WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:23 AM GMT

PDB ID	:	2QIO
Title	:	X-Ray Structure of Enoyl-Acyl Carrier Protein Reductase from Bacillus Anthracis with Triclosan
Authors	:	Klein, G.M.; Santarsiero, B.D.; Mesecar, A.D.
Deposited on	:	2007-07-05
Resolution	:	2.44 Å(reported)

The following versions of software and data (see references (1)) 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 2.44 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		0.186
Clashscore		10
Ramachandran outliers		1.1%
Sidechain outliers		4.5%
RSRZ outliers		2.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
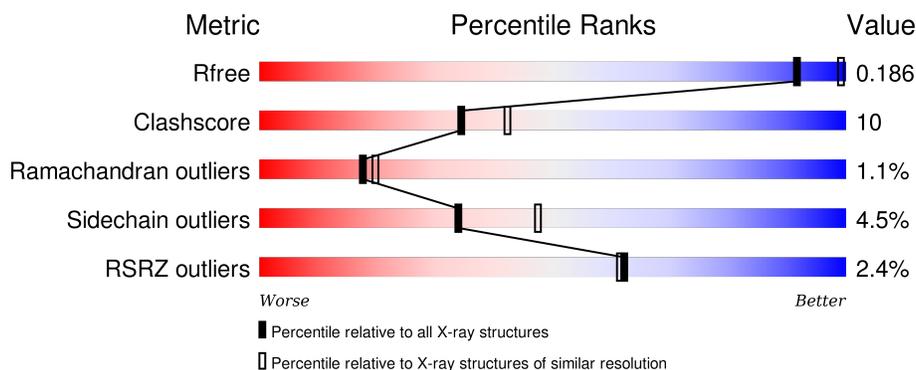
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	256	79% · · · 20% ·
1	B	256	3% · 75% · · 21% ·
1	C	256	2% · 81% · · 18% ·
1	D	256	4% · 77% · · 19% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8460 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 Enoyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1950	1217	347	379	7			
1	B	256	Total	C	N	O	S	0	0	0
			1950	1217	347	379	7			
1	C	256	Total	C	N	O	S	0	0	0
			1950	1217	347	379	7			
1	D	256	Total	C	N	O	S	0	0	0
			1950	1217	347	379	7			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
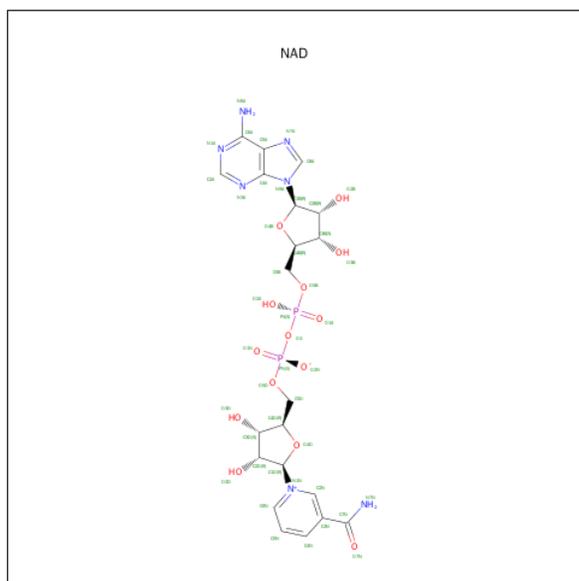
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).
