Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:56 AM GMT

PDB ID	:	3GLM
Title	:	Glutaconyl-coA decarboxylase A subunit from Clostridium symbiosum co-crystallized with crotonyl-coA
Authors	:	Kress, D.; Brugel, D.; Buckel, W.; Essen, L.-O.
Deposited on	:	2009-03-12
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.208
Clashscore		6
Ramachandran outliers		0.0%
Sidechain outliers		1.8%
RSRZ outliers		0.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
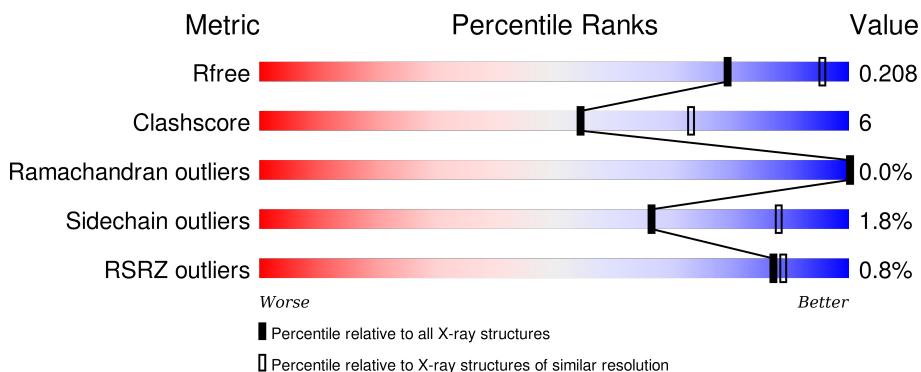
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	588	80% 15% • •
1	B	588	81% 14% • •
1	C	588	80% 14% • 5%
1	D	588	82% 13% • •
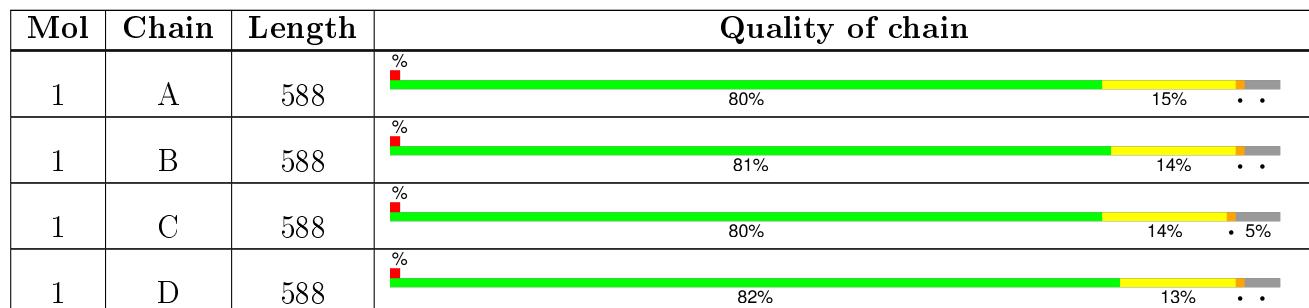
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18142 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 Glutaconyl-CoA decarboxylase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4327	2746	729	824	28			
1	B	562	Total	C	N	O	S	0	0	0
			4330	2749	729	824	28			
1	C	558	Total	C	N	O	S	0	0	0
			4305	2730	726	821	28			
1	D	562	Total	C	N	O	S	0	0	0
			4337	2754	730	825	28			

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

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

- Molecule 3 is CROTONYL COENZYME A (three-letter code: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$).
