			3911	2444	709	740	18			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

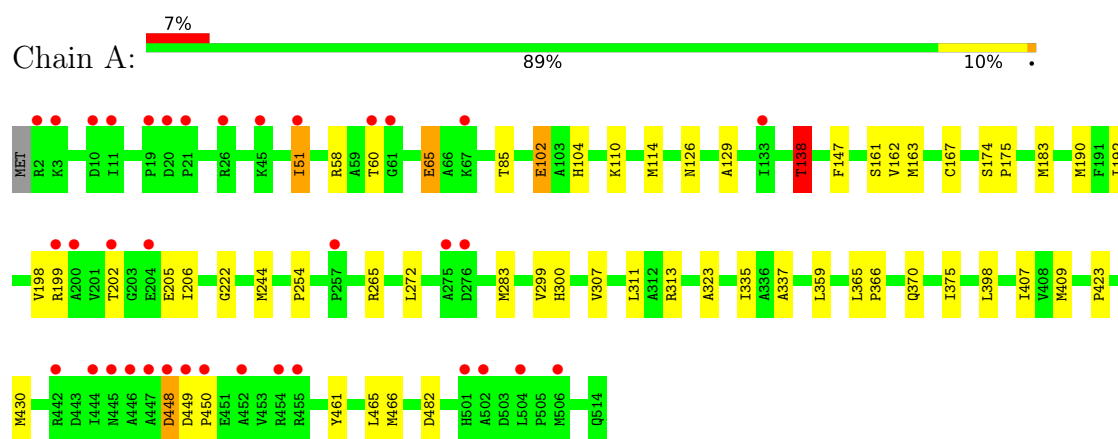
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	17	Total 17	O 17	0	0
4	C	11	Total 11	O 11	0	0
4	D	19	Total 19	O 19	0	0
4	E	13	Total 13	O 13	0	0
4	F	18	Total 18	O 18	0	0

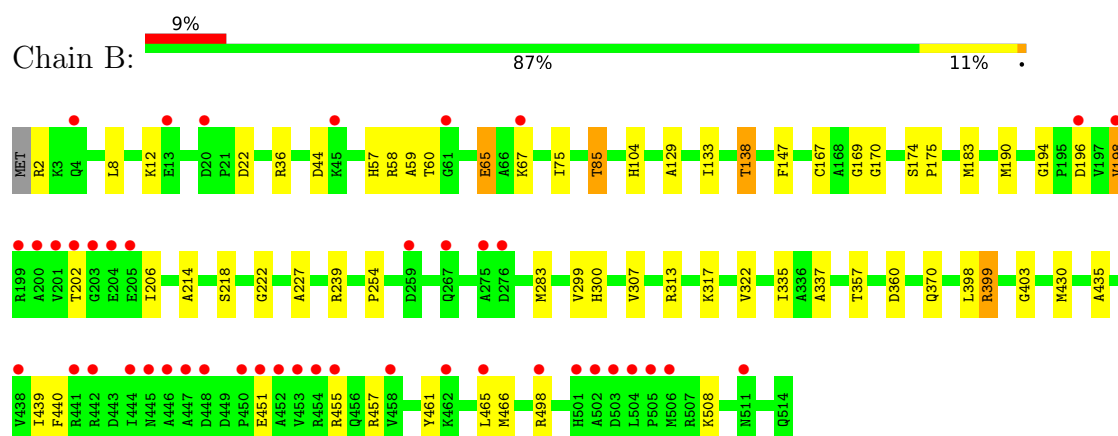
3 Residue-property plots [i](#)

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

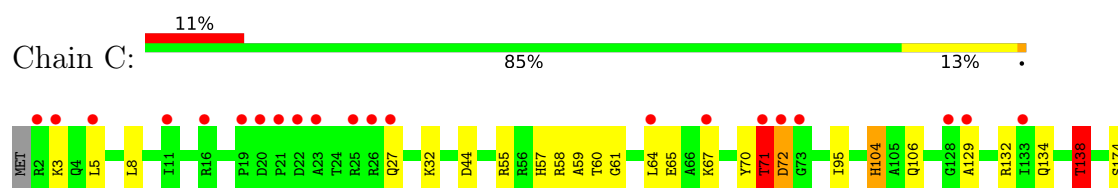
- Molecule 1: Acetyl-CoA carboxylase complex, beta-chain

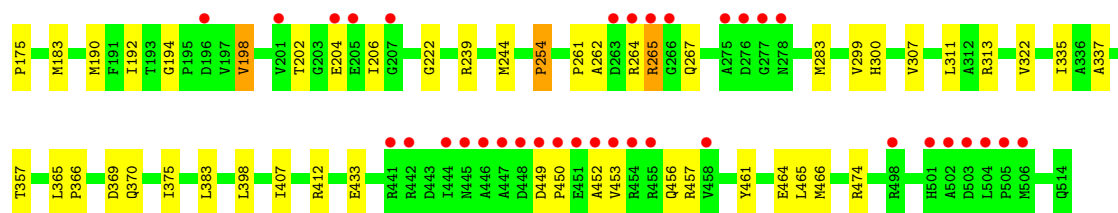


- Molecule 1: Acetyl-CoA carboxylase complex, beta-chain

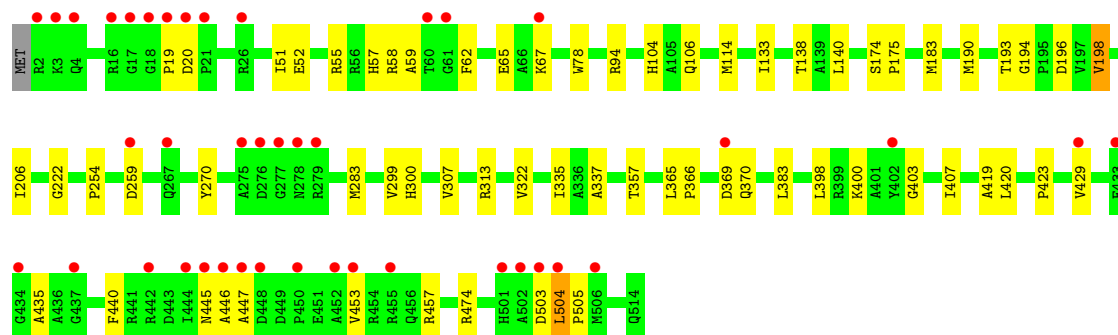
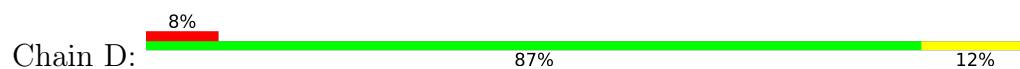


