



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2Y0P
Title : CRYSTAL STRUCTURE OF THE SUCA DOMAIN OF MYCOBACTERIUM SMEGMATIS ALPHA-KETOGLUTARATE DECARBOXYLASE IN COMPLEX WITH THE ENAMINE-THDP INTERMEDIATE AND ACETYL-COA
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Deposited on : 2010-12-07
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

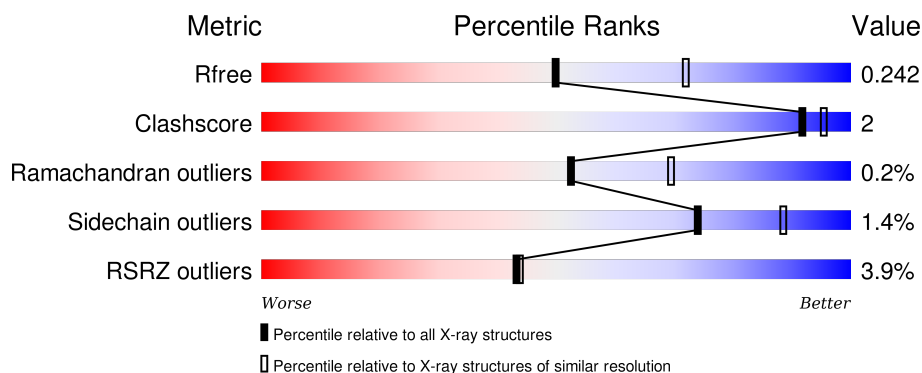
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	868	<div> <div>4%</div> <div>90%</div> <div>7%</div> </div>
1	B	868	<div> <div>4%</div> <div>90%</div> <div>7%</div> </div>
1	C	868	<div> <div>4%</div> <div>92%</div> <div>6%</div> </div>
1	D	868	<div> <div>4%</div> <div>90%</div> <div>6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26809 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.

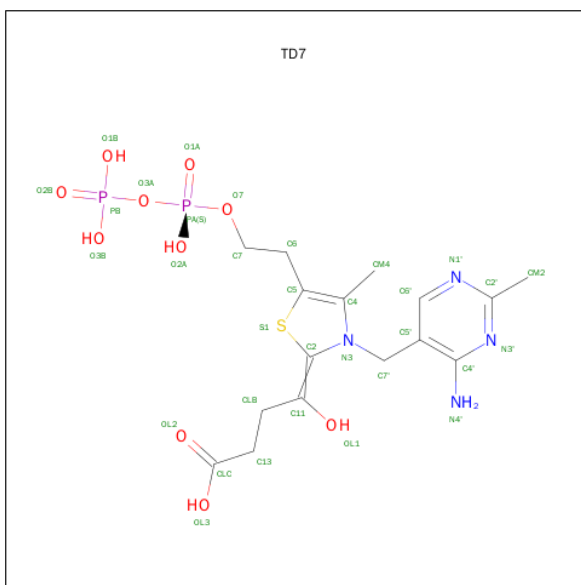
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	847	Total	C	N	O	S	0	0	0
			6518	4102	1151	1241	24			
1	B	839	Total	C	N	O	S	0	0	0
			6459	4065	1136	1234	24			
1	C	856	Total	C	N	O	S	0	0	0
			6577	4142	1157	1254	24			
1	D	837	Total	C	N	O	S	0	0	0
			6414	4043	1128	1219	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
B	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
C	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
D	360	GLY	-	EXPRESSION TAG	UNP A0R2B1

- Molecule 2 is (4E)-4-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-(2-[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY)ETHYL)-4-METHYL-1,3-THIAZOL-2(3H)-YLIDENE}-4-HYDROXYBUTANOIC ACID (three-letter code: TD7) (formula: C₁₆H₂₄N₄O₁₀P₂S).

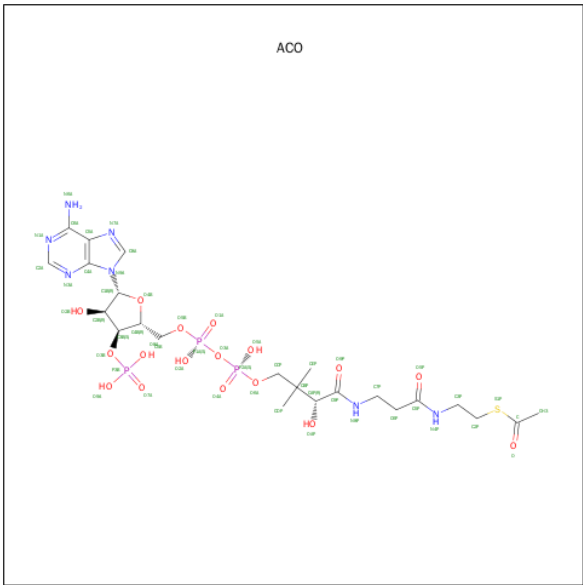


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 33	C 16	N 4	O 10	P 2	S 1	0	0
2	B	1	Total 33	C 16	N 4	O 10	P 2	S 1	0	0
2	C	1	Total 33	C 16	N 4	O 10	P 2	S 1	0	0
2	D	1	Total 33	C 16	N 4	O 10	P 2	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
4	D	1	Total	C	N	O	P		0	0
			38	16	5	14	3			