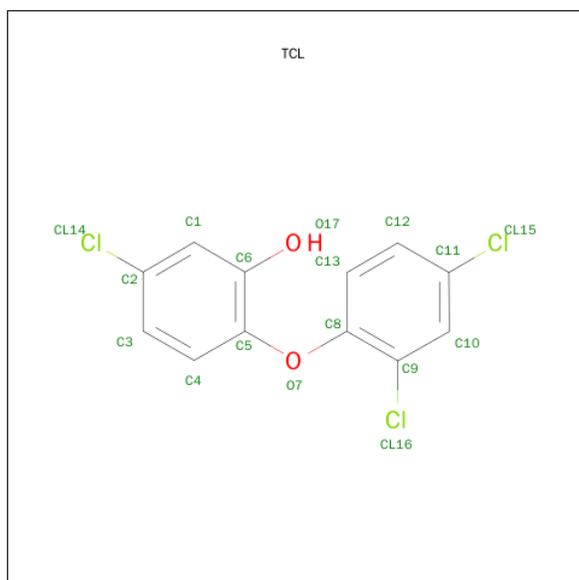
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	100	Total	O	0	0
			100	100		
4	C	104	Total	O	0	0
			104	104		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	87	Total　O 87　　87		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Enoyl-(Acyl-carrier-protein) reductase
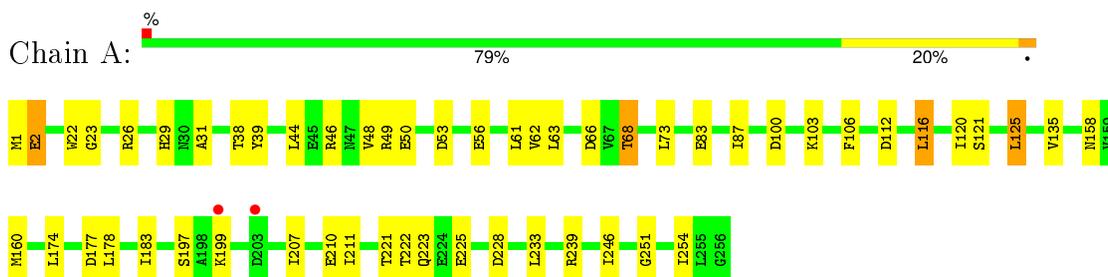
- Molecule 1: Enoyl-(Acyl-carrier-protein) reductase
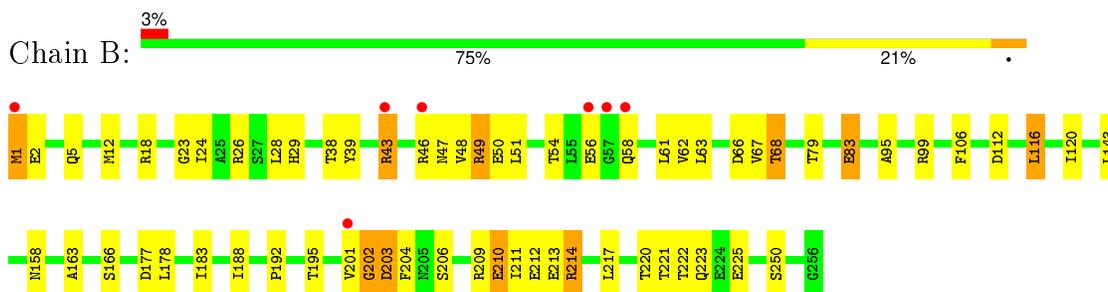
- Molecule 1: Enoyl-(Acyl-carrier-protein) reductase
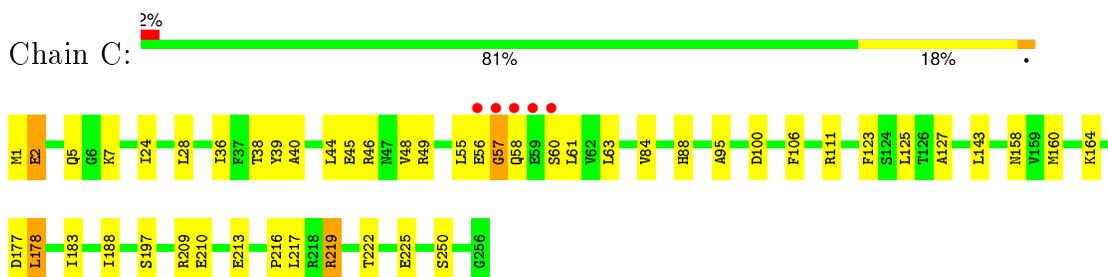
- Molecule 1: Enoyl-(Acyl-carrier-protein) reductase
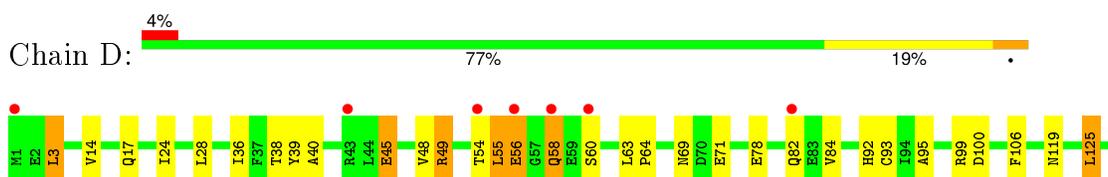
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.37Å 89.02Å 186.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.44 48.07 – 2.42	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.44) 96.7 (48.07-2.42)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.223 0.177 , 0.186	Depositor DCC
R_{free} test set	2221 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	1 of 44930 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8460	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: TCL, NAD

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	0.54	0/1975	0.74	0/2667
1	B	0.53	0/1975	0.71	0/2667
1	C	0.52	0/1975	0.71	0/2667
1	D	0.49	0/1975	0.71	0/2667
All	All	0.52	0/7900	0.72	0/10668

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	1950	0	1952	39	0
1	B	1950	0	1952	48	0
1	C	1950	0	1952	38	0
1	D	1950	0	1952	44	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	17	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	6	1	0
3	C	17	0	7	2	0
3	D	17	0	7	1	0
4	A	125	0	0	5	0
4	B	100	0	0	3	0
4	C	104	0	0	3	0
4	D	87	0	0	7	0
All	All	8460	0	7938	159	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 10.