- Molecule 1: Acetyl-CoA carboxylase complex, beta-chain

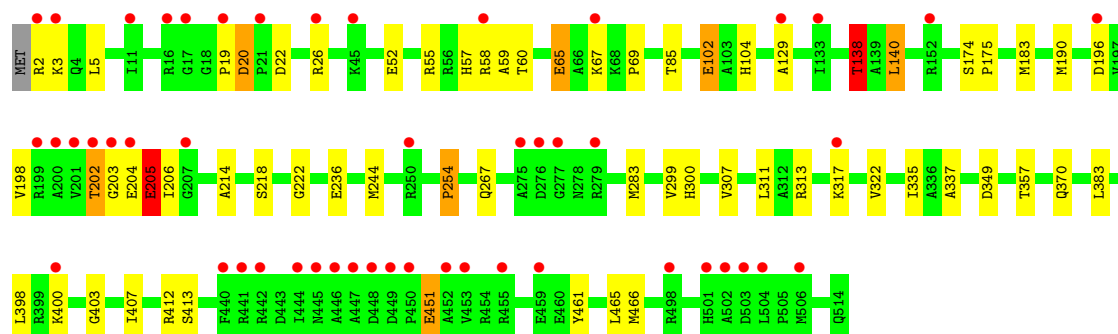
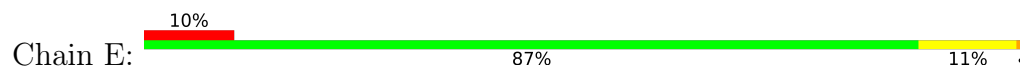




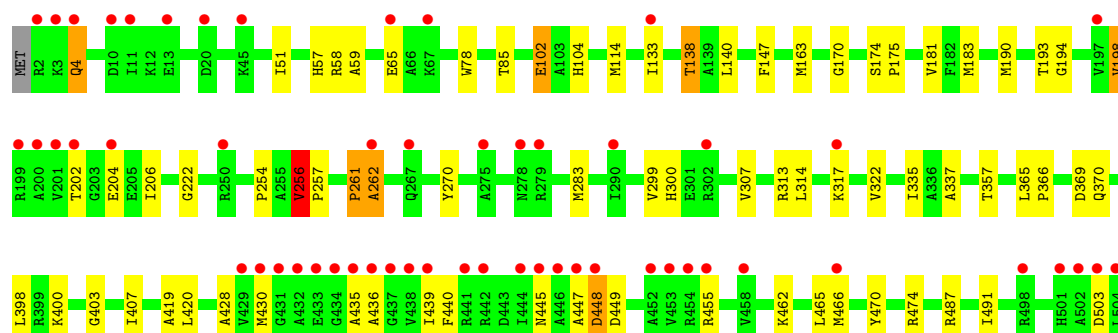
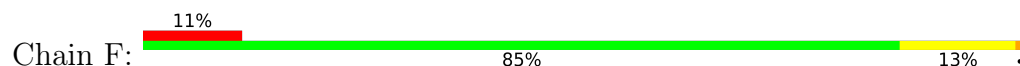
• Molecule 1: Acetyl-CoA carboxylase complex, beta-chain



• Molecule 1: Acetyl-CoA carboxylase complex, beta-chain



• Molecule 1: Acetyl-CoA carboxylase complex, beta-chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.00Å 202.39Å 204.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 2.34 39.74 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.74-2.34) 99.1 (39.74-2.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.217 , 0.239 0.221 , 0.240	Depositor DCC
R_{free} test set	10132 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23603	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/3980	1.42	5/5396 (0.1%)
1	B	1.02	0/3980	1.41	5/5396 (0.1%)
1	C	1.03	2/3982 (0.1%)	1.43	9/5399 (0.2%)
1	D	1.03	0/3986	1.41	3/5404 (0.1%)
1	E	1.02	1/3986 (0.0%)	1.42	7/5404 (0.1%)
1	F	1.05	0/3986	1.42	10/5404 (0.2%)
All	All	1.03	3/23900 (0.0%)	1.42	39/32403 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	PRO	C-O	-5.29	1.17	1.23
1	C	261	PRO	C-O	-5.27	1.17	1.23
1	E	254	PRO	C-O	-5.10	1.18	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	20	ASP	CB-CA-C	7.30	118.17	109.85
1	C	262	ALA	CA-C-N	7.12	132.90	120.87
1	C	262	ALA	C-N-CA	7.12	132.90	120.87
1	A	65	GLU	CB-CG-CD	6.91	124.35	112.60
1	E	104	HIS	CA-CB-CG	6.54	120.34	113.80
1	E	20	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	104	HIS	CA-CB-CG	6.28	120.08	113.80
1	B	104	HIS	CA-CB-CG	6.23	120.03	113.80
1	A	104	HIS	CA-CB-CG	6.08	119.88	113.80
1	F	261	PRO	N-CA-C	6.08	122.62	113.81
1	C	453	VAL	N-CA-C	-5.99	104.67	110.72
1	C	129	ALA	CA-C-O	-5.87	114.01	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	22	ASP	N-CA-C	-5.70	106.32	113.28
1	F	104	HIS	CA-CB-CG	5.68	119.48	113.80
1	D	104	HIS	CA-CB-CG	5.58	119.38	113.80
1	C	265	ARG	CA-C-O	-5.56	113.35	119.08
1	F	445	ASN	CA-C-N	5.54	128.25	120.28
1	F	445	ASN	C-N-CA	5.54	128.25	120.28
1	E	138	THR	CA-CB-OG1	-5.39	101.52	109.60
1	F	448	ASP	N-CA-C	-5.37	104.04	111.28
1	C	204	GLU	CB-CA-C	5.35	118.56	109.53
1	C	433	GLU	CB-CG-CD	5.25	121.52	112.60
1	F	470	TYR	CA-C-O	-5.22	115.33	120.82
1	F	403	GLY	CA-C-N	5.20	125.85	120.03
1	F	403	GLY	C-N-CA	5.20	125.85	120.03
1	A	138	THR	CA-CB-OG1	-5.15	101.87	109.60
1	B	85	THR	CB-CA-C	5.13	118.43	109.65
1	A	430	MET	CA-C-N	5.12	124.96	120.10
1	A	430	MET	C-N-CA	5.12	124.96	120.10
1	D	403	GLY	CA-C-N	5.12	125.76	120.03
1	D	403	GLY	C-N-CA	5.12	125.76	120.03
1	C	138	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	22	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	430	MET	CA-C-N	5.05	124.89	120.10
1	B	430	MET	C-N-CA	5.05	124.89	120.10
1	F	447	ALA	CB-CA-C	-5.04	110.78	116.63
1	F	256	VAL	N-CA-CB	-5.02	108.36	111.83
1	E	403	GLY	CA-C-N	5.00	125.64	120.03
1	E	403	GLY	C-N-CA	5.00	125.64	120.03