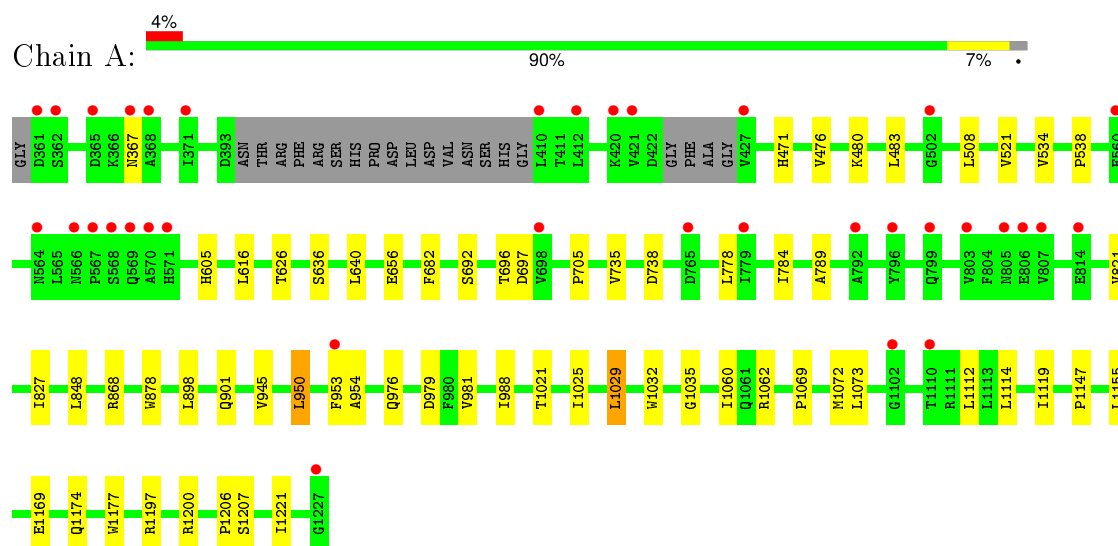
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		
5	B	143	Total	O	0	0
			143	143		
5	C	119	Total	O	0	0
			119	119		
5	D	118	Total	O	0	0
			118	118		

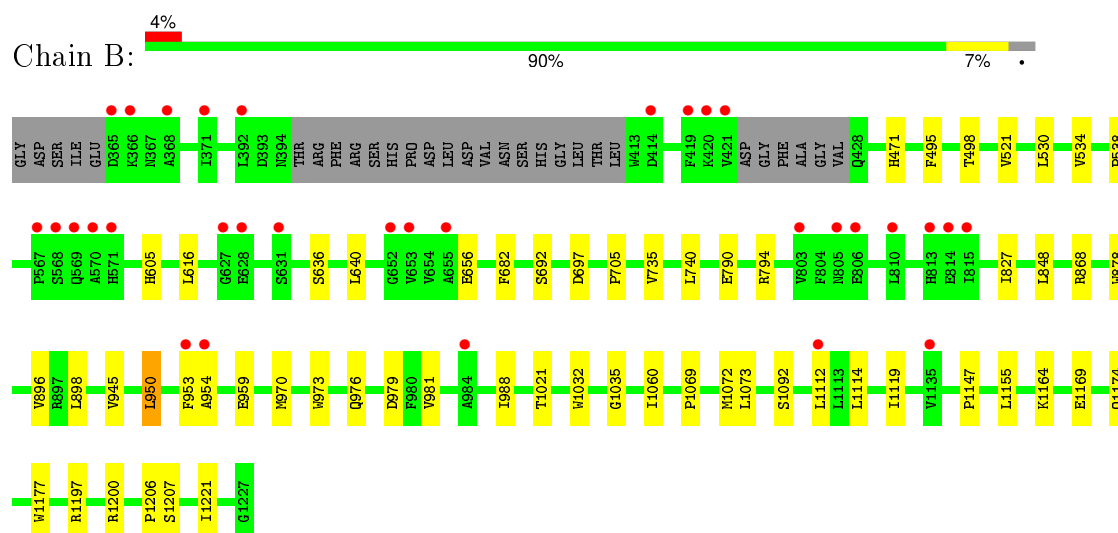
3 Residue-property plots [i](#)

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.

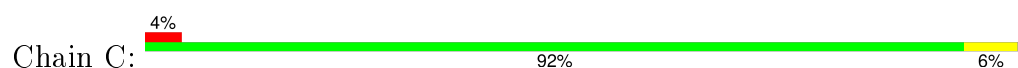
• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE