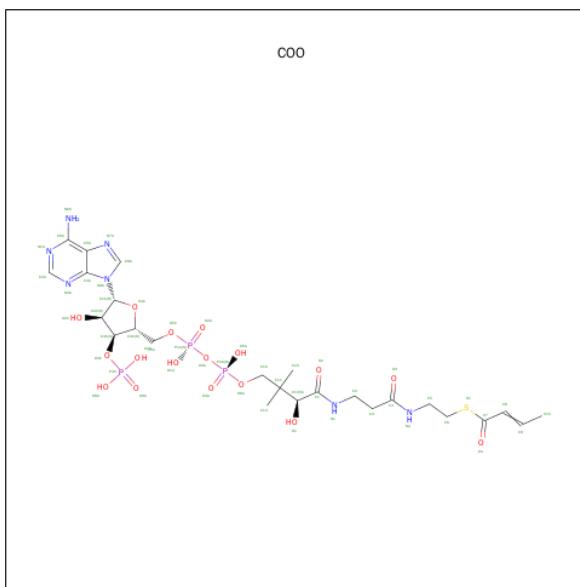
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	176	Total	O	0	0
			176	176		
4	C	161	Total	O	0	0
			161	161		
4	D	153	Total	O	0	0
			153	153		

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: Glutaconyl-CoA decarboxylase subunit A
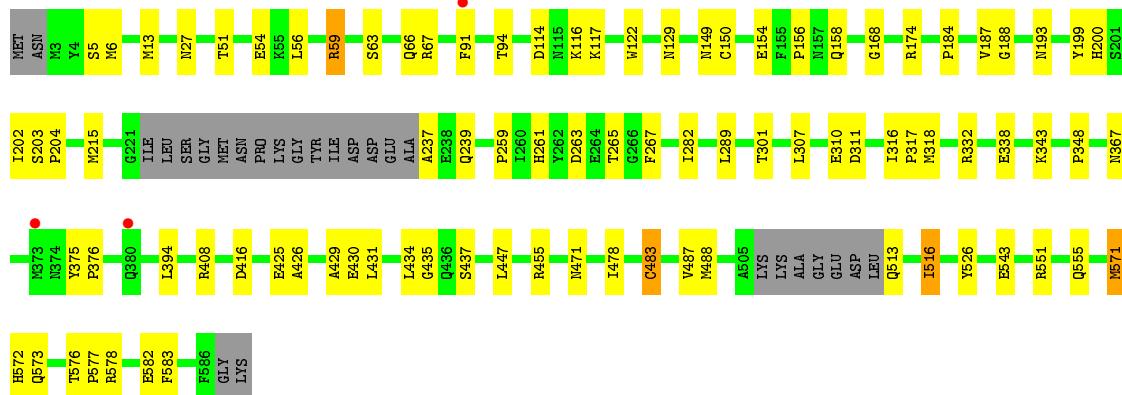
- Molecule 1: Glutaconyl-CoA decarboxylase subunit A

- Molecule 1: Glutaconyl-CoA decarboxylase subunit A

• Molecule 1: Glutaconyl-CoA decarboxylase subunit A

Chain D:
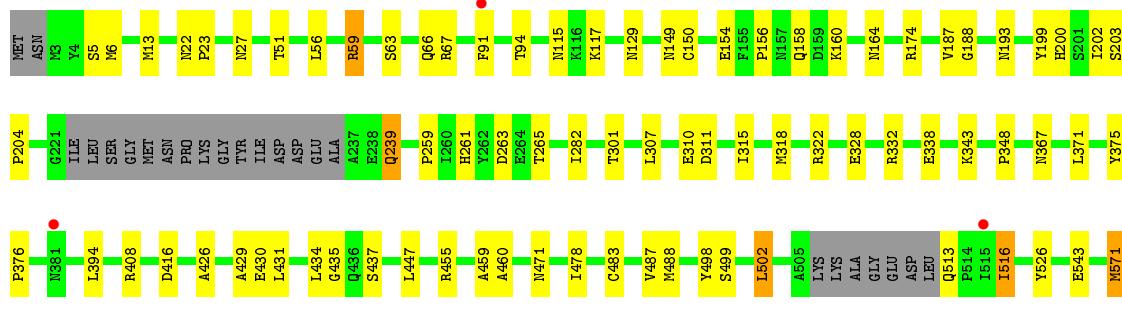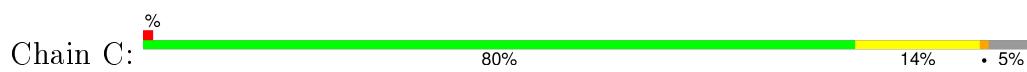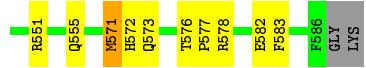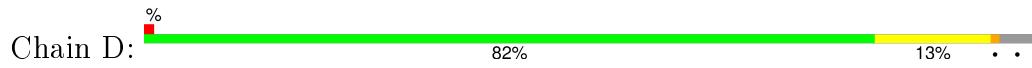
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.50Å　　167.45Å　　138.11Å 90.00°　　89.98°　　90.00°	Depositor
Resolution (Å)	36.76　–　2.50 36.75　–　2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.76-2.50) 99.5 (36.75-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$<I/\sigma(I)>$ [1]	1.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193　,　0.230 0.195　,　0.208	Depositor DCC
R_{free} test set	1005 reflections (1.28%)	DCC
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 11.2	EDS
Estimated twinning fraction	0.000 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.000 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.460 for -h,-k,l	Xtriage
L-test for twinning[2]	$<|L|> = 0.51, <L^2> = 0.34$	Xtriage
Outliers	6 of 79228 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18142	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.0569e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COO, 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	0.45	0/4421	0.55	0/5998
1	B	0.46	0/4424	0.56	0/6002
1	C	0.46	0/4399	0.57	2/5967 (0.0%)
1	D	0.45	0/4431	0.55	0/6011
All	All	0.46	0/17675	0.56	2/23978 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	487	VAL	CB-CA-C	-5.83	100.33	111.40
1	C	487	VAL	CG1-CB-CG2	5.58	119.84	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4327	0	4240	62	0
1	B	4330	0	4249	61	0
1	C	4305	0	4217	63	0
1	D	4337	0	4264	56	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	1	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
3	A	53	0	37	3	0
3	B	53	0	37	2	0
3	C	53	0	37	4	0
3	D	53	0	37	2	0
4	A	137	0	0	6	0
4	B	176	0	0	6	0
4	C	161	0	0	7	0
4	D	153	0	0	3	0
All	All	18142	0	17118	222	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 (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:HD21	1:A:318:MET:H	1.16	0.89
1:B:27:ASN:HD21	1:B:318:MET:H	1.16	0.88