All (159) 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:D:221:THR:HG22	1:D:225:GLU:OE1	1.76	0.86
1:C:38:THR:HA	1:C:63:LEU:O	1.83	0.77
1:C:160:MET:HE1	1:C:164:LYS:HE2	1.69	0.75
1:C:36:ILE:HD11	1:C:84:VAL:HG21	1.71	0.72
1:D:17:GLN:HG2	4:D:668:HOH:O	1.89	0.71
1:A:66:ASP:OD1	1:A:68:THR:HG22	1.89	0.71
1:C:217:LEU:HD12	1:C:250:SER:HA	1.72	0.71
1:B:66:ASP:OD1	1:B:68:THR:HB	1.91	0.71
1:B:192:PRO:HG2	1:B:211:ILE:HD11	1.72	0.70
1:A:87:ILE:HG12	1:A:135:VAL:HG23	1.73	0.70
1:A:2:GLU:O	1:A:2:GLU:HG2	1.91	0.70
1:C:60:SER:HA	4:C:667:HOH:O	1.93	0.69
1:C:160:MET:CE	1:C:164:LYS:HE2	2.22	0.68
1:D:38:THR:HA	1:D:63:LEU:O	1.92	0.68
1:C:222:THR:OG1	1:C:225:GLU:HG3	1.94	0.68
1:D:137:THR:O	1:D:138:GLU:HB2	1.93	0.68
1:B:38:THR:HA	1:B:63:LEU:O	1.93	0.68
1:B:49:ARG:HA	1:B:49:ARG:HH11	1.59	0.68
1:B:203:ASP:OD1	1:B:206:SER:HB3	1.94	0.67
1:D:71:GLU:H	1:D:71:GLU:CD	2.00	0.65
1:C:61:LEU:HD11	1:C:63:LEU:HD21	1.77	0.65
1:B:1:MET:HG3	1:C:1:MET:SD	2.37	0.64
1:A:228:ASP:OD2	1:D:239:ARG:NH2	2.31	0.64
1:D:78:GLU:HG3	1:D:82:GLN:HE21	1.63	0.63
1:C:46:ARG:HB3	4:C:692:HOH:O	1.98	0.63
1:C:2:GLU:OE1	1:C:2:GLU:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:HIS:HD2	4:B:693:HOH:O	1.81	0.62
1:D:55:LEU:O	1:D:56:GLU:HB2	1.99	0.62
1:C:58:GLN:OE1	1:C:60:SER:HB2	1.99	0.61
1:A:26:ARG:HH11	1:A:26:ARG:HG3	1.66	0.61
1:C:209:ARG:HG2	1:C:213:GLU:OE2	2.00	0.60
1:B:212:GLU:HG3	1:B:220:THR:HG23	1.84	0.60
1:D:39:TYR:CZ	1:D:45:GLU:HG3	2.36	0.60
1:A:46:ARG:O	1:A:50:GLU:HG3	2.01	0.60
1:C:2:GLU:O	1:C:5:GLN:HG3	2.01	0.59
1:D:24:ILE:O	1:D:28:LEU:HG	2.03	0.59
1:A:239:ARG:NH1	4:A:663:HOH:O	2.24	0.59
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.69	0.58
1:A:61:LEU:HD22	1:A:83:GLU:HG2	1.85	0.58
1:B:49:ARG:HG3	1:B:49:ARG:NH1	2.19	0.57
1:B:51:LEU:O	1:B:54:THR:HB	2.03	0.57
1:B:221:THR:HG22	1:B:222:THR:N	2.18	0.57
1:C:61:LEU:CD1	1:C:63:LEU:HD21	2.34	0.57
1:B:49:ARG:CG	1:B:49:ARG:HH11	2.18	0.56
1:B:143:LEU:HD11	1:B:188:ILE:HG13	1.87	0.56
1:B:24:ILE:O	1:B:28:LEU:HG	2.06	0.56
1:D:55:LEU:O	1:D:56:GLU:CB	2.54	0.56
1:D:39:TYR:CZ	1:D:64:PRO:HB3	2.41	0.56
1:C:219:ARG:HD2	4:C:647:HOH:O	2.06	0.55
1:A:38:THR:HA	1:A:63:LEU:O	2.05	0.55
1:A:199:LYS:HG3	4:A:681:HOH:O	2.08	0.54
1:B:221:THR:HG22	1:B:222:THR:H	1.73	0.54
1:C:123:PHE:CE1	1:C:127:ALA:HB2	2.43	0.53
1:A:61:LEU:HD11	1:A:63:LEU:HD21	1.89	0.53
1:A:178:LEU:HB3	1:A:183:ILE:HB	1.89	0.53