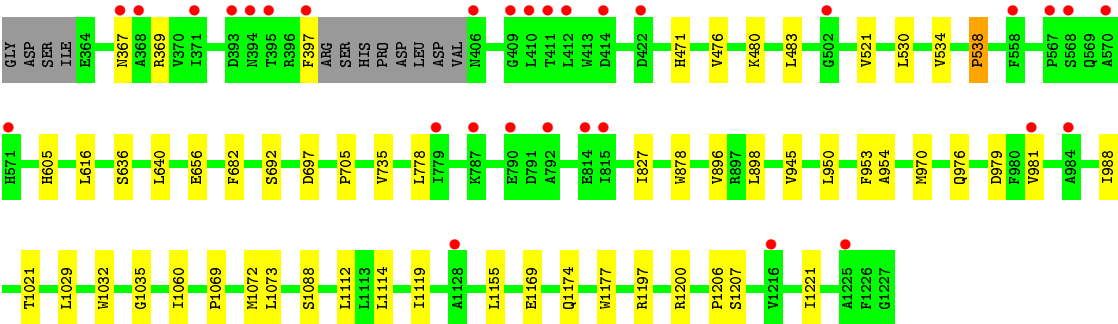


• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE

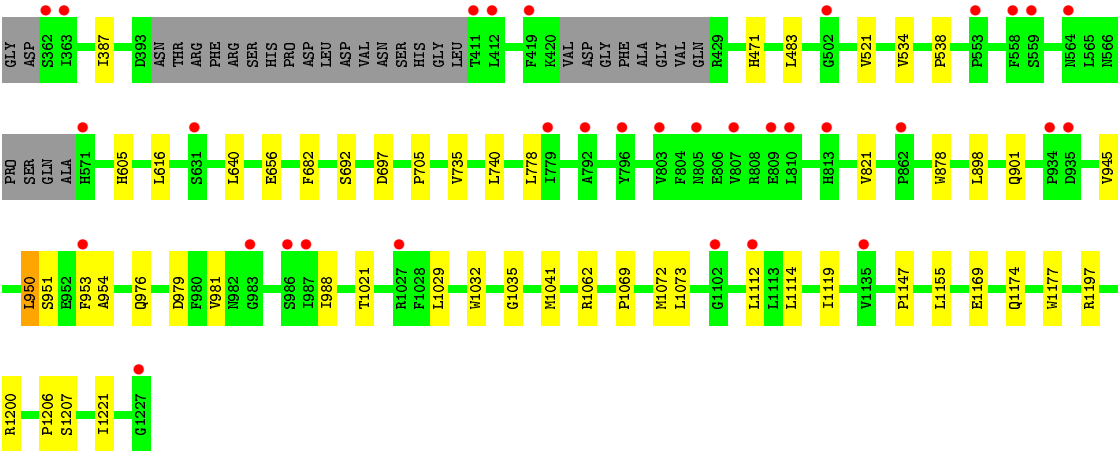
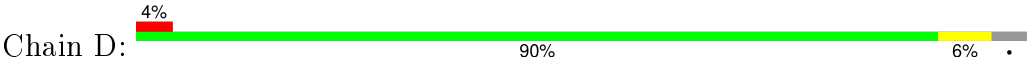


• Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE





● Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.06Å 81.95Å 161.88Å 99.26° 97.09° 100.58°	Depositor
Resolution (Å)	35.14 – 2.40 40.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (35.14-2.40) 89.6 (40.85-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.197 , 0.220 0.215 , 0.242	Depositor DCC
R_{free} test set	7516 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.8	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 149490 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26809	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 16.32% 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, 0.375 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: ACO, MG, TD7

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	0.41	0/6650	0.59	0/9024
1	B	0.42	0/6592	0.59	0/8949
1	C	0.41	0/6713	0.59	0/9112
1	D	0.41	0/6545	0.58	0/8885
All	All	0.41	0/26500	0.59	0/35970

There are no bond length outliers.

There are no bond angle outliers.

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	6518	0	6282	31	0
1	B	6459	0	6214	28	0
1	C	6577	0	6326	23	0
1	D	6414	0	6166	24	0
2	A	33	0	20	2	0
2	B	33	0	20	3	0
2	C	33	0	20	3	0
2	D	33	0	20	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	51	0	34	1	0
4	B	51	0	34	0	0
4	C	51	0	34	0	0
4	D	38	0	21	1	0
5	A	134	0	0	0	0
5	B	143	0	0	0	0
5	C	119	0	0	1	0
5	D	118	0	0	1	0
All	All	26809	0	25191	110	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 2.