1:D:27:ASN:HD21	1:D:318:MET:H	1.17	0.88
1:C:27:ASN:HD21	1:C:318:MET:H	1.17	0.87
1:D:447:LEU:HD12	4:D:668:HOH:O	1.75	0.87
1:B:471:ASN:HD22	1:D:174:ARG:HH21	1.24	0.86
1:A:471:ASN:HD22	1:C:174:ARG:HH21	1.24	0.83
1:B:174:ARG:HH21	1:D:471:ASN:HD22	1.26	0.82
1:B:160:LYS:HE3	4:B:701:HOH:O	1.77	0.81
1:A:367:ASN:ND2	1:A:416:ASP:H	1.80	0.78
1:A:174:ARG:HH21	1:C:471:ASN:HD22	1.29	0.78
1:B:322:ARG:HD3	4:B:691:HOH:O	1.84	0.76
1:C:367:ASN:ND2	1:C:416:ASP:H	1.84	0.74
1:A:63:SER:H	1:A:66:GLN:HE21	1.35	0.74
1:A:158:GLN:HB2	1:C:487:VAL:HG22	1.69	0.73
1:C:160:LYS:HE3	4:C:722:HOH:O	1.88	0.73
1:B:367:ASN:ND2	1:B:416:ASP:H	1.87	0.72
1:D:367:ASN:ND2	1:D:416:ASP:H	1.87	0.72
1:C:63:SER:H	1:C:66:GLN:HE21	1.40	0.69
1:A:158:GLN:HG2	1:C:526:TYR:CZ	2.28	0.69
1:B:158:GLN:HG2	1:D:526:TYR:CZ	2.29	0.68
1:A:526:TYR:CZ	1:C:158:GLN:HG2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:TYR:CZ	1:D:158:GLN:HG2	2.29	0.68
1:A:199:TYR:HA	1:A:202:ILE:HG22	1.76	0.67
1:B:199:TYR:HA	1:B:202:ILE:HG22	1.77	0.66
1:A:367:ASN:HD22	1:A:416:ASP:H	1.43	0.66
1:B:426:ALA:HB1	1:B:431:LEU:HD22	1.77	0.65
1:A:426:ALA:HB1	1:A:431:LEU:HD22	1.78	0.65
1:C:199:TYR:HA	1:C:202:ILE:HG22	1.76	0.65
1:D:199:TYR:HA	1:D:202:ILE:HG22	1.78	0.65
1:A:237:ALA:CB	4:A:659:HOH:O	2.45	0.64
1:A:150:CYS:H	1:A:193:ASN:ND2	1.96	0.64
1:C:367:ASN:HD22	1:C:416:ASP:H	1.44	0.64
1:C:426:ALA:HB1	1:C:431:LEU:HD22	1.79	0.64
1:B:371:LEU:HD12	4:B:768:HOH:O	1.98	0.63
1:B:63:SER:H	1:B:66:GLN:HE21	1.45	0.63
1:D:150:CYS:H	1:D:193:ASN:ND2	1.98	0.62
1:D:426:ALA:HB1	1:D:431:LEU:HD22	1.80	0.61
1:D:63:SER:H	1:D:66:GLN:HE21	1.47	0.60
1:B:322:ARG:CD	4:B:691:HOH:O	2.47	0.60
1:C:150:CYS:H	1:C:193:ASN:ND2	1.99	0.60
1:B:150:CYS:H	1:B:193:ASN:ND2	2.00	0.60
1:A:67:ARG:HH12	1:A:149:ASN:HD22	1.50	0.60
1:B:67:ARG:HH12	1:B:149:ASN:HD22	1.50	0.59
1:D:91:PHE:HB3	1:D:117:LYS:HE3	1.85	0.58
1:D:499:SER:HA	1:D:502:LEU:HD12	1.85	0.58
1:D:67:ARG:HH12	1:D:149:ASN:HD22	1.51	0.58
1:B:91:PHE:HB3	1:B:117:LYS:HE3	1.86	0.57
1:C:91:PHE:HB3	1:C:117:LYS:HE3	1.86	0.57
1:D:371:LEU:HD12	4:D:653:HOH:O	2.03	0.57
1:A:91:PHE:HB3	1:A:117:LYS:HE3	1.86	0.57
1:D:367:ASN:HD22	1:D:416:ASP:H	1.51	0.57
3:C:590:COO:H2X	4:C:674:HOH:O	2.04	0.57
1:A:513:GLN:HA	1:A:516:ILE:HG12	1.88	0.56
1:C:67:ARG:HH12	1:C:149:ASN:HD22	1.54	0.55
1:A:63:SER:H	1:A:66:GLN:NE2	2.04	0.55
1:B:259:PRO:O	1:B:263:ASP:HB2	2.07	0.55
1:D:513:GLN:HA	1:D:516:ILE:HG12	1.89	0.54
1:C:513:GLN:HA	1:C:516:ILE:HG12	1.90	0.54
1:B:367:ASN:HD22	1:B:416:ASP:H	1.52	0.54
1:C:378:TYR:HB3	4:C:713:HOH:O	2.08	0.53
1:D:408:ARG:HA	1:D:447:LEU:HD11	1.89	0.53