1:D:36:ILE:HD11	1:D:84:VAL:HG21	1.89	0.53
1:D:192:PRO:HG2	1:D:211:ILE:HD11	1.91	0.52
1:B:49:ARG:CA	1:B:49:ARG:HH11	2.22	0.52
1:D:3:LEU:HD22	1:D:235:SER:HB2	1.91	0.52
1:D:178:LEU:HB3	1:D:183:ILE:HB	1.91	0.52
1:D:69:ASN:OD1	1:D:71:GLU:OE2	2.27	0.52
1:B:49:ARG:NH1	1:B:62:VAL:HG21	2.25	0.51
1:D:192:PRO:HD2	1:D:211:ILE:HD13	1.93	0.51
1:A:56:GLU:H	1:A:56:GLU:CD	2.14	0.51
1:D:49:ARG:NH2	1:D:60:SER:O	2.43	0.51
1:D:180:GLN:HG3	4:D:627:HOH:O	2.11	0.50
1:B:210:GLU:OE2	1:B:214:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ALA:HB3	3:C:603:TCL:CL16	2.49	0.50
1:A:66:ASP:CG	1:A:68:THR:HG22	2.32	0.50
1:A:1:MET:HG3	1:A:2:GLU:H	1.75	0.50
1:A:177:ASP:OD2	1:B:106:PHE:HB3	2.11	0.49
1:A:106:PHE:HB3	1:B:177:ASP:OD2	2.13	0.49
1:A:39:TYR:HB3	1:A:48:VAL:HG21	1.93	0.49
1:D:159:VAL:HB	4:D:646:HOH:O	2.13	0.49
1:A:39:TYR:HE1	1:A:62:VAL:HG12	1.78	0.49
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.13	0.48
1:D:92:HIS:O	1:D:144:THR:HA	2.13	0.48
1:A:239:ARG:NE	4:A:663:HOH:O	2.41	0.48
1:B:79:THR:O	1:B:83:GLU:HB2	2.14	0.48
1:B:222:THR:OG1	1:B:225:GLU:HG3	2.14	0.48
1:C:106:PHE:HB3	1:D:177:ASP:OD2	2.14	0.47
1:A:39:TYR:CE1	1:A:62:VAL:HG12	2.50	0.47
1:D:217:LEU:HD12	1:D:250:SER:HA	1.97	0.47
1:C:143:LEU:HD11	1:C:188:ILE:HG13	1.97	0.47
1:A:116:LEU:CD2	1:A:120:ILE:HD12	2.44	0.47
1:B:95:ALA:HB3	3:B:602:TCL:CL16	2.52	0.47
1:A:125:LEU:HD13	1:A:174:LEU:HD12	1.97	0.47
1:D:99:ARG:HG3	4:D:657:HOH:O	2.14	0.47
1:B:192:PRO:HG2	1:B:211:ILE:CD1	2.41	0.46
1:B:209:ARG:O	1:B:213:GLU:HG3	2.15	0.46
1:A:68:THR:HG23	4:A:640:HOH:O	2.16	0.46
1:A:29:HIS:HD2	4:A:726:HOH:O	1.98	0.46
1:B:39:TYR:HB3	1:B:48:VAL:HG21	1.97	0.46
1:B:202:GLY:O	1:B:203:ASP:C	2.54	0.46
1:D:219:ARG:HD2	4:D:632:HOH:O	2.15	0.46
1:D:208:LEU:O	1:D:212:GLU:HG3	2.16	0.46
1:D:180:GLN:N	4:D:627:HOH:O	2.48	0.45
1:B:18:ARG:HD2	4:B:685:HOH:O	2.15	0.45
1:C:49:ARG:HD3	1:C:49:ARG:O	2.17	0.45
1:C:111:ARG:NH1	1:D:119:ASN:OD1	2.49	0.45
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.82	0.44
1:D:251:GLY:O	1:D:254:ILE:HG12	2.16	0.44
1:C:39:TYR:CE2	1:C:45:GLU:HB2	2.52	0.44
1:B:23:GLY:HA3	1:B:223:GLN:HB3	2.00	0.44
1:A:251:GLY:O	1:A:254:ILE:HG12	2.18	0.44
1:A:100:ASP:HA	1:A:103:LYS:HE2	1.99	0.44
1:D:125:LEU:HD13	1:D:174:LEU:HD12	1.99	0.44
1:A:22:TRP:CD1	1:A:26:ARG:NH1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:SER:HB3	3:A:601:TCL:C9	2.47	0.44
1:B:46:ARG:HG3	1:B:50:GLU:OE2	2.18	0.44