All (110) 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:1112:LEU:HD21	1:A:1155:LEU:HD22	1.75	0.67
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.81	0.63
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.81	0.62
1:C:827:ILE:HA	1:C:1060:ILE:HD11	1.82	0.60
2:A:2001:TD7:H4'1	2:A:2001:TD7:C11	2.15	0.59
1:B:848:LEU:HD12	1:B:868:ARG:HD3	1.84	0.59
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.83	0.59
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.84	0.59
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.85	0.59
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.85	0.59
2:C:2001:TD7:C11	2:C:2001:TD7:H4'1	2.16	0.59
2:D:2001:TD7:C11	2:D:2001:TD7:H4'1	2.15	0.58
2:B:2001:TD7:C11	2:B:2001:TD7:H4'1	2.16	0.58
1:A:1032:TRP:CZ2	1:A:1035:GLY:HA2	2.39	0.58
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.87	0.57
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.88	0.56
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	1.88	0.56
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	1.88	0.55
1:D:1041:MET:HE1	5:D:2106:HOH:O	2.06	0.55
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	1.89	0.54
2:C:2001:TD7:HM43	1:D:950:LEU:HD11	1.89	0.54
1:B:1032:TRP:CZ2	1:B:1035:GLY:HA2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:PRO:HG2	1:D:735:VAL:HG13	1.91	0.52
1:A:705:PRO:HG2	1:A:735:VAL:HG13	1.91	0.51
1:C:534:VAL:HG11	1:C:616:LEU:HD23	1.92	0.51
1:B:705:PRO:HG2	1:B:735:VAL:HG13	1.92	0.51
1:C:705:PRO:HG2	1:C:735:VAL:HG13	1.93	0.51
1:D:534:VAL:HG11	1:D:616:LEU:HD23	1.94	0.50
1:A:534:VAL:HG11	1:A:616:LEU:HD23	1.93	0.50
1:D:483:LEU:HD22	1:D:778:LEU:HD12	1.94	0.50
1:B:534:VAL:HG11	1:B:616:LEU:HD23	1.93	0.49
1:C:530:LEU:HD22	1:C:636:SER:HA	1.94	0.49
1:A:656:GLU:HB3	1:A:954:ALA:HB2	1.95	0.49
1:B:656:GLU:HB3	1:B:954:ALA:HB2	1.95	0.48
1:A:1021:THR:HG21	1:A:1207:SER:HB3	1.95	0.48
1:D:1147:PRO:HA	4:D:2228:ACO:H143	1.96	0.48
2:A:2001:TD7:HM43	1:B:950:LEU:HD11	1.96	0.48
1:C:656:GLU:HB3	1:C:954:ALA:HB2	1.94	0.48
1:D:1021:THR:HG21	1:D:1207:SER:HB3	1.95	0.48
1:B:1021:THR:HG21	1:B:1207:SER:HB3	1.96	0.47
1:D:898:LEU:O	1:D:945:VAL:HA	2.15	0.47
1:D:656:GLU:HB3	1:D:954:ALA:HB2	1.96	0.47
1:C:1119:ILE:HD12	1:C:1169:GLU:HG2	1.96	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.15	0.47
1:B:1119:ILE:HD12	1:B:1169:GLU:HG2	1.97	0.47
1:C:1021:THR:HG21	1:C:1207:SER:HB3	1.96	0.46
1:B:1200:ARG:HG3	1:B:1221:ILE:HD11	1.98	0.46
1:A:626:THR:HG21	1:A:636:SER:OG	2.16	0.46
1:B:898:LEU:O	1:B:945:VAL:HA	2.16	0.46
1:B:790:GLU:O	1:B:794:ARG:HG2	2.15	0.46
1:D:1119:ILE:HD12	1:D:1169:GLU:HG2	1.98	0.46
1:A:1025:ILE:HG22	1:A:1029:LEU:HD22	1.98	0.46
1:D:1200:ARG:HG3	1:D:1221:ILE:HD11	1.98	0.45
1:C:898:LEU:O	1:C:945:VAL:HA	2.16	0.45
1:A:1119:ILE:HD12	1:A:1169:GLU:HG2	1.98	0.45
1:C:538:PRO:HD2	5:C:2012:HOH:O	2.17	0.45
1:C:1032:TRP:CZ2	1:C:1035:GLY:HA2	2.51	0.45
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.17	0.45
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.46	0.45
1:A:483:LEU:HD22	1:A:778:LEU:HD12	1.99	0.44
1:A:1174:GLN:OE1	1:A:1206:PRO:HA	2.17	0.44
1:A:950:LEU:HD11	2:B:2001:TD7:HM43	1.99	0.44