3:A:590:COO:H2X	4:A:718:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:SER:O	1:B:502:LEU:HB2	2.09	0.53
1:D:375:TYR:CG	1:D:376:PRO:HA	2.44	0.53
1:B:375:TYR:CG	1:B:376:PRO:HA	2.45	0.52
1:C:63:SER:H	1:C:66:GLN:NE2	2.06	0.52
1:A:158:GLN:CB	1:C:487:VAL:HG22	2.38	0.52
1:A:434:LEU:HD21	1:B:578:ARG:HG2	1.92	0.52
1:C:94:THR:OG1	1:C:129:ASN:ND2	2.43	0.52
1:A:408:ARG:HA	1:A:447:LEU:HD11	1.91	0.52
1:A:154:GLU:HA	3:A:590:COO:N1A	2.25	0.52
1:B:513:GLN:HA	1:B:516:ILE:HG12	1.92	0.52
1:D:259:PRO:O	1:D:263:ASP:HB2	2.10	0.51
1:D:154:GLU:HA	3:D:590:COO:N1A	2.25	0.51
1:A:154:GLU:HG2	1:A:156:PRO:HD2	1.92	0.51
1:C:154:GLU:HA	3:C:590:COO:N1A	2.26	0.51
1:B:154:GLU:HA	3:B:590:COO:N1A	2.26	0.51
1:C:322:ARG:HD3	4:C:695:HOH:O	2.10	0.51
1:D:94:THR:OG1	1:D:129:ASN:ND2	2.42	0.51
1:B:94:THR:OG1	1:B:129:ASN:ND2	2.42	0.50
1:C:408:ARG:HA	1:C:447:LEU:HD11	1.92	0.50
1:A:375:TYR:CG	1:A:376:PRO:HA	2.46	0.50
1:B:63:SER:H	1:B:66:GLN:NE2	2.10	0.50
1:C:375:TYR:CG	1:C:376:PRO:HA	2.46	0.50
1:D:200:HIS:HD2	4:D:624:HOH:O	1.96	0.49
1:A:578:ARG:HG2	1:B:434:LEU:HD21	1.95	0.49
1:C:154:GLU:HG2	1:C:156:PRO:HD2	1.93	0.49
1:B:27:ASN:ND2	1:B:318:MET:H	1.99	0.49
1:C:434:LEU:HD21	1:D:578:ARG:HG2	1.95	0.48
1:B:311:ASP:HB2	1:B:332:ARG:HE	1.78	0.48
1:D:27:ASN:ND2	1:D:318:MET:H	1.99	0.48
1:B:261:HIS:HA	1:B:265:THR:OG1	2.13	0.48
1:D:154:GLU:HG2	1:D:156:PRO:HD2	1.96	0.48
1:A:94:THR:OG1	1:A:129:ASN:ND2	2.43	0.48
4:B:690:HOH:O	1:C:571:MET:HG2	2.13	0.48
1:D:63:SER:H	1:D:66:GLN:NE2	2.11	0.48
1:A:51:THR:HG21	1:A:59:ARG:HH21	1.79	0.48
1:C:51:THR:HG21	1:C:59:ARG:HH21	1.79	0.47
1:A:259:PRO:O	1:A:263:ASP:HB2	2.14	0.47
1:C:259:PRO:O	1:C:263:ASP:HB2	2.14	0.47
1:A:5:SER:HB2	1:A:571:MET:HG3	1.96	0.47
1:B:471:ASN:ND2	1:D:174:ARG:HH21	2.04	0.47
1:A:237:ALA:HB3	4:A:656:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASP:HB2	1:C:332:ARG:HE	1.79	0.47
1:B:408:ARG:HA	1:B:447:LEU:HD11	1.96	0.47
1:D:261:HIS:HA	1:D:265:THR:OG1	2.15	0.46
1:C:261:HIS:HA	1:C:265:THR:OG1	2.16	0.46
1:D:455:ARG:HA	1:D:483:CYS:HA	1.97	0.46
1:A:429:ALA:O	1:A:430:GLU:HB2	2.16	0.46
1:B:394:LEU:HD22	1:B:435:GLY:HA2	1.97	0.46
1:B:174:ARG:HH21	1:D:471:ASN:ND2	2.04	0.46
1:C:5:SER:HB2	1:C:571:MET:HG3	1.97	0.46
1:D:394:LEU:HD22	1:D:435:GLY:HA2	1.97	0.46
1:A:150:CYS:H	1:A:193:ASN:HD21	1.61	0.46
1:B:455:ARG:HA	1:B:483:CYS:HA	1.97	0.46
1:B:460:ALA:HB3	2:B:589:CL:CL	2.53	0.45
1:A:6:MET:SD	1:A:572:HIS:HA	2.56	0.45
1:C:578:ARG:HG2	1:D:434:LEU:HD21	1.98	0.45
1:C:576:THR:HB	1:C:577:PRO:HD3	1.99	0.45
1:A:27:ASN:ND2	1:A:318:MET:H	1.98	0.45