1:A:221:THR:HG22	1:A:222:THR:N	2.33	0.43
1:B:116:LEU:CD2	1:B:120:ILE:HD12	2.48	0.43
1:B:46:ARG:HD2	4:B:701:HOH:O	2.18	0.43
1:B:217:LEU:HD12	1:B:250:SER:HA	2.01	0.43
1:B:18:ARG:O	1:B:195:THR:HG22	2.19	0.43
1:A:207:ILE:O	1:A:211:ILE:HG12	2.18	0.43
1:B:178:LEU:HB3	1:B:183:ILE:HB	1.99	0.43
1:C:7:LYS:HD2	1:C:88:HIS:CG	2.54	0.43
1:B:221:THR:HG23	1:B:225:GLU:OE1	2.18	0.43
1:C:56:GLU:CD	1:C:56:GLU:H	2.22	0.42
1:C:177:ASP:OD2	1:D:106:PHE:HB3	2.19	0.42
1:D:93:CYS:HB3	1:D:145:LEU:HD12	2.02	0.42
1:A:1:MET:N	1:A:31:ALA:HA	2.35	0.42
1:D:222:THR:OG1	1:D:225:GLU:HG3	2.19	0.42
1:C:106:PHE:N	1:D:177:ASP:OD2	2.53	0.42
1:C:39:TYR:HB3	1:C:48:VAL:HG21	2.02	0.42
1:C:56:GLU:O	1:C:57:GLY:C	2.57	0.42
1:A:112:ASP:O	1:A:116:LEU:HB2	2.20	0.42
1:A:121:SER:CB	1:A:160:MET:HE3	2.50	0.42
1:C:178:LEU:HB3	1:C:183:ILE:HB	2.02	0.42
1:C:1:MET:HB3	1:C:2:GLU:H	1.73	0.42
1:B:2:GLU:HB3	1:B:5:GLN:NE2	2.35	0.42
1:D:95:ALA:HB3	3:D:604:TCL:CL16	2.57	0.42
1:D:14:VAL:HG23	4:D:625:HOH:O	2.19	0.42
1:A:26:ARG:NH1	1:A:26:ARG:HG3	2.32	0.41
1:B:112:ASP:O	1:B:116:LEU:HB2	2.21	0.41
1:C:55:LEU:HB2	1:C:58:GLN:HG2	2.02	0.41
1:B:163:ALA:O	1:B:166:SER:HB3	2.21	0.41
1:D:137:THR:O	1:D:138:GLU:CB	2.64	0.41
1:B:201:VAL:O	1:B:202:GLY:O	2.39	0.41
1:B:202:GLY:O	1:B:204:PHE:N	2.54	0.41
1:A:49:ARG:HD2	1:A:53:ASP:OD2	2.21	0.41
1:C:217:LEU:HB2	1:C:250:SER:HB3	2.02	0.41
1:C:24:ILE:O	1:C:28:LEU:HG	2.20	0.41
1:B:67:VAL:HG22	2:B:502:NAD:N1A	2.35	0.41
1:D:54:THR:O	1:D:54:THR:HG22	2.21	0.41
1:D:58:GLN:HA	1:D:58:GLN:OE1	2.21	0.41
1:D:180:GLN:HG3	1:D:180:GLN:H	1.63	0.41
1:B:43:ARG:H	1:B:43:ARG:HG2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG3	1:C:1:MET:CE	2.50	0.41
1:D:39:TYR:HB3	1:D:48:VAL:HG21	2.02	0.41
1:C:197:SER:HB3	3:C:603:TCL:C9	2.50	0.41
1:B:1:MET:O	1:B:2:GLU:OE2	2.38	0.41
1:C:58:GLN:CD	1:C:60:SER:HB2	2.41	0.40
1:D:137:THR:C	1:D:139:GLY:H	2.22	0.40
1:A:233:LEU:HD11	1:A:246:ILE:HD12	2.02	0.40
1:C:177:ASP:OD2	1:D:106:PHE:N	2.55	0.40
1:B:12:MET:HG2	1:B:38:THR:OG1	2.22	0.40
1:A:23:GLY:HA3	1:A:223:GLN:HB3	2.04	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	254/256 (99%)	245 (96%)	8 (3%)	1 (0%)	39	49
1	B	254/256 (99%)	238 (94%)	13 (5%)	3 (1%)	16	17
1	C	254/256 (99%)	237 (93%)	14 (6%)	3 (1%)	16	17
1	D	254/256 (99%)	239 (94%)	11 (4%)	4 (2%)	12	11
All	All	1016/1024 (99%)	959 (94%)	46 (4%)	11 (1%)	17	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	GLY
