Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:43 PM GMT

PDB ID	:	4PS9
Title	:	Apo structure of Aldehyde Dehydrogenase from Bacillus cereus
Authors	:	Ngo, H.P.T.; Hong, S.H.; Oh, D.K.; Kang, L.W.
Deposited on	:	2014-03-07
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

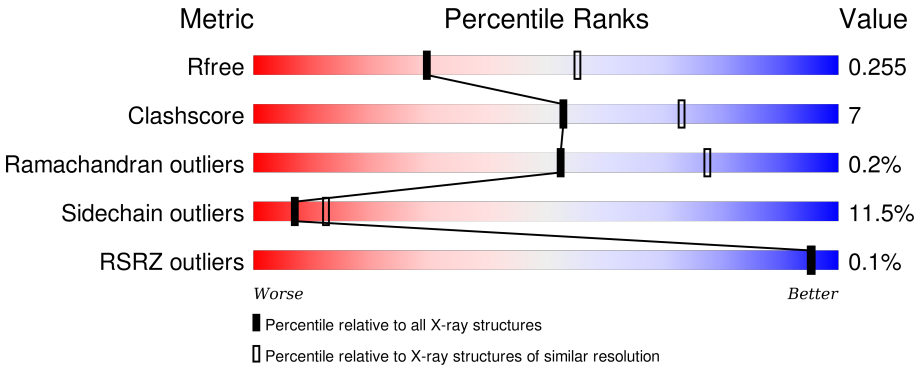
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	494	80% 17%
1	B	494	79% 17%
1	C	494	79% 16%
1	D	494	79% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	501	-	-	-	X
2	NA	B	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15211 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			
1	C	487	Total	C	N	O	S	0	0	0
			3759	2395	625	725	14			
1	D	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is water.

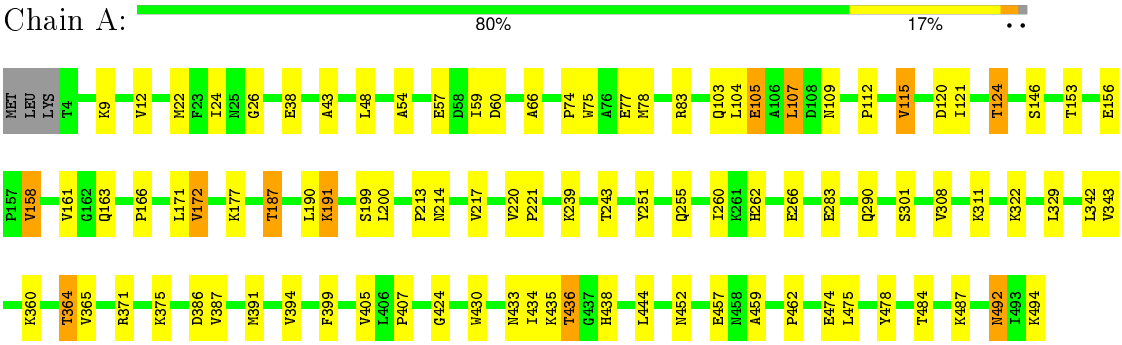
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	24	Total	O	0	0
			24	24		
3	C	23	Total	O	0	0
			23	23		
3	D	16	Total	O	0	0
			16	16		

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.