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	3905	0	3854	45	0
1	B	3905	0	3854	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3907	0	3863	64	0
1	D	3911	0	3867	44	0
1	E	3911	0	3867	52	0
1	F	3911	0	3867	55	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	D	10	0	0	0	0
3	B	6	0	8	3	0
3	C	6	0	8	2	0
3	E	6	0	8	3	0
3	F	6	0	8	1	0
4	A	21	0	0	1	0
4	B	17	0	0	0	0
4	C	11	0	0	0	0
4	D	19	0	0	1	0
4	E	13	0	0	0	0
4	F	18	0	0	0	0
All	All	23603	0	23204	273	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:TYR:O	1:C:71:THR:HB	1.43	1.13
1:C:72:ASP:OD2	1:C:104:HIS:HB2	1.50	1.10
1:C:27:GLN:HE22	1:C:32:LYS:HE2	1.26	0.97
1:E:204:GLU:O	1:E:205:GLU:HB2	1.63	0.96
1:F:51:ILE:CD1	1:F:114:MET:HE1	2.05	0.87
1:F:439:ILE:HG23	1:F:440:PHE:CD2	2.10	0.87
1:B:307:VAL:CG2	1:B:337:ALA:HB1	2.05	0.86
1:E:307:VAL:CG2	1:E:337:ALA:HB1	2.06	0.86
1:F:307:VAL:CG2	1:F:337:ALA:HB1	2.05	0.86
1:A:307:VAL:CG2	1:A:337:ALA:HB1	2.06	0.85
1:F:51:ILE:HD13	1:F:114:MET:HE1	1.57	0.85
1:D:307:VAL:CG2	1:D:337:ALA:HB1	2.06	0.85
1:C:307:VAL:CG2	1:C:337:ALA:HB1	2.06	0.84
1:C:72:ASP:OD2	1:C:104:HIS:CB	2.26	0.82
1:E:202:THR:HG23	1:E:204:GLU:N	1.95	0.82
1:C:70:TYR:O	1:C:71:THR:CB	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:THR:CG2	1:E:204:GLU:H	1.96	0.79
1:A:162:VAL:C	1:A:163:MET:HE2	2.09	0.78
1:A:51:ILE:HD11	1:A:110:LYS:HD3	1.67	0.77
1:C:198:VAL:O	1:C:202:THR:HG22	1.86	0.76
1:B:198:VAL:O	1:B:202:THR:HG22	1.86	0.76
1:E:412:ARG:HE	3:E:601:GOL:H32	1.51	0.75
1:F:198:VAL:O	1:F:202:THR:HG22	1.86	0.75
1:A:254:PRO:O	1:A:313:ARG:NH2	2.20	0.74
1:E:204:GLU:O	1:E:205:GLU:CB	2.35	0.74
1:A:198:VAL:O	1:A:202:THR:HG22	1.87	0.74
1:F:307:VAL:HG21	1:F:337:ALA:HB1	1.70	0.73
1:E:307:VAL:HG21	1:E:337:ALA:HB1	1.70	0.73
1:C:335:ILE:H	1:C:370:GLN:HE22	1.37	0.73
1:B:307:VAL:HG21	1:B:337:ALA:HB1	1.70	0.73
1:A:335:ILE:H	1:A:370:GLN:HE22	1.37	0.73
1:C:412:ARG:HE	3:C:601:GOL:H2	1.53	0.73
1:D:335:ILE:H	1:D:370:GLN:HE22	1.37	0.73
1:F:335:ILE:H	1:F:370:GLN:HE22	1.37	0.73
1:A:265:ARG:NH1	1:A:482:ASP:OD2	2.23	0.72
1:E:335:ILE:H	1:E:370:GLN:HE22	1.36	0.72
1:B:335:ILE:H	1:B:370:GLN:HE22	1.36	0.71
1:A:307:VAL:HG21	1:A:337:ALA:HB1	1.71	0.71
1:C:72:ASP:CG	1:C:104:HIS:HB2	2.14	0.71
1:B:218:SER:OG	1:B:227:ALA:HB2	1.91	0.71
1:C:307:VAL:HG21	1:C:337:ALA:HB1	1.70	0.71
1:D:307:VAL:HG21	1:D:337:ALA:HB1	1.71	0.70
1:A:102:GLU:OE1	1:A:138:THR:HG23	1.90	0.70
1:C:138:THR:HG21	1:F:58:ARG:HH22	1.56	0.70
1:C:307:VAL:HG23	1:C:337:ALA:HB1	1.74	0.70
1:C:72:ASP:O	1:C:95:ILE:HD13	1.92	0.69
1:D:307:VAL:HG23	1:D:337:ALA:HB1	1.72	0.69
1:A:307:VAL:HG23	1:A:337:ALA:HB1	1.74	0.69
1:E:307:VAL:HG23	1:E:337:ALA:HB1	1.73	0.69
1:E:202:THR:CG2	1:E:204:GLU:N	2.55	0.69
1:B:360:ASP:OD2	1:B:399:ARG:HD3	1.91	0.69
1:B:307:VAL:HG23	1:B:337:ALA:HB1	1.72	0.68
1:D:58:ARG:HH22	1:E:138:THR:HG21	1.57	0.68
1:F:307:VAL:HG23	1:F:337:ALA:HB1	1.73	0.68
1:E:19:PRO:HG3	1:E:69:PRO:HB3	1.73	0.68
1:C:72:ASP:OD1	1:C:132:ARG:NH2	2.23	0.68
1:E:198:VAL:O	1:E:202:THR:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLU:OE1	1:E:138:THR:HG23	1.95	0.67
1:C:71:THR:HG22	1:C:72:ASP:O	1.95	0.66
1:C:456:GLN:NE2	1:C:457:ARG:HH21	1.94	0.65
1:A:126:ASN:OD1	1:A:163:MET:HE1	1.97	0.65
1:F:102:GLU:OE1	1:F:138:THR:HG23	1.97	0.65
1:F:314:LEU:HB3	1:F:491:ILE:CD1	2.26	0.65
1:D:133:ILE:HG13	1:F:435:ALA:HB2	1.78	0.64
1:B:44:ASP:OD1	1:B:239:ARG:NH1	2.30	0.64
1:A:58:ARG:HH22	1:B:138:THR:HG21	1.62	0.64
1:F:439:ILE:CG2	1:F:440:PHE:CD2	2.81	0.64
1:E:451:GLU:HA	1:E:451:GLU:OE1	1.98	0.64
1:C:27:GLN:NE2	1:C:32:LYS:HE2	2.05	0.64
1:A:192:ILE:HD12	1:C:375:ILE:HG23	1.81	0.63
1:D:51:ILE:HD11	1:D:78:TRP:HZ3	1.63	0.63
1:E:461:TYR:CE2	1:E:465:LEU:HD12	2.33	0.63
1:F:261:PRO:O	1:F:262:ALA:HB3	1.99	0.63
1:A:449:ASP:N	1:A:450:PRO:HD3	2.13	0.63
1:D:140:LEU:HG	1:F:407:ILE:HD11	1.79	0.63
1:C:61:GLY:O	1:C:64:LEU:HD13	1.99	0.63
1:D:19:PRO:HG2	1:D:94:ARG:HB3	1.80	0.63
1:B:461:TYR:CE2	1:B:465:LEU:HD12	2.35	0.62
1:F:254:PRO:O	1:F:313:ARG:NH2	2.33	0.61
1:A:461:TYR:CE2	1:A:465:LEU:HD12	2.35	0.61
1:C:72:ASP:OD2	1:C:104:HIS:N	2.32	0.61
1:F:163:MET:CE	1:F:181:VAL:HG13	2.30	0.61
1:C:44:ASP:OD1	1:C:239:ARG:NH2	2.33	0.61
1:E:254:PRO:O	1:E:313:ARG:NH2	2.34	0.61
1:B:254:PRO:O	1:B:313:ARG:NH2	2.33	0.61
1:C:254:PRO:O	1:C:313:ARG:NH2	2.34	0.61