1:A:551:ARG:O	1:A:555:GLN:HG3	2.17	0.45
1:A:261:HIS:HA	1:A:265:THR:OG1	2.17	0.45
1:C:455:ARG:HA	1:C:483:CYS:HA	1.99	0.45
1:B:154:GLU:HG2	1:B:156:PRO:HD2	1.99	0.45
1:A:437:SER:OG	1:B:573:GLN:HA	2.16	0.45
1:A:311:ASP:HB2	1:A:332:ARG:HE	1.81	0.45
1:D:311:ASP:HB2	1:D:332:ARG:HE	1.81	0.45
1:A:455:ARG:HA	1:A:483:CYS:HA	1.99	0.44
1:C:429:ALA:O	1:C:430:GLU:HB2	2.17	0.44
1:B:498:TYR:O	1:B:502:LEU:HD22	2.17	0.44
1:B:200:HIS:HD2	4:B:727:HOH:O	2.01	0.44
1:B:5:SER:HB2	1:B:571:MET:HG3	1.99	0.44
1:C:13:MET:HB2	1:C:338:GLU:HB3	1.98	0.44
1:B:115:ASN:HD22	1:B:149:ASN:ND2	2.15	0.44
1:D:578:ARG:O	1:D:582:GLU:HG2	2.18	0.44
1:D:375:TYR:CD1	1:D:376:PRO:HA	2.52	0.44
1:C:27:ASN:ND2	1:C:318:MET:H	1.99	0.44
3:A:590:COO:H8	1:C:487:VAL:HG12	1.99	0.44
1:C:578:ARG:O	1:C:582:GLU:HG2	2.17	0.44
1:B:239:GLN:H	1:B:239:GLN:HG3	1.60	0.44
1:B:429:ALA:O	1:B:430:GLU:HB2	2.18	0.44
1:A:576:THR:HB	1:A:577:PRO:HD3	2.01	0.43
1:D:5:SER:HB2	1:D:571:MET:HG3	1.99	0.43
1:B:6:MET:SD	1:B:572:HIS:HA	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:MET:HB2	1:D:338:GLU:HB3	2.00	0.43
1:A:394:LEU:HD22	1:A:435:GLY:HA2	2.00	0.43
1:A:573:GLN:HA	1:B:437:SER:OG	2.19	0.43
1:C:455:ARG:NH2	4:C:709:HOH:O	2.51	0.43
1:A:478:ILE:HG22	1:A:543:GLU:HB3	2.01	0.43
1:A:13:MET:HB2	1:A:338:GLU:HB3	1.99	0.43
1:C:122:TRP:CZ3	1:C:168:GLY:HA3	2.54	0.43
1:D:115:ASN:HD22	1:D:149:ASN:ND2	2.16	0.43
1:B:487:VAL:HG23	3:D:590:COO:H8	2.01	0.43
1:D:188:GLY:HA3	1:D:282:ILE:HD11	2.01	0.43
1:C:478:ILE:HG22	1:C:543:GLU:HB3	2.01	0.43
1:D:6:MET:SD	1:D:572:HIS:HA	2.59	0.43
1:A:487:VAL:HG13	1:A:488:MET:HG2	2.01	0.43
1:A:54:GLU:HB2	4:A:607:HOH:O	2.18	0.43
1:B:478:ILE:HG22	1:B:543:GLU:HB3	2.01	0.43
1:C:188:GLY:HA3	1:C:282:ILE:HD11	2.00	0.43
1:D:487:VAL:HG13	1:D:488:MET:HG2	2.01	0.42
1:C:348:PRO:HD2	1:C:375:TYR:CZ	2.54	0.42
1:C:573:GLN:HA	1:D:437:SER:OG	2.20	0.42
1:B:13:MET:HB2	1:B:338:GLU:HB3	2.01	0.42
1:D:203:SER:N	1:D:204:PRO:CD	2.83	0.42
1:D:348:PRO:HD2	1:D:375:TYR:CZ	2.55	0.42
1:B:487:VAL:HG13	1:B:488:MET:HG2	2.01	0.42
1:D:429:ALA:O	1:D:430:GLU:HB2	2.19	0.42
1:C:6:MET:SD	1:C:572:HIS:HA	2.60	0.42
1:D:187:VAL:HB	1:D:204:PRO:HG2	2.00	0.42
1:A:487:VAL:HG23	3:C:590:COO:H8	2.02	0.42
1:A:375:TYR:CD1	1:A:376:PRO:HA	2.54	0.42
1:B:51:THR:HG21	1:B:59:ARG:HH21	1.84	0.42
1:B:187:VAL:HB	1:B:204:PRO:HG2	2.01	0.42
1:C:425:GLU:HB2	4:C:595:HOH:O	2.18	0.42
1:B:188:GLY:HA3	1:B:282:ILE:HD11	2.02	0.42
1:A:184:PRO:HG3	1:A:289:LEU:HD22	2.02	0.41
1:C:203:SER:N	1:C:204:PRO:CD	2.83	0.41
1:C:460:ALA:HB3	2:C:589:CL:CL	2.57	0.41
1:C:375:TYR:CD1	1:C:376:PRO:HA	2.55	0.41