1	B	203	ASP
1	C	57	GLY
1	D	56	GLU
1	C	40	ALA

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Mol	Chain	Res	Type
1	C	158	ASN
1	D	158	ASN
1	A	158	ASN
1	B	158	ASN
1	D	55	LEU
1	D	40	ALA

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	205/205 (100%)	198 (97%)	7 (3%)	44	60
1	B	205/205 (100%)	191 (93%)	14 (7%)	20	26
1	C	205/205 (100%)	197 (96%)	8 (4%)	39	54
1	D	205/205 (100%)	197 (96%)	8 (4%)	39	54
All	All	820/820 (100%)	783 (96%)	37 (4%)	34	47

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

Mol	Chain	Res	Type
1	A	2	GLU
1	A	44	LEU
1	A	68	THR
1	A	73	LEU
1	A	116	LEU
1	A	125	LEU
1	A	210	GLU
1	B	1	MET
1	B	26	ARG
1	B	43	ARG
1	B	47	ASN
1	B	49	ARG
1	B	56	GLU
1	B	58	GLN
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	68	THR
1	B	83	GLU
1	B	99	ARG
1	B	116	LEU
1	B	210	GLU
1	B	214	ARG
1	C	2	GLU
1	C	44	LEU
1	C	100	ASP
1	C	125	LEU
1	C	178	LEU
1	C	210	GLU
1	C	216	PRO
1	C	219	ARG
1	D	3	LEU
1	D	45	GLU
1	D	49	ARG
1	D	58	GLN
1	D	100	ASP
1	D	125	LEU
1	D	180	GLN
1	D	221	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	5	GLN
1	B	30	ASN
1	B	47	ASN
1	B	58	GLN
1	D	82	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)

8 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	#$|Z| > 2$
2	NAD	A	501	-	38,48,48	1.48	5 (13%)	47,73,73	2.30	6 (12%)
3	TCL	A	601	-	18,18,18	2.60	10 (55%)	25,25,25	0.98	1 (4%)
2	NAD	B	502	-	38,48,48	1.33	7 (18%)	47,73,73	2.23	5 (10%)
3	TCL	B	602	-	18,18,18	2.49	12 (66%)	25,25,25	0.91	1 (4%)
2	NAD	C	503	-	38,48,48	1.28	5 (13%)	47,73,73	2.24	5 (10%)
3	TCL	C	603	-	18,18,18	2.51	10 (55%)	25,25,25	0.96	1 (4%)
2	NAD	D	504	-	38,48,48	1.36	5 (13%)	47,73,73	2.27	5 (10%)
3	TCL	D	604	-	18,18,18	2.72	12 (66%)	25,25,25	0.82	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
2	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	TCL	A	601	-	-	0/4/4/4	0/2/2/2
2	NAD	B	502	-	-	0/22/62/62	0/5/5/5
3	TCL	B	602	-	-	0/4/4/4	0/2/2/2
2	NAD	C	503	-	-	0/22/62/62	0/5/5/5
3	TCL	C	603	-	-	0/4/4/4	0/2/2/2
2	NAD	D	504	-	-	0/22/62/62	0/5/5/5
3	TCL	D	604	-	-	0/4/4/4	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	604	TCL	C2-CL14	-2.65	1.68	1.74
3	B	602	TCL	C2-CL14	-2.51	1.68	1.74
3	B	602	TCL	C11-CL15	-2.29	1.69	1.74
3	A	601	TCL	C2-CL14	-2.24	1.69	1.74
3	C	603	TCL	C2-CL14	-2.14	1.69	1.74
3	C	603	TCL	C3-C2	2.08	1.42	1.38
2	B	502	NAD	C4N-C3N	2.13	1.42	1.39