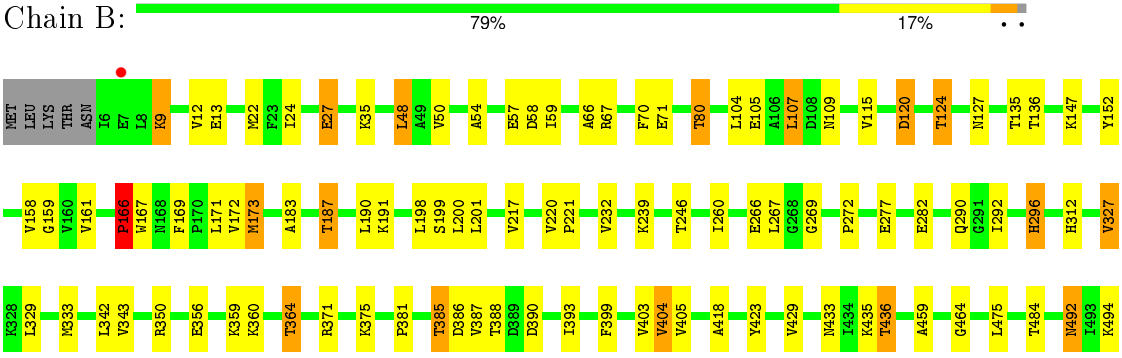
- Molecule 1: Aldehyde dehydrogenase

Chain A:



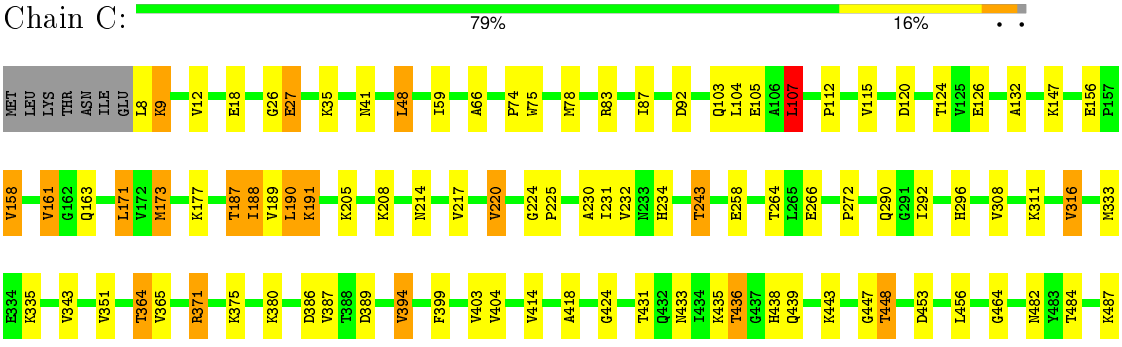
- Molecule 1: Aldehyde dehydrogenase

Chain B:



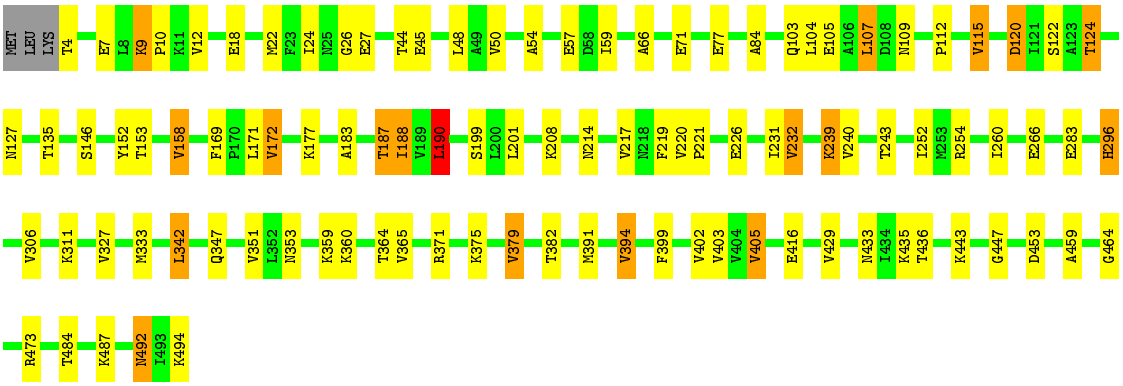
- Molecule 1: Aldehyde dehydrogenase

Chain C:



• Molecule 1: Aldehyde dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.53Å 93.28Å 145.47Å 90.00° 98.05° 90.00°	Depositor
Resolution (Å)	49.57 – 2.60 49.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.57-2.60) 99.1 (49.57-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	38.30 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.252 0.190 , 0.255	Depositor DCC
R_{free} test set	3423 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 27.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 67445 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15211	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.75	0/3870	0.85	1/5250 (0.0%)
1	B	0.74	0/3855	0.85	3/5229 (0.1%)
1	C	0.73	1/3838 (0.0%)	0.84	6/5206 (0.1%)
1	D	0.72	0/3870	0.83	3/5250 (0.1%)
All	All	0.73	1/15433 (0.0%)	0.84	13/20935 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	126	GLU	CG-CD	5.10	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	LEU	CA-CB-CG	7.34	132.17	115.30
1	B	350	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	350	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	92	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	371	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	158	VAL	CB-CA-C	-6.08	99.85	111.40
1	D	158	VAL	CB-CA-C	-5.96	100.08	111.40
1	C	158	VAL	CB-CA-C	-5.62	100.73	111.40
1	D	254	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	190	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	92	ASP	CB-CG-OD1	5.24	123.01	118.30
1	C	107	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	173	MET	CB-CG-SD	-5.01	97.36	112.40

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	3791	0	3740	48	0
1	B	3776	0	3727	53	0
1	C	3759	0	3710	51	0
1	D	3791	0	3740	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	0	1	0
3	B	24	0	0	1	0
3	C	23	0	0	1	0
3	D	16	0	0	0	0
All	All	15211	0	14917	197	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 7.