1:D:215:MET:HE1	1:D:267:PHE:HB3	2.02	0.41
1:D:343:LYS:HA	1:D:583:PHE:CD2	2.56	0.41
1:D:22:ASN:HA	1:D:23:PRO:HD2	1.96	0.41
1:D:150:CYS:H	1:D:193:ASN:HD21	1.66	0.41
1:B:375:TYR:CD1	1:B:376:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PRO:HD2	1:A:375:TYR:CZ	2.56	0.41
1:C:394:LEU:HD22	1:C:435:GLY:HA2	2.02	0.41
1:A:343:LYS:HA	1:A:583:PHE:CD2	2.56	0.41
1:C:343:LYS:HA	1:C:583:PHE:CD2	2.55	0.41
1:C:165:ARG:NE	4:C:708:HOH:O	2.54	0.41
1:A:122:TRP:CZ3	1:A:168:GLY:HA3	2.56	0.41
1:B:343:LYS:HA	1:B:583:PHE:CD2	2.56	0.41
1:B:203:SER:N	1:B:204:PRO:CD	2.84	0.41
1:A:200:HIS:HD2	4:A:634:HOH:O	2.03	0.41
1:A:203:SER:N	1:A:204:PRO:CD	2.84	0.41
1:A:425:GLU:HB2	4:A:602:HOH:O	2.20	0.41
1:A:188:GLY:HA3	1:A:282:ILE:HD11	2.02	0.41
1:A:471:ASN:ND2	1:C:174:ARG:HH21	2.04	0.41
1:B:348:PRO:HD2	1:B:375:TYR:CZ	2.56	0.41
3:B:590:COO:H8	1:D:487:VAL:HG23	2.03	0.41
1:A:578:ARG:O	1:A:582:GLU:HG2	2.20	0.41
1:B:164:ASN:OD1	1:D:132:ARG:NH2	2.53	0.41
1:B:22:ASN:HA	1:B:23:PRO:HD2	1.97	0.41
1:B:315:ILE:HD13	1:B:328:GLU:HB3	2.03	0.41
1:B:311:ASP:HB2	1:B:332:ARG:NE	2.36	0.41
1:D:122:TRP:CZ3	1:D:168:GLY:HA3	2.55	0.41
1:C:150:CYS:H	1:C:193:ASN:HD21	1.66	0.40
1:C:455:ARG:O	1:C:483:CYS:HA	2.21	0.40
1:A:114:ASP:OD1	1:A:116:LYS:HB2	2.21	0.40
1:A:316:ILE:HA	1:A:317:PRO:HD3	1.92	0.40
1:C:316:ILE:HA	1:C:317:PRO:HD3	1.91	0.40
1:B:578:ARG:O	1:B:582:GLU:HG2	2.21	0.40
1:A:187:VAL:HB	1:A:204:PRO:HG2	2.03	0.40
1:C:437:SER:OG	1:D:573:GLN:HA	2.20	0.40
1:A:215:MET:HE1	1:A:267:PHE:HB3	2.02	0.40
1:A:27:ASN:HD21	1:A:318:MET:N	1.99	0.40
1:C:551:ARG:O	1:C:555:GLN:HG3	2.22	0.40
1:C:196:GLY:N	3:C:590:COO:H9	2.36	0.40
1:D:51:THR:HG21	1:D:59:ARG:HH21	1.85	0.40
1:C:311:ASP:HB2	1:C:332:ARG:NE	2.37	0.40
1:C:275:ASP:O	1:C:279:ILE:HG12	2.22	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	556/588 (95%)	541 (97%)	15 (3%)	0	100	100
1	B	556/588 (95%)	538 (97%)	17 (3%)	1 (0%)	52	75
1	C	552/588 (94%)	535 (97%)	17 (3%)	0	100	100
1	D	556/588 (95%)	538 (97%)	18 (3%)	0	100	100
All	All	2220/2352 (94%)	2152 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	ALA

5.3.2 Protein sidechains (i)

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	460/491 (94%)	451 (98%)	9 (2%)	63	86
1	B	461/491 (94%)	452 (98%)	9 (2%)	63	86
1	C	459/491 (94%)	451 (98%)	8 (2%)	68	89
1	D	463/491 (94%)	456 (98%)	7 (2%)	72	91
All	All	1843/1964 (94%)	1810 (98%)	33 (2%)	66	88

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	59	ARG
1	A	239	GLN
1	A	301	THR
1	A	307	LEU
1	A	310	GLU
1	A	483	CYS
1	A	516	ILE
1	A	571	MET
1	B	56	LEU