2	B	502	NAD	C3N-C7N	2.13	1.53	1.50
3	B	602	TCL	C3-C2	2.14	1.42	1.38
3	B	602	TCL	C4-C5	2.19	1.44	1.39
2	C	503	NAD	C4A-N3A	2.20	1.38	1.35
2	D	504	NAD	C3N-C7N	2.28	1.54	1.50
2	B	502	NAD	C2A-N3A	2.29	1.36	1.32
3	D	604	TCL	C4-C5	2.33	1.44	1.39
3	C	603	TCL	C12-C11	2.34	1.42	1.38
2	B	502	NAD	C2A-N1A	2.40	1.38	1.33
2	C	503	NAD	C2N-C3N	2.43	1.42	1.39
3	B	602	TCL	C12-C11	2.43	1.42	1.38
3	A	601	TCL	C3-C2	2.47	1.42	1.38
2	B	502	NAD	C2N-C3N	2.48	1.42	1.39
3	C	603	TCL	C13-C8	2.48	1.44	1.39
3	C	603	TCL	C10-C9	2.51	1.42	1.38
2	D	504	NAD	C2A-N1A	2.56	1.38	1.33
3	B	602	TCL	C10-C9	2.57	1.42	1.38
2	A	501	NAD	C4A-N3A	2.66	1.39	1.35
3	D	604	TCL	C13-C12	2.67	1.43	1.38
2	C	503	NAD	C6N-N1N	2.69	1.42	1.35
2	D	504	NAD	C2A-N3A	2.76	1.37	1.32
2	A	501	NAD	C6N-N1N	2.77	1.42	1.35
3	D	604	TCL	C1-C2	2.79	1.43	1.38
3	B	602	TCL	C13-C8	2.83	1.45	1.39
3	A	601	TCL	C10-C9	2.88	1.43	1.38
2	C	503	NAD	C2A-N3A	2.89	1.37	1.32
2	A	501	NAD	C2N-C3N	2.91	1.43	1.39
3	A	601	TCL	C12-C11	2.91	1.43	1.38
3	B	602	TCL	C3-C4	2.93	1.44	1.38
2	A	501	NAD	C3N-C7N	2.96	1.55	1.50
3	A	601	TCL	C13-C8	3.01	1.46	1.39
3	D	604	TCL	C12-C11	3.03	1.43	1.38
3	D	604	TCL	C13-C8	3.07	1.46	1.39
2	D	504	NAD	C6N-N1N	3.08	1.43	1.35
3	D	604	TCL	C3-C2	3.10	1.44	1.38
3	A	601	TCL	C3-C4	3.16	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	NAD	C6N-N1N	3.16	1.43	1.35
3	C	603	TCL	C1-C2	3.18	1.43	1.38
3	A	601	TCL	C8-C9	3.18	1.45	1.39
3	D	604	TCL	C10-C9	3.20	1.43	1.38
3	A	601	TCL	C1-C2	3.22	1.43	1.38
3	D	604	TCL	C10-C11	3.36	1.44	1.38
3	B	602	TCL	C1-C2	3.38	1.44	1.38
2	C	503	NAD	O4D-C1D	3.55	1.45	1.41
3	B	602	TCL	C8-C9	3.57	1.46	1.39
2	B	502	NAD	O4D-C1D	3.62	1.45	1.41
3	C	603	TCL	C3-C4	3.68	1.45	1.38
3	B	602	TCL	C1-C6	3.77	1.44	1.38
2	D	504	NAD	O4D-C1D	3.88	1.46	1.41
3	D	604	TCL	C8-C9	3.91	1.46	1.39
3	A	601	TCL	C10-C11	3.95	1.45	1.38
3	D	604	TCL	C3-C4	3.97	1.45	1.38
3	C	603	TCL	C10-C11	4.04	1.45	1.38
3	C	603	TCL	C1-C6	4.04	1.44	1.38
3	B	602	TCL	C10-C11	4.08	1.45	1.38
3	C	603	TCL	C8-C9	4.23	1.47	1.39
3	D	604	TCL	C1-C6	4.38	1.45	1.38
2	A	501	NAD	O4D-C1D	4.46	1.46	1.41
3	A	601	TCL	C1-C6	5.16	1.46	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	N3A-C2A-N1A	-9.58	121.56	128.89
2	D	504	NAD	N3A-C2A-N1A	-9.44	121.67	128.89
2	C	503	NAD	N3A-C2A-N1A	-9.11	121.92	128.89
2	B	502	NAD	N3A-C2A-N1A	-9.10	121.92	128.89
2	B	502	NAD	C4B-O4B-C1B	-6.11	103.00	109.72