All (197) 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:188:ILE:HD11	1:C:190:LEU:HB2	1.57	0.87
1:D:266:GLU:OE1	1:D:464:GLY:HA2	1.76	0.84
1:A:105:GLU:OE1	1:A:199:SER:OG	2.00	0.78
1:C:448:THR:HG23	3:C:620:HOH:O	1.85	0.76
1:C:220:VAL:O	1:C:220:VAL:HG12	1.87	0.75
1:C:59:ILE:CD1	1:C:220:VAL:HG11	2.17	0.74
1:A:22:MET:HG2	1:A:221:PRO:HD2	1.70	0.74
1:B:66:ALA:O	1:B:187:THR:HG21	1.89	0.71
1:A:54:ALA:CB	1:A:220:VAL:HG12	2.22	0.70
1:B:80:THR:HG23	1:B:136:THR:HG22	1.74	0.69
1:D:120:ASP:O	1:D:124:THR:HG23	1.93	0.68
1:C:59:ILE:HD11	1:C:220:VAL:HG11	1.78	0.66
1:B:190:LEU:HD13	1:B:191:LYS:N	2.12	0.65
1:A:364:THR:CG2	1:A:386:ASP:OD2	2.44	0.65
1:A:66:ALA:O	1:A:187:THR:HG21	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HD13	1:B:333:MET:HG3	1.77	0.64
1:B:327:VAL:HG13	1:B:381:PRO:HG2	1.79	0.64
1:D:342:LEU:HD22	1:D:379:VAL:HG13	1.79	0.64
1:A:433:ASN:HD22	1:A:436:THR:H	1.45	0.64
1:B:127:ASN:OD1	3:B:614:HOH:O	2.14	0.63
1:C:66:ALA:O	1:C:187:THR:HG21	1.98	0.63
1:C:243:THR:HB	1:C:266:GLU:HB2	1.79	0.63
1:D:66:ALA:HB1	1:D:187:THR:CG2	2.29	0.63
1:B:66:ALA:HB1	1:B:187:THR:CG2	2.28	0.63
1:A:492:ASN:HD21	1:A:494:LYS:HA	1.64	0.63
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.80	0.62
1:C:220:VAL:O	1:C:220:VAL:CG1	2.48	0.62
1:B:59:ILE:HD13	1:B:220:VAL:HG11	1.81	0.62
1:A:75:TRP:CH2	1:A:83:ARG:HD2	2.34	0.62
1:D:169:PHE:HB3	1:D:172:VAL:HG13	1.81	0.61
1:A:38:GLU:OE1	1:C:35:LYS:NZ	2.32	0.60
1:A:364:THR:HG21	1:A:386:ASP:OD2	2.02	0.59
1:C:188:ILE:CD1	1:C:190:LEU:HB2	2.29	0.59
1:C:177:LYS:HZ1	1:C:243:THR:HG22	1.67	0.59
1:C:59:ILE:HD12	1:C:231:ILE:HG13	1.84	0.58
1:A:59:ILE:HD13	1:A:220:VAL:HG11	1.83	0.58
1:B:356:GLU:OE1	1:B:359:LYS:NZ	2.37	0.58
1:C:433:ASN:HB3	1:C:436:THR:HG23	1.84	0.58
1:D:492:ASN:ND2	1:D:494:LYS:H	2.01	0.58
1:D:54:ALA:CB	1:D:220:VAL:HG13	2.33	0.58
1:B:433:ASN:HD22	1:B:436:THR:H	1.52	0.58
1:B:166:PRO:HD2	1:B:173:MET:HG2	1.84	0.58
1:A:9:LYS:HB3	1:A:12:VAL:HG13	1.85	0.58
1:D:124:THR:HG22	1:D:172:VAL:HB	1.85	0.58
1:B:54:ALA:CB	1:B:220:VAL:HG13	2.34	0.57
1:A:120:ASP:O	1:A:124:THR:HG23	2.05	0.57
1:B:266:GLU:OE1	1:B:464:GLY:HA2	2.05	0.56
1:B:152:TYR:OH	1:C:438:HIS:HD2	1.88	0.56
1:D:135:THR:HG22	1:D:183:ALA:HA	1.88	0.56
1:B:67:ARG:O	1:B:71:GLU:HG3	2.06	0.56
1:D:66:ALA:HB1	1:D:187:THR:HG23	1.89	0.55
1:C:66:ALA:HB1	1:C:187:THR:CG2	2.37	0.55
1:B:492:ASN:ND2	1:B:494:LYS:H	2.05	0.55