1:D:254:PRO:O	1:D:313:ARG:NH2	2.34	0.61
1:E:461:TYR:CE1	1:E:466:MET:HE3	2.35	0.60
1:F:51:ILE:HD11	1:F:78:TRP:HZ3	1.65	0.60
1:E:60:THR:O	1:E:65:GLU:OE1	2.21	0.58
1:C:27:GLN:NE2	1:C:32:LYS:HB3	2.18	0.58
1:C:58:ARG:HD3	1:D:474:ARG:CD	2.33	0.58
1:C:449:ASP:N	1:C:450:PRO:HD3	2.18	0.58
1:A:60:THR:O	1:A:65:GLU:OE2	2.21	0.58
1:A:375:ILE:HG23	1:C:192:ILE:HD12	1.85	0.57
1:B:435:ALA:O	1:B:439:ILE:HG13	2.04	0.57
1:B:461:TYR:CE1	1:B:466:MET:HE3	2.38	0.57
1:A:449:ASP:N	1:A:450:PRO:CD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:MET:HE3	1:F:181:VAL:HG13	1.86	0.57
1:C:60:THR:O	1:C:65:GLU:OE1	2.22	0.57
1:D:222:GLY:O	1:D:300:HIS:HE1	1.87	0.57
1:D:140:LEU:HG	1:F:407:ILE:CD1	2.34	0.57
1:D:407:ILE:HD11	1:F:140:LEU:HG	1.87	0.57
1:F:420:LEU:N	1:F:420:LEU:HD22	2.20	0.57
1:B:183:MET:SD	1:B:190:MET:HE2	2.44	0.56
1:E:202:THR:HG22	1:E:204:GLU:H	1.68	0.56
1:D:440:PHE:CD2	1:D:457:ARG:HB3	2.41	0.56
1:C:412:ARG:HB3	3:C:601:GOL:H31	1.88	0.56
1:B:60:THR:O	1:B:65:GLU:OE1	2.23	0.56
1:C:57:HIS:HD2	1:C:59:ALA:H	1.53	0.55
1:A:222:GLY:O	1:A:300:HIS:HE1	1.89	0.55
1:C:174:SER:HB3	1:C:175:PRO:HD3	1.88	0.55
1:D:420:LEU:N	1:D:420:LEU:HD22	2.21	0.55
1:B:58:ARG:HD3	1:C:474:ARG:HG2	1.88	0.55
1:C:194:GLY:O	1:C:198:VAL:HG13	2.06	0.55
1:B:8:LEU:HD11	1:B:12:LYS:HE2	1.88	0.55
1:D:194:GLY:O	1:D:198:VAL:HG13	2.06	0.55
1:C:222:GLY:O	1:C:300:HIS:HE1	1.90	0.55
1:B:57:HIS:HD2	1:B:59:ALA:H	1.54	0.55
1:E:222:GLY:O	1:E:300:HIS:HE1	1.90	0.55
1:F:194:GLY:O	1:F:198:VAL:HG13	2.08	0.55
1:F:436:ALA:HA	1:F:439:ILE:HG22	1.88	0.55
1:A:174:SER:HB3	1:A:175:PRO:HD3	1.88	0.54
1:A:183:MET:SD	1:A:190:MET:HE2	2.47	0.54
1:D:183:MET:SD	1:D:190:MET:HE2	2.47	0.54
1:E:202:THR:HG21	1:E:204:GLU:CB	2.38	0.54
1:B:194:GLY:O	1:B:198:VAL:HG13	2.07	0.54
1:F:174:SER:HB3	1:F:175:PRO:HD3	1.89	0.54
1:E:202:THR:CG2	1:E:204:GLU:CB	2.85	0.54
1:F:222:GLY:O	1:F:300:HIS:HE1	1.89	0.54
1:F:256:VAL:HG13	1:F:257:PRO:O	2.07	0.54
1:B:222:GLY:O	1:B:300:HIS:HE1	1.89	0.54
1:E:183:MET:SD	1:E:190:MET:HE2	2.48	0.54
1:C:461:TYR:CE1	1:C:466:MET:HE3	2.43	0.54
1:B:174:SER:HB3	1:B:175:PRO:HD3	1.90	0.53
1:E:57:HIS:HD2	1:E:59:ALA:H	1.56	0.53
1:B:169:GLY:HA3	3:B:603:GOL:H12	1.89	0.53
1:C:138:THR:HG21	1:F:58:ARG:NH2	2.23	0.53
1:E:174:SER:HB3	1:E:175:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE2	1:A:163:MET:N	2.24	0.53
1:D:57:HIS:HD2	1:D:59:ALA:H	1.56	0.53
1:A:300:HIS:HD2	4:A:716:HOH:O	1.91	0.53
1:A:461:TYR:CE1	1:A:466:MET:HE3	2.44	0.53
1:C:55:ARG:HH12	1:C:106:GLN:NE2	2.07	0.53
1:D:55:ARG:HH12	1:D:106:GLN:NE2	2.06	0.53
1:C:183:MET:SD	1:C:190:MET:HE2	2.49	0.53
1:D:407:ILE:CD1	1:F:140:LEU:HG	2.39	0.53
1:D:174:SER:HB3	1:D:175:PRO:HD3	1.89	0.53
1:F:57:HIS:HD2	1:F:59:ALA:H	1.57	0.52
1:B:307:VAL:HG23	1:B:337:ALA:CB	2.39	0.52
1:D:365:LEU:HD13	1:D:366:PRO:O	2.10	0.52
1:C:456:GLN:NE2	1:C:457:ARG:NH2	2.58	0.52
1:A:448:ASP:N	1:A:448:ASP:OD1	2.42	0.52
1:F:428:ALA:HB1	1:F:466:MET:HE2	1.92	0.52
1:F:261:PRO:O	1:F:262:ALA:CB	2.57	0.51
1:A:58:ARG:NH2	1:B:138:THR:HG21	2.24	0.51
1:E:307:VAL:HG23	1:E:337:ALA:CB	2.40	0.51
1:A:51:ILE:HD13	1:A:114:MET:HE1	1.92	0.51
1:C:64:LEU:HD11	1:C:134:GLN:CB	2.41	0.51
1:B:214:ALA:O	1:B:218:SER:HB2	2.11	0.51
1:E:202:THR:CG2	1:E:203:GLY:N	2.73	0.51
1:F:365:LEU:HD13	1:F:366:PRO:O	2.11	0.50
1:A:161:SER:HB3	1:A:163:MET:HE3	1.93	0.50
1:A:161:SER:HB3	1:A:163:MET:CE	2.41	0.50
1:F:51:ILE:HD11	1:F:78:TRP:CZ3	2.45	0.50
1:A:461:TYR:CD1	1:A:466:MET:HE3	2.47	0.50
1:E:202:THR:CG2	1:E:204:GLU:HB2	2.42	0.49
1:A:129:ALA:HB2	1:A:167:CYS:HA	1.93	0.49
1:A:307:VAL:HG23	1:A:337:ALA:CB	2.41	0.49
1:B:461:TYR:CD1	1:B:466:MET:HE3	2.47	0.49
1:D:51:ILE:HG13	1:D:114:MET:HE1	1.93	0.49
1:A:147:PHE:CG	1:C:383:LEU:HD21	2.48	0.48
1:C:264:ARG:HH11	1:C:267:GLN:NE2	2.10	0.48
1:E:202:THR:HG21	1:E:204:GLU:HB3	1.94	0.48
1:B:508:LYS:CE	1:E:349:ASP:O	2.61	0.48
1:C:307:VAL:HG23	1:C:337:ALA:CB	2.41	0.48
1:E:461:TYR:CD1	1:E:466:MET:HE3	2.48	0.48
1:B:129:ALA:HB2	1:B:167:CYS:HA	1.96	0.48
1:E:214:ALA:O	1:E:218:SER:HB3	2.14	0.48
1:C:72:ASP:O	1:C:95:ILE:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:THR:HG23	1:F:204:GLU:H	1.79	0.47
1:D:307:VAL:HG23	1:D:337:ALA:CB	2.40	0.47
1:F:307:VAL:HG23	1:F:337:ALA:CB	2.41	0.47
1:C:64:LEU:HD11	1:C:134:GLN:HB3	1.97	0.47