2	A	501	NAD	C1B-N9A-C4A	-5.86	118.11	126.94
2	A	501	NAD	C4B-O4B-C1B	-5.60	103.56	109.72
2	D	504	NAD	C4B-O4B-C1B	-5.56	103.60	109.72
2	B	502	NAD	C1B-N9A-C4A	-5.43	118.75	126.94
2	C	503	NAD	C4B-O4B-C1B	-5.42	103.76	109.72
2	C	503	NAD	C1B-N9A-C4A	-5.37	118.84	126.94
2	D	504	NAD	C1B-N9A-C4A	-4.80	119.70	126.94
2	A	501	NAD	O2B-C2B-C3B	-2.45	103.86	111.83
3	A	601	TCL	O7-C5-C6	2.06	120.16	116.12
3	B	602	TCL	C8-C9-CL16	2.11	122.01	119.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	603	TCL	C8-C9-CL16	2.52	122.52	119.42
2	B	502	NAD	C4A-C5A-N7A	3.23	112.45	109.48
2	C	503	NAD	C4A-C5A-N7A	3.33	112.54	109.48
2	A	501	NAD	C4A-C5A-N7A	3.38	112.59	109.48
2	D	504	NAD	C4A-C5A-N7A	3.50	112.70	109.48
2	B	502	NAD	O4D-C1D-N1N	5.78	114.48	108.13
2	A	501	NAD	O4D-C1D-N1N	5.91	114.63	108.13
2	C	503	NAD	O4D-C1D-N1N	6.29	115.04	108.13
2	D	504	NAD	O4D-C1D-N1N	6.63	115.42	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TCL	1	0
2	B	502	NAD	1	0
3	B	602	TCL	1	0
3	C	603	TCL	2	0
3	D	604	TCL	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 (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	256/256 (100%)	-0.36	2 (0%)	87	88	11, 21, 44, 60	0
1	B	256/256 (100%)	-0.28	7 (2%)	58	57	12, 25, 50, 68	0
1	C	256/256 (100%)	-0.07	5 (1%)	68	68	14, 26, 51, 69	0
1	D	256/256 (100%)	0.13	11 (4%)	39	37	13, 28, 60, 77	0
All	All	1024/1024 (100%)	-0.15	25 (2%)	62	61	11, 25, 54, 77	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.1
1	A	199	LYS	3.7
1	C	59	GLU	3.7
1	B	57	GLY	3.6
1	D	203	ASP	3.5
1	C	57	GLY	3.5
1	B	201	VAL	3.5
1	D	56	GLU	3.3
1	D	58	GLN	3.3
1	D	199	LYS	3.1
1	B	58	GLN	2.9
1	C	60	SER	2.9
1	D	43	ARG	2.6
1	C	58	GLN	2.5
1	B	43	ARG	2.1
1	D	54	THR	2.1
1	D	201	VAL	2.1
1	D	1	MET	2.1
1	D	60	SER	2.1
1	B	46	ARG	2.0
1	B	56	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	82	GLN	2.0
1	C	56	GLU	2.0
1	D	165	ALA	2.0
1	A	203	ASP	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	TCL	C	603	17/17	0.81	0.19	1.53	4,18,21,22	0
3	TCL	D	604	17/17	0.80	0.21	1.51	7,22,26,26	0
3	TCL	A	601	17/17	0.85	0.20	1.10	7,19,22,22	0
3	TCL	B	602	17/17	0.85	0.20	0.96	7,19,21,21	0
2	NAD	A	501	44/44	0.98	0.10	-0.47	18,21,24,25	0
2	NAD	C	503	44/44	0.97	0.11	-0.76	15,19,21,24	0
2	NAD	B	502	44/44	0.97	0.10	-0.95	18,21,25,26	0
2	NAD	D	504	44/44	0.97	0.10	-1.19	21,25,28,31	0

6.5 Other polymers (i)

There are no such residues in this entry.