1:B:22:MET:CE	1:B:24:ILE:HD11	2.36	0.54
1:B:120:ASP:O	1:B:124:THR:HG23	2.07	0.54
1:C:243:THR:HA	1:C:266:GLU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ALA:O	1:D:187:THR:HG21	2.06	0.54
1:C:66:ALA:HB1	1:C:187:THR:HG23	1.88	0.54
1:B:169:PHE:O	1:B:173:MET:HB2	2.08	0.54
1:B:364:THR:HG21	1:B:386:ASP:OD2	2.08	0.54
1:C:9:LYS:H	1:C:103:GLN:HE22	1.56	0.53
1:D:107:LEU:HD13	1:D:333:MET:HG3	1.91	0.53
1:C:264:THR:HG21	1:C:482:ASN:ND2	2.23	0.53
1:D:464:GLY:HA3	1:D:473:ARG:HD3	1.90	0.53
1:C:48:LEU:HD11	1:C:107:LEU:HB3	1.91	0.52
1:D:217:VAL:HG13	1:D:219:PHE:CZ	2.45	0.52
1:D:232:VAL:HG21	1:D:252:ILE:HG12	1.92	0.52
1:D:188:ILE:CD1	1:D:190:LEU:HB2	2.40	0.52
1:D:177:LYS:NZ	1:D:243:THR:OG1	2.42	0.52
1:D:433:ASN:HD22	1:D:436:THR:H	1.56	0.52
1:D:22:MET:CE	1:D:24:ILE:HD11	2.40	0.52
1:B:80:THR:CG2	1:B:136:THR:HG22	2.40	0.51
1:A:9:LYS:H	1:A:103:GLN:HE22	1.57	0.51
1:C:26:GLY:HA3	1:C:214:ASN:ND2	2.26	0.51
1:B:246:THR:HA	1:B:267:LEU:HD13	1.92	0.51
1:B:22:MET:HE3	1:B:24:ILE:HD11	1.93	0.51
1:B:459:ALA:HA	1:B:475:LEU:HD22	1.93	0.51
1:C:439:GLN:O	1:C:443:LYS:HD3	2.11	0.51
1:A:66:ALA:HB1	1:A:187:THR:CG2	2.41	0.51
1:A:260:ILE:HG22	1:A:260:ILE:O	2.11	0.50
1:A:191:LYS:HG2	1:A:220:VAL:O	2.11	0.50
1:C:59:ILE:HD13	1:C:220:VAL:HG11	1.90	0.50
1:A:438:HIS:HD2	1:D:152:TYR:OH	1.94	0.50
1:C:156:GLU:OE2	1:C:487:LYS:HE3	2.12	0.50
1:C:161:VAL:HG23	1:C:163:GLN:HG3	1.93	0.50
1:D:492:ASN:HD22	1:D:494:LYS:H	1.59	0.49
1:C:389:ASP:HA	1:C:394:VAL:HG21	1.93	0.49
1:D:59:ILE:HD12	1:D:231:ILE:HG13	1.94	0.48
1:A:74:PRO:O	1:A:78:MET:HB2	2.14	0.48
1:B:327:VAL:CG1	1:B:381:PRO:HG2	2.43	0.48
1:B:54:ALA:CB	1:B:220:VAL:CG1	2.91	0.48
1:C:447:GLY:HA3	1:C:464:GLY:O	2.13	0.48
1:A:161:VAL:HG12	1:A:187:THR:O	2.13	0.48
1:B:22:MET:HE1	1:B:58:ASP:HB3	1.96	0.48
1:B:190:LEU:HD12	1:B:200:LEU:HD21	1.96	0.47
1:A:433:ASN:HB3	1:A:436:THR:HG23	1.96	0.47
1:D:201:LEU:HD11	1:D:221:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:HIS:CD2	1:C:296:HIS:N	2.83	0.47
1:A:239:LYS:NZ	1:A:262:HIS:HD2	2.12	0.47
1:B:59:ILE:CD1	1:B:220:VAL:HG11	2.43	0.47
1:B:292:ILE:HG12	1:B:403:VAL:HB	1.95	0.47
1:D:127:ASN:OD1	1:D:459:ALA:HB2	2.15	0.47
1:D:26:GLY:HA3	1:D:214:ASN:ND2	2.30	0.47
1:C:87:ILE:HG22	1:C:132:ALA:HB2	1.96	0.47
1:A:190:LEU:HD12	1:A:200:LEU:HD21	1.96	0.47
1:D:153:THR:HA	1:D:487:LYS:O	2.15	0.47
1:C:308:VAL:HG11	1:C:316:VAL:CG1	2.45	0.46