1:A:1069:PRO:CB	1:A:1072:MET:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:ARG:HG3	1:A:1221:ILE:HD11	1.99	0.44
1:B:1174:GLN:OE1	1:B:1206:PRO:HA	2.17	0.44
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.18	0.44
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.47	0.44
1:A:784:ILE:HD12	1:A:789:ALA:HB2	1.99	0.44
1:D:821:VAL:O	1:D:1062:ARG:NH2	2.51	0.44
1:C:1200:ARG:HG3	1:C:1221:ILE:HD11	1.98	0.44
1:A:821:VAL:O	1:A:1062:ARG:NH2	2.50	0.44
1:D:1174:GLN:OE1	1:D:1206:PRO:HA	2.17	0.44
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.47	0.44
1:B:1112:LEU:HB3	1:B:1164:LYS:HG2	2.00	0.43
1:A:878:TRP:HB3	1:A:1073:LEU:HD23	2.01	0.43
1:A:1147:PRO:HA	4:A:2228:ACO:H143	1.99	0.43
1:B:521:VAL:HG11	1:B:640:LEU:HD13	2.00	0.43
1:D:692:SER:HB2	1:D:697:ASP:OD2	2.18	0.43
1:A:508:LEU:O	1:A:508:LEU:HG	2.18	0.43
1:D:387:ILE:HD12	1:D:740:LEU:HD12	2.01	0.42
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.19	0.42
1:D:1032:TRP:CZ2	1:D:1035:GLY:HA2	2.54	0.42
1:A:827:ILE:HA	1:A:1060:ILE:HD11	2.01	0.42
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.55	0.42
1:A:476:VAL:HG12	1:A:480:LYS:HE3	2.01	0.42
2:C:2001:TD7:H6'	1:D:901:GLN:OE1	2.20	0.42
1:C:521:VAL:HG11	1:C:640:LEU:HD13	2.02	0.42
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.20	0.41
1:B:896:VAL:HG22	1:B:970:MET:HB3	2.02	0.41
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.55	0.41
1:A:901:GLN:OE1	2:B:2001:TD7:H6'	2.21	0.41
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.56	0.41
1:D:878:TRP:HB3	1:D:1073:LEU:HD23	2.03	0.41
1:B:1092:SER:HB2	1:B:1147:PRO:HG3	2.03	0.41
1:C:476:VAL:HG12	1:C:480:LYS:HE3	2.02	0.41
1:B:530:LEU:HD22	1:B:636:SER:HA	2.01	0.41
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.02	0.41
1:A:521:VAL:HG11	1:A:640:LEU:HD13	2.03	0.41
1:C:878:TRP:HB3	1:C:1073:LEU:HD23	2.02	0.41
1:C:896:VAL:HG22	1:C:970:MET:HB3	2.03	0.41
1:B:959:GLU:HG3	1:B:973:TRP:HB2	2.03	0.40
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.56	0.40
1:C:483:LEU:HD22	1:C:778:LEU:HD12	2.02	0.40
1:B:827:ILE:HA	1:B:1060:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:LEU:HD12	1:A:1029:LEU:HA	1.93	0.40
1:B:878:TRP:HB3	1:B:1073:LEU:HD23	2.02	0.40
1:A:848:LEU:HD12	1:A:868:ARG:HD2	2.04	0.40
1:D:521:VAL:HG11	1:D:640:LEU:HD13	2.02	0.40
1:B:495:PHE:O	1:B:498:THR:HG22	2.21	0.40
1:B:740:LEU:HA	1:B:740:LEU:HD23	1.99	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	841/868 (97%)	817 (97%)	22 (3%)	2 (0%)	52	69
1	B	833/868 (96%)	808 (97%)	23 (3%)	2 (0%)	52	69
1	C	852/868 (98%)	824 (97%)	26 (3%)	2 (0%)	52	69
1	D	829/868 (96%)	804 (97%)	23 (3%)	2 (0%)	52	69
All	All	3355/3472 (97%)	3253 (97%)	94 (3%)	8 (0%)	52	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	HIS
1	B	605	HIS
1	D	605	HIS
1	A	605	HIS
1	A	538	PRO
1	D	538	PRO
1	B	538	PRO
1	C	538	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	669/726 (92%)	660 (99%)	9 (1%)	76	89
1	B	665/726 (92%)	658 (99%)	7 (1%)	80	92
1	C	674/726 (93%)	662 (98%)	12 (2%)	66	84
1	D	656/726 (90%)	647 (99%)	9 (1%)	74	88
All	All	2664/2904 (92%)	2627 (99%)	37 (1%)	74	88