1:E:58:ARG:HD3	1:F:474:ARG:HD3	1.96	0.47
1:A:129:ALA:CB	1:A:167:CYS:HA	2.43	0.47
1:B:169:GLY:CA	3:B:603:GOL:H12	2.43	0.47
1:C:264:ARG:HH11	1:C:267:GLN:HE21	1.62	0.47
1:C:464:GLU:C	1:C:465:LEU:HD22	2.40	0.47
1:B:317:LYS:HD3	1:B:498:ARG:NH2	2.30	0.47
1:C:244:MET:HE3	1:C:311:LEU:HB3	1.97	0.46
1:D:20:ASP:N	4:D:702:HOH:O	2.47	0.46
1:B:283:MET:HE1	1:B:398:LEU:HD22	1.98	0.46
1:F:4:GLN:H	1:F:4:GLN:HE21	1.64	0.46
1:A:244:MET:HE3	1:A:311:LEU:HB3	1.98	0.46
1:B:451:GLU:HA	1:B:451:GLU:OE1	2.14	0.46
1:C:55:ARG:HH12	1:C:106:GLN:HE21	1.63	0.46
1:A:51:ILE:HD13	1:A:114:MET:CE	2.45	0.46
1:D:365:LEU:HD12	1:D:370:GLN:HG3	1.98	0.46
1:F:283:MET:HE1	1:F:398:LEU:HD22	1.98	0.46
1:A:51:ILE:HD11	1:A:110:LYS:CD	2.40	0.46
1:F:183:MET:SD	1:F:190:MET:HE2	2.56	0.46
1:B:129:ALA:CB	1:B:167:CYS:HA	2.46	0.45
1:C:283:MET:HE1	1:C:398:LEU:HD22	1.97	0.45
1:C:27:GLN:NE2	1:C:32:LYS:CB	2.78	0.45
1:E:198:VAL:O	1:E:202:THR:N	2.49	0.45
1:C:72:ASP:O	1:C:95:ILE:CD1	2.63	0.45
1:C:5:LEU:HD11	1:D:270:TYR:CE1	2.52	0.45
1:A:199:ARG:NE	1:A:205:GLU:OE1	2.50	0.45
1:A:423:PRO:HB2	1:F:4:GLN:HB3	1.99	0.45
1:B:57:HIS:CD2	1:B:59:ALA:H	2.35	0.45
1:C:461:TYR:CD1	1:C:466:MET:HE3	2.51	0.44
1:E:283:MET:HE1	1:E:398:LEU:HD22	1.99	0.44
1:C:58:ARG:HH12	1:F:138:THR:HG21	1.81	0.44
1:F:430:MET:HE1	1:F:462:LYS:NZ	2.33	0.44
1:B:170:GLY:H	3:B:603:GOL:C1	2.30	0.44
1:D:62:PHE:HB3	1:F:439:ILE:HD11	2.00	0.44
1:F:487:ARG:O	1:F:491:ILE:HG12	2.17	0.44
1:E:57:HIS:HE1	1:E:67:LYS:O	2.01	0.44
1:B:57:HIS:HE1	1:B:67:LYS:O	2.02	0.43
1:C:72:ASP:OD2	1:C:104:HIS:CA	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:HIS:HE1	1:C:67:LYS:O	2.02	0.43
1:D:65:GLU:H	1:D:65:GLU:HG3	1.56	0.43
1:B:147:PHE:CG	1:E:383:LEU:HD21	2.52	0.43
1:C:449:ASP:N	1:C:450:PRO:CD	2.81	0.43
1:E:52:GLU:OE1	1:E:55:ARG:HD3	2.17	0.43
1:F:57:HIS:CD2	1:F:59:ALA:H	2.37	0.43
1:A:283:MET:HE1	1:A:398:LEU:HD22	2.01	0.43
1:E:198:VAL:O	1:E:202:THR:CG2	2.63	0.43
1:E:412:ARG:NE	3:E:601:GOL:H32	2.27	0.43
1:D:383:LEU:HD21	1:F:147:PHE:CG	2.53	0.43
1:E:244:MET:HE3	1:E:311:LEU:HB3	2.00	0.43
1:E:5:LEU:HD11	1:F:270:TYR:CE1	2.54	0.42
1:B:403:GLY:HA2	1:E:140:LEU:HD11	2.01	0.42
1:B:440:PHE:CE2	1:B:457:ARG:HG3	2.54	0.42
1:C:58:ARG:HD3	1:D:474:ARG:NE	2.35	0.42
1:D:419:ALA:C	1:D:420:LEU:HD22	2.45	0.42
1:D:504:LEU:HD12	1:D:505:PRO:HD3	2.01	0.42
1:E:461:TYR:HE1	1:E:466:MET:HE3	1.81	0.42
1:F:365:LEU:HD12	1:F:370:GLN:HG3	2.01	0.42
1:D:445:ASN:C	1:D:445:ASN:HD22	2.27	0.42
1:A:198:VAL:HG13	1:A:202:THR:CG2	2.50	0.42
1:D:58:ARG:NH2	1:E:138:THR:HG21	2.29	0.41
1:D:453:VAL:O	1:D:457:ARG:HG2	2.20	0.41
1:E:413:SER:HA	3:E:601:GOL:O1	2.20	0.41
1:F:322:VAL:O	1:F:357:THR:HA	2.20	0.41
1:F:419:ALA:C	1:F:420:LEU:HD22	2.45	0.41
1:B:322:VAL:O	1:B:357:THR:HA	2.20	0.41
1:D:283:MET:HE1	1:D:398:LEU:HD22	2.01	0.41
1:E:57:HIS:CD2	1:E:59:ALA:H	2.37	0.41
1:A:102:GLU:CD	1:A:138:THR:HG23	2.45	0.41
1:F:170:GLY:H	3:F:701:GOL:H11	1.84	0.41
1:A:359:LEU:HD21	1:A:409:MET:HB2	2.02	0.41
1:E:102:GLU:CD	1:E:138:THR:HG23	2.45	0.41
1:E:202:THR:HG23	1:E:204:GLU:HB2	2.01	0.41
1:C:27:GLN:OE1	1:C:27:GLN:HA	2.21	0.41
1:C:265:ARG:HH11	1:C:265:ARG:HB3	1.86	0.41
1:C:365:LEU:HA	1:C:366:PRO:HD3	1.93	0.41
1:D:57:HIS:CD2	1:D:59:ALA:H	2.37	0.41
1:D:52:GLU:OE1	1:D:55:ARG:HD3	2.21	0.41
1:D:57:HIS:HE1	1:D:67:LYS:O	2.03	0.41
1:A:365:LEU:HA	1:A:366:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HD22	1:D:423:PRO:HG3	2.02	0.40
1:C:322:VAL:O	1:C:357:THR:HA	2.22	0.40
1:D:435:ALA:HB1	1:F:133:ILE:CG2	2.52	0.40
1:F:428:ALA:HB1	1:F:466:MET:CE	2.51	0.40
1:A:283:MET:HG2	1:A:323:ALA:HB1	2.02	0.40
1:E:2:ARG:HG3	1:E:3:LYS:H	1.87	0.40
1:F:335:ILE:N	1:F:370:GLN:HE22	2.13	0.40
1:D:322:VAL:O	1:D:357:THR:HA	2.21	0.40
1:E:322:VAL:O	1:E:357:THR:HA	2.22	0.40
1:B:36:ARG:HG3	1:B:75:ILE:HD13	2.03	0.40
1:B:440:PHE:CD2	1:B:457:ARG:HG3	2.56	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	511/514 (99%)	493 (96%)	18 (4%)	0	100	100
1	B	511/514 (99%)	496 (97%)	15 (3%)	0	100	100
1	C	511/514 (99%)	497 (97%)	11 (2%)	3 (1%)	21	22
1	D	511/514 (99%)	492 (96%)	17 (3%)	2 (0%)	30	32
1	E	511/514 (99%)	490 (96%)	19 (4%)	2 (0%)	30	32
1	F	511/514 (99%)	493 (96%)	16 (3%)	2 (0%)	30	32
All	All	3066/3084 (99%)	2961 (97%)	96 (3%)	9 (0%)	36	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	129	ALA