1	B	59	ARG
1	B	239	GLN
1	B	301	THR
1	B	307	LEU
1	B	310	GLU
1	B	502	LEU
1	B	516	ILE
1	B	571	MET
1	C	56	LEU
1	C	59	ARG
1	C	301	THR
1	C	307	LEU
1	C	483	CYS
1	C	487	VAL
1	C	516	ILE
1	C	571	MET
1	D	56	LEU
1	D	59	ARG
1	D	301	THR
1	D	307	LEU
1	D	310	GLU
1	D	516	ILE
1	D	571	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	57	ASN
1	A	66	GLN
1	A	129	ASN
1	A	149	ASN
1	A	175	ASN

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Mol	Chain	Res	Type
1	A	179	ASN
1	A	193	ASN
1	A	200	HIS
1	A	367	ASN
1	A	471	ASN
1	A	520	ASN
1	A	566	GLN
1	B	27	ASN
1	B	57	ASN
1	B	66	GLN
1	B	129	ASN
1	B	149	ASN
1	B	175	ASN
1	B	179	ASN
1	B	193	ASN
1	B	200	HIS
1	B	367	ASN
1	B	471	ASN
1	C	27	ASN
1	C	57	ASN
1	C	66	GLN
1	C	129	ASN
1	C	149	ASN
1	C	175	ASN
1	C	179	ASN
1	C	193	ASN
1	C	200	HIS
1	C	367	ASN
1	C	471	ASN
1	C	566	GLN
1	D	27	ASN
1	D	57	ASN
1	D	66	GLN
1	D	129	ASN
1	D	141	HIS
1	D	149	ASN
1	D	175	ASN
1	D	179	ASN
1	D	193	ASN
1	D	200	HIS
1	D	367	ASN
1	D	471	ASN

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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	COO	A	590	-	43,55,55	0.66	1 (2%)	56,81,81	2.32	11 (19%)
3	COO	B	590	-	43,55,55	0.71	1 (2%)	56,81,81	2.36	12 (21%)
3	COO	C	590	-	43,55,55	0.66	1 (2%)	56,81,81	2.35	12 (21%)
3	COO	D	590	-	43,55,55	0.68	1 (2%)	56,81,81	2.47	12 (21%)

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	COO	A	590	-	-	0/49/70/70	0/3/3/3
3	COO	B	590	-	-	0/49/70/70	0/3/3/3
3	COO	C	590	-	-	0/49/70/70	0/3/3/3
3	COO	D	590	-	-	0/49/70/70	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	590	COO	O4X-C1X	2.18	1.44	1.41
3	C	590	COO	O4X-C1X	2.30	1.44	1.41
3	D	590	COO	O4X-C1X	2.37	1.44	1.41
3	B	590	COO	O4X-C1X	2.56	1.44	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	590	COO	N3A-C2A-N1A	-10.83	120.60	128.89
3	A	590	COO	N3A-C2A-N1A	-10.59	120.79	128.89
3	B	590	COO	N3A-C2A-N1A	-10.46	120.89	128.89
3	C	590	COO	N3A-C2A-N1A	-10.35	120.97	128.89
3	D	590	COO	C3-C2-N1	-5.13	100.62	111.88
3	B	590	COO	C3-C2-N1	-5.03	100.84	111.88
3	A	590	COO	C3-C2-N1	-4.68	101.61	111.88
3	C	590	COO	C3-C2-N1	-4.64	101.69	111.88
3	B	590	COO	C6-C5-N2	-3.55	105.26	112.36
3	C	590	COO	C10-C9-C8	-3.43	118.86	125.27
3	A	590	COO	C10-C9-C8	-3.36	118.99	125.27
3	D	590	COO	C10-C9-C8	-3.33	119.05	125.27
3	D	590	COO	C6-C5-N2	-3.33	105.71	112.36
3	C	590	COO	C6-C5-N2	-3.20	105.96	112.36
3	B	590	COO	C10-C9-C8	-3.08	119.51	125.27
3	A	590	COO	C6-C5-N2	-3.08	106.21	112.36
3	D	590	COO	C2X-C1X-N9A	-2.77	110.06	114.29
3	C	590	COO	C4A-C5A-N7A	-2.72	106.98	109.48
3	D	590	COO	C4A-C5A-N7A	-2.62	107.07	109.48