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	471	HIS
1	A	682	PHE
1	A	950	LEU
1	A	953	PHE
1	A	976	GLN
1	A	979	ASP
1	A	1029	LEU
1	A	1114	LEU
1	B	471	HIS
1	B	682	PHE
1	B	950	LEU
1	B	953	PHE
1	B	976	GLN
1	B	979	ASP
1	B	1114	LEU
1	C	367	ASN
1	C	369	ARG
1	C	397	PHE
1	C	471	HIS
1	C	682	PHE
1	C	950	LEU
1	C	953	PHE
1	C	976	GLN

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Mol	Chain	Res	Type
1	C	979	ASP
1	C	1029	LEU
1	C	1088	SER
1	C	1114	LEU
1	D	471	HIS
1	D	682	PHE
1	D	950	LEU
1	D	951	SER
1	D	953	PHE
1	D	976	GLN
1	D	979	ASP
1	D	1029	LEU
1	D	1114	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	428	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
2	TD7	A	2001	3	25,34,34	1.79	4 (16%)	36,50,50	1.97	13 (36%)
4	ACO	A	2228	-	43,53,53	1.32	5 (11%)	55,79,79	1.91	10 (18%)
2	TD7	B	2001	3	25,34,34	1.77	4 (16%)	36,50,50	1.94	12 (33%)
4	ACO	B	2228	-	43,53,53	1.46	3 (6%)	55,79,79	1.97	11 (20%)
2	TD7	C	2001	3	25,34,34	1.80	4 (16%)	36,50,50	1.98	14 (38%)
4	ACO	C	2228	-	43,53,53	1.43	7 (16%)	55,79,79	2.00	8 (14%)
2	TD7	D	2001	3	25,34,34	1.78	4 (16%)	36,50,50	1.98	13 (36%)
4	ACO	D	2228	-	32,40,53	1.34	3 (9%)	40,63,79	1.99	6 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TD7	A	2001	3	-	0/19/26/26	0/2/2/2
4	ACO	A	2228	-	-	0/47/67/67	0/3/3/3
2	TD7	B	2001	3	-	0/19/26/26	0/2/2/2
4	ACO	B	2228	-	-	0/47/67/67	0/3/3/3
2	TD7	C	2001	3	-	0/19/26/26	0/2/2/2
4	ACO	C	2228	-	-	0/47/67/67	0/3/3/3
2	TD7	D	2001	3	-	0/19/26/26	0/2/2/2
4	ACO	D	2228	-	-	0/30/50/67	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD7	C2-N3	-4.92	1.30	1.38
2	A	2001	TD7	C2-N3	-4.88	1.30	1.38
2	D	2001	TD7	C2-N3	-4.75	1.30	1.38
2	B	2001	TD7	C2-N3	-4.72	1.30	1.38
2	A	2001	TD7	C4-N3	-3.21	1.32	1.39
2	D	2001	TD7	C4-N3	-3.14	1.33	1.39
2	C	2001	TD7	C4-N3	-3.11	1.33	1.39
2	B	2001	TD7	C4-N3	-3.06	1.33	1.39
4	A	2228	ACO	C8A-N7A	-2.30	1.30	1.34
4	C	2228	ACO	P1A-O2A	-2.05	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2228	ACO	P3B-O8A	2.23	1.62	1.54
4	C	2228	ACO	P2A-O4A	2.27	1.59	1.51
4	D	2228	ACO	O4B-C1B	2.43	1.44	1.41
4	C	2228	ACO	P3B-O8A	2.60	1.64	1.54
4	C	2228	ACO	C2A-N3A	2.68	1.36	1.32
4	C	2228	ACO	P1A-O1A	2.73	1.61	1.51
4	D	2228	ACO	P3B-O7A	2.83	1.60	1.51
2	B	2001	TD7	PB-O2B	2.89	1.60	1.51
2	D	2001	TD7	PB-O2B	2.97	1.60	1.51
2	A	2001	TD7	PB-O2B	3.01	1.61	1.51
4	D	2228	ACO	P1A-O1A	3.05	1.62	1.51
2	C	2001	TD7	PB-O2B	3.05	1.61	1.51
4	A	2228	ACO	P1A-O1A	3.10	1.62	1.51
4	A	2228	ACO	P3B-O7A	3.21	1.61	1.51
4	A	2228	ACO	O4B-C1B	3.39	1.45	1.41
4	B	2228	ACO	P1A-O1A	3.44	1.63	1.51
4	C	2228	ACO	O4B-C1B	3.59	1.45	1.41
4	B	2228	ACO	P3B-O7A	3.61	1.63	1.51
4	C	2228	ACO	P3B-O7A	3.97	1.64	1.51
2	A	2001	TD7	OL1-C11	4.30	1.43	1.32
2	D	2001	TD7	OL1-C11	4.45	1.43	1.32
2	B	2001	TD7	OL1-C11	4.49	1.43	1.32
2	C	2001	TD7	OL1-C11	4.49	1.43	1.32
4	B	2228	ACO	O4B-C1B	5.30	1.47	1.41