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Mol	Chain	Res	Type
1	E	205	GLU
1	C	72	ASP
1	C	452	ALA
1	F	262	ALA
1	D	447	ALA
1	C	71	THR
1	D	446	ALA
1	F	449	ASP

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	399/402 (99%)	390 (98%)	9 (2%)	44	56
1	B	399/402 (99%)	388 (97%)	11 (3%)	38	50
1	C	400/402 (100%)	392 (98%)	8 (2%)	48	61
1	D	401/402 (100%)	389 (97%)	12 (3%)	36	47
1	E	401/402 (100%)	383 (96%)	18 (4%)	24	32
1	F	401/402 (100%)	384 (96%)	17 (4%)	26	34
All	All	2401/2412 (100%)	2326 (97%)	75 (3%)	35	45

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	85	THR
1	A	102	GLU
1	A	138	THR
1	A	206	ILE
1	A	272	LEU
1	A	299	VAL
1	A	407	ILE
1	A	448	ASP
1	B	2	ARG

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Mol	Chain	Res	Type
1	B	65	GLU
1	B	85	THR
1	B	133	ILE
1	B	138	THR
1	B	196	ASP
1	B	198	VAL
1	B	206	ILE
1	B	299	VAL
1	B	399	ARG
1	B	455	ARG
1	C	3	LYS
1	C	71	THR
1	C	138	THR
1	C	198	VAL
1	C	206	ILE
1	C	299	VAL
1	C	369	ASP
1	C	407	ILE
1	D	138	THR
1	D	193	THR
1	D	196	ASP
1	D	198	VAL
1	D	206	ILE
1	D	259	ASP
1	D	299	VAL
1	D	369	ASP
1	D	400	LYS
1	D	429	VAL
1	D	503	ASP
1	D	504	LEU
1	E	20	ASP
1	E	26	ARG
1	E	65	GLU
1	E	85	THR
1	E	102	GLU
1	E	138	THR
1	E	140	LEU
1	E	196	ASP
1	E	202	THR
1	E	205	GLU
1	E	206	ILE
1	E	236	GLU

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Mol	Chain	Res	Type
1	E	267	GLN
1	E	299	VAL
1	E	317	LYS
1	E	400	LYS
1	E	407	ILE
1	E	451	GLU
1	F	4	GLN
1	F	65	GLU
1	F	85	THR
1	F	102	GLU
1	F	138	THR
1	F	193	THR
1	F	198	VAL
1	F	206	ILE
1	F	256	VAL
1	F	299	VAL
1	F	317	LYS
1	F	369	ASP
1	F	400	LYS
1	F	448	ASP
1	F	455	ARG
1	F	465	LEU
1	F	503	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	82	HIS
1	A	150	ASN
1	A	296	HIS
1	A	300	HIS
1	A	370	GLN
1	A	378	HIS
1	A	425	ASN
1	A	511	ASN
1	A	514	GLN
1	B	57	HIS
1	B	126	ASN
1	B	148	GLN
1	B	150	ASN
1	B	296	HIS