3	A	590	COO	C4A-C5A-N7A	-2.57	107.12	109.48
3	C	590	COO	C2X-C1X-N9A	-2.48	110.51	114.29
3	B	590	COO	C4A-C5A-N7A	-2.44	107.24	109.48
3	B	590	COO	C2X-C1X-N9A	-2.40	110.63	114.29
3	B	590	COO	P1A-O3A-P2A	-2.40	126.00	132.73
3	C	590	COO	P1A-O3A-P2A	-2.28	126.31	132.73
3	C	590	COO	C5-C6-S1	-2.27	105.29	111.36
3	A	590	COO	P1A-O3A-P2A	-2.25	126.40	132.73
3	D	590	COO	P1A-O3A-P2A	-2.24	126.43	132.73
3	D	590	COO	C5-C6-S1	-2.22	105.43	111.36
3	A	590	COO	C2X-C1X-N9A	-2.20	110.93	114.29
3	B	590	COO	C5-C6-S1	-2.13	105.66	111.36
3	A	590	COO	C5-C6-S1	-2.09	105.78	111.36
3	C	590	COO	C14-C11-C13	2.02	113.04	109.34
3	C	590	COO	C5-N2-C4	2.05	126.82	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	590	COO	C14-C11-C13	2.10	113.18	109.34
3	D	590	COO	O4X-C1X-N9A	2.11	112.51	108.10
3	B	590	COO	O4X-C1X-N9A	2.14	112.58	108.10
3	D	590	COO	C14-C11-C13	2.51	113.93	109.34
3	B	590	COO	C14-C11-C13	2.54	113.98	109.34
3	A	590	COO	C2-N1-C1	3.15	128.77	122.53
3	C	590	COO	C2-N1-C1	3.25	128.96	122.53
3	D	590	COO	C2-N1-C1	3.35	129.17	122.53
3	B	590	COO	C2-N1-C1	3.43	129.32	122.53
3	A	590	COO	C6-S1-C7	8.49	110.39	99.59
3	B	590	COO	C6-S1-C7	8.81	110.80	99.59
3	C	590	COO	C6-S1-C7	8.85	110.86	99.59
3	D	590	COO	C6-S1-C7	9.64	111.86	99.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	590	COO	3	0
3	B	590	COO	2	0
3	C	590	COO	4	0
3	D	590	COO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	562/588 (95%)	-0.47	3 (0%)	91 92	24, 33, 56, 75	1 (0%)
1	B	562/588 (95%)	-0.47	3 (0%)	91 92	24, 33, 56, 74	1 (0%)
1	C	558/588 (94%)	-0.48	6 (1%)	82 84	24, 33, 55, 74	1 (0%)
1	D	562/588 (95%)	-0.45	7 (1%)	81 83	24, 33, 56, 74	1 (0%)
All	All	2244/2352 (95%)	-0.47	19 (0%)	87 89	24, 33, 56, 75	4 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	ALA	4.5
1	A	373	MET	3.7
1	D	241	ILE	3.4
1	C	373	MET	2.9
1	A	380	GLN	2.9
1	C	22	ASN	2.7
1	D	91	PHE	2.7
1	D	373	MET	2.6
1	B	91	PHE	2.5
1	D	516	ILE	2.4
1	A	91	PHE	2.3
1	B	515	ILE	2.3
1	C	91	PHE	2.3
1	C	514	PRO	2.3
1	D	22	ASN	2.2
1	D	515	ILE	2.2
1	C	249	LYS	2.1
1	C	246	GLU	2.0
1	B	381	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	COO	A	590	53/53	0.94	0.17	1.33	39,55,67,68	0
3	COO	C	590	53/53	0.93	0.15	1.12	39,55,67,68	0
3	COO	B	590	53/53	0.94	0.15	0.69	38,55,67,68	0
3	COO	D	590	53/53	0.94	0.13	0.51	39,55,67,68	0
2	CL	A	589	1/1	0.98	0.09	-1.09	46,46,46,46	0
2	CL	C	589	1/1	0.99	0.06	-2.03	45,45,45,45	0
2	CL	B	589	1/1	0.98	0.06	-2.07	38,38,38,38	0
2	CL	D	589	1/1	0.99	0.03	-3.57	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.