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2228	ACO	N3A-C2A-N1A	-8.72	122.22	128.89
4	D	2228	ACO	N3A-C2A-N1A	-7.65	123.03	128.89
4	A	2228	ACO	N3A-C2A-N1A	-7.13	123.44	128.89
4	B	2228	ACO	N3A-C2A-N1A	-6.97	123.56	128.89
4	D	2228	ACO	P2A-O3A-P1A	-6.61	114.16	132.73
4	C	2228	ACO	P2A-O3A-P1A	-6.22	115.27	132.73
4	B	2228	ACO	P2A-O3A-P1A	-6.14	115.48	132.73
4	A	2228	ACO	P3B-O3B-C3B	-5.77	107.74	121.56
4	A	2228	ACO	P2A-O3A-P1A	-5.58	117.05	132.73
2	D	2001	TD7	CM4-C4-C5	-5.09	117.45	128.90
4	C	2228	ACO	P3B-O3B-C3B	-5.07	109.41	121.56
2	A	2001	TD7	CM4-C4-C5	-5.05	117.55	128.90
2	B	2001	TD7	CM4-C4-C5	-5.03	117.59	128.90
2	C	2001	TD7	CM4-C4-C5	-4.96	117.75	128.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2228	ACO	P3B-O3B-C3B	-4.45	110.88	121.56
4	C	2228	ACO	C2P-C3P-N4P	-4.34	103.69	112.36
4	B	2228	ACO	C2P-C3P-N4P	-3.63	105.10	112.36
4	C	2228	ACO	C4A-C5A-N7A	-3.23	106.51	109.48
4	D	2228	ACO	P3B-O3B-C3B	-3.12	114.07	121.56
2	D	2001	TD7	CLB-C11-C2	-3.02	117.44	124.27
2	A	2001	TD7	CLB-C11-C2	-2.91	117.68	124.27
4	B	2228	ACO	C6P-C7P-N8P	-2.91	105.49	111.88
2	A	2001	TD7	CLB-C13-CLC	-2.88	107.47	112.75
2	C	2001	TD7	CLB-C11-C2	-2.88	117.76	124.27
2	B	2001	TD7	CLB-C11-C2	-2.88	117.76	124.27
4	D	2228	ACO	C4A-C5A-N7A	-2.79	106.92	109.48
4	B	2228	ACO	C2B-C1B-N9A	-2.74	110.11	114.29
4	B	2228	ACO	O6A-P2A-O4A	-2.71	99.09	109.62
2	C	2001	TD7	CLB-C13-CLC	-2.60	107.98	112.75
4	A	2228	ACO	O6A-CCP-CBP	-2.57	106.42	110.55
2	A	2001	TD7	C5'-C6'-N1'	-2.53	119.47	123.86
2	C	2001	TD7	C5'-C6'-N1'	-2.52	119.49	123.86
2	B	2001	TD7	C5'-C6'-N1'	-2.47	119.56	123.86
4	A	2228	ACO	CEP-CBP-CCP	-2.46	105.31	108.50
2	B	2001	TD7	CLB-C13-CLC	-2.44	108.28	112.75
2	D	2001	TD7	CLB-C13-CLC	-2.42	108.32	112.75
4	A	2228	ACO	C4A-C5A-N7A	-2.37	107.30	109.48
2	D	2001	TD7	N1'-C2'-N3'	-2.32	121.30	125.60
4	A	2228	ACO	C2B-C1B-N9A	-2.31	110.76	114.29
2	D	2001	TD7	C5'-C6'-N1'	-2.30	119.87	123.86
2	C	2001	TD7	N1'-C2'-N3'	-2.21	121.52	125.60
4	A	2228	ACO	O6A-P2A-O4A	-2.18	101.15	109.62
4	C	2228	ACO	C6P-C7P-N8P	-2.16	107.14	111.88
2	A	2001	TD7	N1'-C2'-N3'	-2.08	121.75	125.60
2	C	2001	TD7	C6-C5-C4	2.07	129.41	127.56
4	B	2228	ACO	O3A-P1A-O5B	2.16	108.68	102.94
2	C	2001	TD7	C6-C5-S1	2.19	123.30	120.24
4	C	2228	ACO	O5A-P2A-O3A	2.23	115.19	105.09
2	A	2001	TD7	CM2-C2'-N1'	2.24	119.72	117.03
4	A	2228	ACO	O5A-P2A-O3A	2.30	115.53	105.09
2	B	2001	TD7	CM2-C2'-N1'	2.35	119.84	117.03
4	B	2228	ACO	O5A-P2A-O3A	2.37	115.84	105.09
2	D	2001	TD7	C6-C5-S1	2.38	123.56	120.24
4	D	2228	ACO	O5A-P2A-O3A	2.42	116.08	105.09
4	B	2228	ACO	C7P-N8P-C9P	2.44	127.35	122.53
2	A	2001	TD7	OL1-C11-CLB	2.44	120.55	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	TD7	O3A-PA-O7	2.46	109.47	102.94
2	B	2001	TD7	C6-C5-S1	2.48	123.71	120.24
2	A	2001	TD7	O3A-PA-O7	2.50	109.56	102.94
2	D	2001	TD7	CM2-C2'-N1'	2.53	120.06	117.03
2	C	2001	TD7	OL1-C11-CLB	2.53	120.82	113.86
2	A	2001	TD7	CM4-C4-N3	2.54	126.18	122.82
2	D	2001	TD7	CM4-C4-N3	2.56	126.21	122.82
2	B	2001	TD7	OL1-C11-CLB	2.57	120.91	113.86
2	A	2001	TD7	C6-C5-S1	2.57	123.83	120.24
4	C	2228	ACO	O3A-P2A-O6A	2.62	109.89	102.94
2	D	2001	TD7	O3A-PA-O7	2.63	109.91	102.94
2	C	2001	TD7	CM2-C2'-N1'	2.63	120.19	117.03
2	C	2001	TD7	O3A-PA-O7	2.67	110.02	102.94
2	C	2001	TD7	CM4-C4-N3	2.67	126.36	122.82
4	D	2228	ACO	O3A-P2A-O6A	2.70	110.11	102.94
2	D	2001	TD7	OL1-C11-CLB	2.74	121.39	113.86
2	B	2001	TD7	CM4-C4-N3	2.78	126.50	122.82
4	B	2228	ACO	O3A-P2A-O6A	2.96	110.80	102.94
2	A	2001	TD7	C6'-N1'-C2'	3.01	121.03	115.77
2	B	2001	TD7	C6'-N1'-C2'	3.01	121.03	115.77
2	D	2001	TD7	C6'-N1'-C2'	3.13	121.24	115.77
2	C	2001	TD7	C6'-N1'-C2'	3.23	121.41	115.77
4	A	2228	ACO	O3A-P2A-O6A	3.30	111.69	102.94
2	C	2001	TD7	C5-C4-N3	3.47	115.89	107.83
2	B	2001	TD7	C5-C4-N3	3.48	115.91	107.83