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Mol	Chain	Res	Type
1	B	300	HIS
1	B	346	GLN
1	B	352	ASN
1	B	370	GLN
1	B	378	HIS
1	B	425	ASN
1	B	514	GLN
1	C	4	GLN
1	C	27	GLN
1	C	57	HIS
1	C	82	HIS
1	C	106	GLN
1	C	126	ASN
1	C	150	ASN
1	C	189	GLN
1	C	267	GLN
1	C	296	HIS
1	C	300	HIS
1	C	370	GLN
1	C	378	HIS
1	C	425	ASN
1	C	456	GLN
1	D	4	GLN
1	D	57	HIS
1	D	106	GLN
1	D	126	ASN
1	D	150	ASN
1	D	267	GLN
1	D	296	HIS
1	D	300	HIS
1	D	370	GLN
1	D	378	HIS
1	D	425	ASN
1	D	445	ASN
1	D	514	GLN
1	E	27	GLN
1	E	57	HIS
1	E	150	ASN
1	E	300	HIS
1	E	346	GLN
1	E	370	GLN
1	E	372	HIS

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Mol	Chain	Res	Type
1	E	378	HIS
1	E	445	ASN
1	E	514	GLN
1	F	4	GLN
1	F	57	HIS
1	F	126	ASN
1	F	148	GLN
1	F	150	ASN
1	F	296	HIS
1	F	300	HIS
1	F	370	GLN
1	F	372	HIS
1	F	378	HIS
1	F	425	ASN
1	F	456	GLN
1	F	467	HIS
1	F	514	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
3	GOL	C	601	-	5,5,5	0.61	0	5,5,5	1.31	1 (20%)
3	GOL	F	701	-	5,5,5	0.23	0	5,5,5	0.58	0
2	SO4	A	602	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	B	601	-	4,4,4	0.28	0	6,6,6	0.30	0
3	GOL	B	603	-	5,5,5	0.26	0	5,5,5	0.64	0
2	SO4	D	601	-	4,4,4	0.37	0	6,6,6	0.12	0
2	SO4	B	602	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	A	601	-	4,4,4	0.28	0	6,6,6	0.35	0
3	GOL	E	601	-	5,5,5	0.69	0	5,5,5	1.10	0
2	SO4	D	602	-	4,4,4	0.33	0	6,6,6	0.25	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	601	-	-	3/4/4/4	-
3	GOL	F	701	-	-	2/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	E	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	GOL	O2-C2-C3	-2.24	99.89	109.18