2	D	2001	TD7	C2-N3-C4	3.60	114.17	109.14
2	A	2001	TD7	C5-C4-N3	3.63	116.26	107.83
2	D	2001	TD7	C5-C4-N3	3.66	116.33	107.83
2	A	2001	TD7	C2-N3-C4	3.69	114.29	109.14
2	B	2001	TD7	C2-N3-C4	3.75	114.38	109.14
2	C	2001	TD7	C2-N3-C4	3.90	114.58	109.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TD7	2	0
4	A	2228	ACO	1	0
2	B	2001	TD7	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	TD7	3	0
2	D	2001	TD7	1	0
4	D	2228	ACO	1	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	847/868 (97%)	0.02	35 (4%) 41 42	24, 41, 75, 106	0
1	B	839/868 (96%)	-0.02	32 (3%) 44 45	22, 39, 66, 95	0
1	C	856/868 (98%)	0.01	31 (3%) 46 47	25, 43, 71, 101	0
1	D	837/868 (96%)	0.16	33 (3%) 43 44	27, 45, 73, 107	0
All	All	3379/3472 (97%)	0.05	131 (3%) 43 44	22, 42, 71, 107	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	ALA	5.8
1	A	567	PRO	5.1
1	D	803	VAL	4.8
1	A	568	SER	4.5
1	A	569	GLN	4.5
1	D	807	VAL	4.4
1	D	571	HIS	4.4
1	C	568	SER	4.3
1	C	394	ASN	4.3
1	C	779	ILE	4.1
1	B	421	VAL	4.0
1	A	368	ALA	3.8
1	C	570	ALA	3.8
1	D	502	GLY	3.8
1	A	570	ALA	3.8
1	D	1102	GLY	3.7
1	B	570	ALA	3.7
1	C	502	GLY	3.6
1	A	361	ASP	3.5
1	A	571	HIS	3.5
1	D	1227	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	571	HIS	3.5
1	D	631	SER	3.5
1	C	410	LEU	3.4
1	B	366	LYS	3.4
1	C	567	PRO	3.4
1	D	796	TYR	3.4
1	D	419	PHE	3.3
1	C	409	GLY	3.3
1	D	935	ASP	3.2
1	A	421	VAL	3.2
1	C	414	ASP	3.2
1	C	395	THR	3.1
1	A	796	TYR	3.1
1	B	567	PRO	3.0
1	A	803	VAL	3.0
1	C	368	ALA	3.0
1	A	806	GLU	3.0
1	B	414	ASP	3.0
1	A	1102	GLY	3.0
1	C	406	ASN	3.0
1	D	1135	VAL	2.9
1	B	365	ASP	2.9
1	B	813	HIS	2.9
1	A	365	ASP	2.9
1	D	934	PRO	2.8
1	D	983	GLY	2.8
1	D	779	ILE	2.8
1	C	792	ALA	2.8
1	A	410	LEU	2.8
1	A	564	ASN	2.8
1	D	559	SER	2.8
1	A	502	GLY	2.7
1	A	1227	GLY	2.7
1	C	815	ILE	2.7
1	A	807	VAL	2.7
1	B	568	SER	2.7
1	C	422	ASP	2.7
1	A	420	LYS	2.7
1	A	427	VAL	2.7
1	A	367	ASN	2.7
1	B	805	ASN	2.6
1	A	412	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	787	LYS	2.6
1	D	809	GLU	2.5
1	D	813	HIS	2.5
1	B	806	GLU	2.5
1	D	363	ILE	2.5
1	B	420	LYS	2.5
1	A	792	ALA	2.5
1	B	571	HIS	2.5
1	A	779	ILE	2.5
1	A	698	VAL	2.5
1	B	631	SER	2.5
1	B	627	GLY	2.4
1	B	953	PHE	2.4
1	C	981	VAL	2.4
1	D	986	SER	2.4
1	B	655	ALA	2.4
1	B	803	VAL	2.4
1	B	814	GLU	2.4
1	C	790	GLU	2.4
1	B	815	ILE	2.4
1	A	560	GLU	2.4
1	D	987	ILE	2.4
1	D	862	PRO	2.3
1	B	1112	LEU	2.3
1	D	810	LEU	2.3
1	D	412	LEU	2.3
1	B	653	VAL	2.3
1	B	1135	VAL	2.3
1	C	984	ALA	2.3
1	D	792	ALA	2.3
1	C	393	ASP	2.3
1	B	569	GLN	2.3
1	A	371	ILE	2.3
1	A	799	GLN	2.3
1	A	814	GLU	2.2
1	B	984	ALA	2.2
1	D	805	ASN	2.2
1	C	367	ASN	2.2
1	C	558	PHE	2.2
1	D	553	PRO	2.2
1	C	1225	ALA	2.2
1	C	371	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	558	PHE	2.2
1	C	1128	ALA	2.2
1	C	411	THR	2.2
1	B	810	LEU	2.1
1	A	805	ASN	2.1
1	B	371	ILE	2.1
1	A	765	ASP	2.1
1	B	419	PHE	2.1
1	A	566	ASN	2.1
1	D	1112	LEU	2.1
1	B	628	GLU	2.1
1	B	954	ALA	2.1
1	C	1216	VAL	2.1
1	D	411	THR	2.1
1	D	1027	ARG	2.1
1	D	362	SER	2.1
1	C	814	GLU	2.1
1	C	397	PHE	2.1
1	C	412	LEU	2.1
1	A	1110	THR	2.1
1	B	392	LEU	2.0
1	D	564	ASN	2.0
1	A	953	PHE	2.0
1	D	953	PHE	2.0
1	B	652	GLY	2.0
1	A	362	SER	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(\AA^2)	Q<0.9
2	TD7	A	2001	33/33	0.98	0.18	0.28	15,29,115,173	0
4	ACO	A	2228	51/51	0.95	0.13	0.03	37,50,63,66	0
2	TD7	D	2001	33/33	0.98	0.15	-0.42	18,33,71,103	0
2	TD7	C	2001	33/33	0.98	0.13	-0.58	17,29,68,190	0
4	ACO	B	2228	51/51	0.96	0.12	-0.66	22,36,48,51	0
4	ACO	C	2228	51/51	0.96	0.12	-0.71	24,38,48,50	0
2	TD7	B	2001	33/33	0.98	0.13	-0.78	8,26,58,86	0
4	ACO	D	2228	38/51	0.96	0.11	-1.05	43,57,63,65	0
3	MG	A	2002	1/1	0.99	0.11	-2.15	17,17,17,17	0
3	MG	D	2002	1/1	0.99	0.07	-3.38	20,20,20,20	0
3	MG	C	2002	1/1	0.98	0.07	-3.95	16,16,16,16	0
3	MG	B	2002	1/1	0.99	0.05	-4.88	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.