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-C3
3	F	701	GOL	C1-C2-C3-O3
3	C	601	GOL	O1-C1-C2-O2
3	F	701	GOL	O2-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	C	601	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	GOL	2	0
3	F	701	GOL	1	0
3	B	603	GOL	3	0
3	E	601	GOL	3	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	513/514 (99%)	0.26	36 (7%)	22 26	23, 35, 79, 127	0
1	B	513/514 (99%)	0.31	44 (8%)	16 19	23, 36, 81, 143	0
1	C	513/514 (99%)	0.51	56 (10%)	10 12	26, 41, 89, 124	0
1	D	513/514 (99%)	0.39	41 (7%)	18 22	25, 38, 78, 118	0
1	E	513/514 (99%)	0.40	49 (9%)	13 16	25, 40, 87, 118	0
1	F	513/514 (99%)	0.43	56 (10%)	10 12	24, 37, 84, 119	0
All	All	3078/3084 (99%)	0.38	282 (9%)	14 18	23, 38, 83, 143	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	PRO	7.6
1	C	72	ASP	6.9
1	B	445	ASN	6.5
1	D	504	LEU	6.2
1	A	445	ASN	6.1
1	A	447	ALA	6.0
1	A	504	LEU	6.0
1	B	504	LEU	5.8
1	D	20	ASP	5.6
1	F	504	LEU	5.6
1	C	504	LEU	5.6
1	E	506	MET	5.6
1	C	501	HIS	5.5
1	C	264	ARG	5.4
1	C	447	ALA	5.4
1	C	19	PRO	5.3
1	E	447	ALA	5.2
1	F	453	VAL	5.1
1	F	2	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	438	VAL	5.0
1	F	431	GLY	4.9
1	C	133	ILE	4.9
1	B	447	ALA	4.8
1	E	133	ILE	4.8
1	E	19	PRO	4.8
1	D	506	MET	4.8
1	F	429	VAL	4.7
1	A	446	ALA	4.6
1	C	506	MET	4.6
1	E	446	ALA	4.6
1	D	447	ALA	4.5
1	D	21	PRO	4.5
1	C	265	ARG	4.5
1	D	448	ASP	4.4
1	C	446	ALA	4.4
1	C	73	GLY	4.4
1	C	21	PRO	4.3
1	F	430	MET	4.3
1	E	129	ALA	4.3
1	E	2	ARG	4.3
1	F	506	MET	4.3
1	A	502	ALA	4.3
1	B	446	ALA	4.2
1	D	455	ARG	4.2
1	A	501	HIS	4.2
1	F	275	ALA	4.1
1	C	451	GLU	4.1
1	F	446	ALA	4.1
1	E	317	LYS	4.1
1	E	504	LEU	4.0
1	A	2	ARG	4.0
1	A	20	ASP	4.0
1	A	67	LYS	4.0
1	C	277	GLY	3.9
1	F	437	GLY	3.9
1	A	3	LYS	3.9
1	C	201	VAL	3.9
1	C	67	LYS	3.9
1	E	501	HIS	3.9
1	A	506	MET	3.8
1	A	11	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	23	ALA	3.8
1	D	3	LYS	3.8
1	C	453	VAL	3.8
1	C	129	ALA	3.8
1	F	432	ALA	3.7
1	A	275	ALA	3.7
1	C	441	ARG	3.7
1	E	275	ALA	3.7
1	F	133	ILE	3.6
1	B	450	PRO	3.6
1	D	275	ALA	3.6
1	F	435	ALA	3.6
1	F	442	ARG	3.6
1	C	450	PRO	3.6
1	F	447	ALA	3.6
1	F	200	ALA	3.5
1	F	45	LYS	3.5
1	F	67	LYS	3.5
1	E	11	ILE	3.5
1	D	67	LYS	3.5
1	F	317	LYS	3.5
1	A	200	ALA	3.4
1	C	275	ALA	3.4
1	D	17	GLY	3.4
1	D	18	GLY	3.4
1	C	11	ILE	3.4
1	F	11	ILE	3.4
1	C	3	LYS	3.4
1	B	204	GLU	3.4
1	C	2	ARG	3.4
1	D	2	ARG	3.4
1	E	17	GLY	3.4
1	B	455	ARG	3.4
1	F	279	ARG	3.4
1	C	502	ALA	3.4
1	F	444	ILE	3.3
1	B	501	HIS	3.3
1	D	445	ASN	3.3
1	F	433	GLU	3.3
1	E	502	ALA	3.3
1	F	448	ASP	3.3
1	B	502	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	452	ALA	3.3
1	F	502	ALA	3.3
1	B	448	ASP	3.3
1	E	450	PRO	3.3
1	C	448	ASP	3.2
1	C	26	ARG	3.2
1	B	20	ASP	3.2
1	C	449	ASP	3.2
1	D	501	HIS	3.1
1	F	10	ASP	3.1
1	D	450	PRO	3.1
1	F	445	ASN	3.1
1	B	506	MET	3.1
1	E	202	THR	3.1
1	F	501	HIS	3.1
1	D	277	GLY	3.1
1	E	67	LYS	3.1
1	C	196	ASP	3.1
1	B	498	ARG	3.1
1	F	498	ARG	3.1
1	D	61	GLY	3.0
1	F	503	ASP	3.0
1	E	3	LYS	3.0
1	E	276	ASP	3.0
1	A	450	PRO	3.0
1	E	201	VAL	3.0
1	F	455	ARG	3.0
1	C	266	GLY	3.0
1	E	200	ALA	3.0
1	E	58	ARG	3.0
1	F	454	ARG	3.0
1	F	434	GLY	3.0
1	B	275	ALA	2.9
1	A	45	LYS	2.9
1	F	278	ASN	2.9
1	D	60	THR	2.9
1	C	64	LEU	2.9
1	E	498	ARG	2.9
1	B	201	VAL	2.9
1	D	437	GLY	2.9
1	B	199	ARG	2.9
1	C	455	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	511	ASN	2.9
1	A	455	ARG	2.8
1	B	454	ARG	2.8
1	D	442	ARG	2.8
1	E	442	ARG	2.8
1	C	505	PRO	2.8
1	F	204	GLU	2.8
1	A	444	ILE	2.8
1	E	26	ARG	2.8
1	E	449	ASP	2.8
1	D	402	TYR	2.8
1	E	452	ALA	2.8
1	F	439	ILE	2.8
1	F	201	VAL	2.8
1	E	207	GLY	2.7
1	A	19	PRO	2.7
1	A	26	ARG	2.7
1	F	458	VAL	2.7
1	A	133	ILE	2.7
1	D	278	ASN	2.7
1	E	445	ASN	2.7
1	E	277	GLY	2.7
1	B	67	LYS	2.7
1	E	16	ARG	2.7
1	F	452	ALA	2.7
1	B	462	LYS	2.7
1	C	204	GLU	2.7
1	E	455	ARG	2.7
1	D	446	ALA	2.6
1	B	451	GLU	2.6
1	C	20	ASP	2.6
1	F	202	THR	2.6
1	C	442	ARG	2.6
1	F	199	ARG	2.6
1	C	25	ARG	2.6
1	F	65	GLU	2.6
1	B	441	ARG	2.6
1	F	250	ARG	2.6
1	B	203	GLY	2.6
1	E	21	PRO	2.6
1	C	5	LEU	2.6
1	D	26	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	452	ALA	2.6
1	C	22	ASP	2.6
1	B	205	GLU	2.5
1	A	442	ARG	2.5
1	B	505	PRO	2.5
1	A	454	ARG	2.5
1	D	279	ARG	2.5
1	F	302	ARG	2.5
1	C	278	ASN	2.5
1	A	51	ILE	2.5
1	F	20	ASP	2.5
1	C	263	ASP	2.5
1	B	442	ARG	2.4
1	D	453	VAL	2.4
1	E	453	VAL	2.4
1	A	452	ALA	2.4
1	E	444	ILE	2.4
1	E	503	ASP	2.4
1	B	13	GLU	2.4
1	F	262	ALA	2.4
1	F	4	GLN	2.4
1	C	445	ASN	2.4
1	E	196	ASP	2.4
1	E	204	GLU	2.4
1	B	200	ALA	2.4
1	F	441	ARG	2.4
1	B	196	ASP	2.3
1	C	207	GLY	2.3
1	D	444	ILE	2.3
1	B	267	GLN	2.3
1	D	276	ASP	2.3
1	D	434	GLY	2.3
1	A	202	THR	2.3
1	E	441	ARG	2.3
1	C	205	GLU	2.3
1	B	276	ASP	2.3
1	A	61	GLY	2.3
1	D	16	ARG	2.3
1	F	267	GLN	2.3
1	E	440	PHE	2.3
1	D	259	ASP	2.3
1	F	466	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	THR	2.3
1	C	27	GLN	2.3
1	B	198	VAL	2.3
1	E	203	GLY	2.2
1	B	4	GLN	2.2
1	C	458	VAL	2.2
1	B	503	ASP	2.2
1	C	498	ARG	2.2
1	B	61	GLY	2.2
1	A	204	GLU	2.2
1	B	438	VAL	2.2
1	B	453	VAL	2.2
1	C	454	ARG	2.2
1	E	250	ARG	2.2
1	E	279	ARG	2.2
1	A	21	PRO	2.2
1	E	45	LYS	2.2
1	D	502	ALA	2.2
1	F	436	ALA	2.2
1	B	259	ASP	2.2
1	D	503	ASP	2.2
1	E	448	ASP	2.2
1	E	459	GLU	2.2
1	A	199	ARG	2.1
1	E	199	ARG	2.1
1	D	433	GLU	2.1
1	B	202	THR	2.1
1	C	16	ARG	2.1
1	A	448	ASP	2.1
1	F	13	GLU	2.1
1	C	128	GLY	2.1
1	B	45	LYS	2.1
1	C	276	ASP	2.1
1	D	4	GLN	2.1
1	D	267	GLN	2.1
1	B	458	VAL	2.1
1	F	197	VAL	2.1
1	F	3	LYS	2.1
1	B	465	LEU	2.1
1	A	276	ASP	2.1
1	A	449	ASP	2.1
1	C	503	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	429	VAL	2.1
1	D	369	ASP	2.0
1	B	444	ILE	2.0
1	C	444	ILE	2.0
1	A	257	PRO	2.0
1	E	152	ARG	2.0
1	C	71	THR	2.0
1	B	452	ALA	2.0
1	A	10	ASP	2.0
1	F	290	ILE	2.0
1	E	400	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	GOL	B	603	6/6	0.79	0.22	37,51,60,65	0
3	GOL	E	601	6/6	0.80	0.25	34,39,53,53	0
3	GOL	F	701	6/6	0.83	0.23	38,57,68,72	0
2	SO4	A	602	5/5	0.88	0.17	61,63,73,73	0
3	GOL	C	601	6/6	0.88	0.22	26,43,51,60	0
2	SO4	A	601	5/5	0.89	0.12	46,49,59,76	0
2	SO4	B	602	5/5	0.91	0.12	66,66,67,80	0
2	SO4	B	601	5/5	0.93	0.12	41,48,52,55	0
2	SO4	D	602	5/5	0.93	0.21	46,49,52,54	0
2	SO4	D	601	5/5	0.95	0.10	50,53,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.