1:D:84:ALA:HB2	1:D:135:THR:OG1	2.15	0.46
1:C:124:THR:HG21	1:C:171:LEU:HD13	1.97	0.46
1:B:269:GLY:HA2	1:B:423:TYR:HB3	1.97	0.46
1:A:364:THR:HG23	1:A:386:ASP:HB2	1.98	0.46
1:D:391:MET:HB2	1:D:394:VAL:HG13	1.98	0.46
1:C:188:ILE:HD12	1:C:189:VAL:N	2.30	0.46
1:C:177:LYS:NZ	1:C:243:THR:CG2	2.79	0.46
1:C:387:VAL:HG11	1:C:404:VAL:HG13	1.98	0.46
1:A:190:LEU:HD12	1:A:200:LEU:CD2	2.46	0.46
1:D:44:THR:O	1:D:45:GLU:HB2	2.16	0.46
1:A:166:PRO:HD3	1:A:243:THR:HB	1.98	0.46
1:D:169:PHE:HB3	1:D:172:VAL:CG1	2.47	0.45
1:B:54:ALA:HB2	1:B:220:VAL:HG13	1.98	0.45
1:D:296:HIS:N	1:D:296:HIS:CD2	2.84	0.45
1:C:27:GLU:HA	1:C:27:GLU:OE2	2.15	0.45
1:A:153:THR:HA	1:A:487:LYS:O	2.17	0.45
1:A:251:TYR:O	1:A:255:GLN:HG2	2.17	0.45
1:D:359:LYS:HE3	1:D:365:VAL:HG21	1.97	0.45
1:B:35:LYS:HE2	1:D:226:GLU:OE2	2.16	0.45
1:D:112:PRO:HB2	1:D:115:VAL:HG13	1.99	0.45
1:A:54:ALA:CB	1:A:220:VAL:CG1	2.94	0.45
1:B:190:LEU:HD13	1:B:190:LEU:C	2.38	0.44
1:D:120:ASP:O	1:D:124:THR:CG2	2.63	0.44
1:B:492:ASN:C	1:B:492:ASN:HD22	2.20	0.44
1:B:27:GLU:HA	1:B:27:GLU:OE2	2.18	0.44
1:B:296:HIS:N	1:B:296:HIS:CD2	2.84	0.44
1:D:382:THR:HB	1:D:402:VAL:HG22	2.00	0.44
1:D:239:LYS:HE3	1:D:240:VAL:O	2.17	0.44
1:A:120:ASP:O	1:A:124:THR:CG2	2.65	0.44
1:A:43:ALA:HB2	3:A:610:HOH:O	2.18	0.44
1:C:190:LEU:HD12	1:C:191:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ALA:HB1	1:B:187:THR:HG23	2.00	0.44
1:C:453:ASP:CG	1:C:456:LEU:HD11	2.38	0.44
1:D:59:ILE:CD1	1:D:220:VAL:HG11	2.48	0.44
1:A:391:MET:HB2	1:A:394:VAL:HG13	1.99	0.44
1:A:430:TRP:CE3	1:A:452:ASN:HA	2.53	0.43
1:C:59:ILE:HD11	1:C:220:VAL:CG1	2.44	0.43
1:D:9:LYS:H	1:D:103:GLN:HE22	1.66	0.43
1:D:54:ALA:HB1	1:D:220:VAL:HG13	1.99	0.43
1:C:112:PRO:HB2	1:C:115:VAL:HG13	2.00	0.43
1:C:74:PRO:O	1:C:78:MET:HB2	2.18	0.43
1:D:306:VAL:HG13	1:D:405:VAL:HB	2.00	0.43
1:A:103:GLN:O	1:A:107:LEU:HB2	2.18	0.43
1:C:41:ASN:OD1	1:C:41:ASN:C	2.56	0.43
1:D:22:MET:HE2	1:D:24:ILE:HD11	2.00	0.43
1:B:22:MET:CG	1:B:221:PRO:HD2	2.47	0.43
1:B:364:THR:HG22	1:B:386:ASP:HB2	1.99	0.43
1:D:124:THR:HG22	1:D:172:VAL:HA	1.99	0.43
1:A:266:GLU:HG3	1:A:474:GLU:OE1	2.19	0.43
1:B:433:ASN:HD21	1:B:435:LYS:HB2	1.85	0.42
1:B:364:THR:HG23	1:B:385:THR:HG22	2.01	0.42
1:A:112:PRO:HB2	1:A:115:VAL:HG13	2.01	0.42
1:D:9:LYS:HA	1:D:10:PRO:HD2	1.87	0.42
1:A:492:ASN:C	1:A:492:ASN:HD22	2.23	0.42
1:B:201:LEU:HD11	1:B:221:PRO:HG3	2.01	0.42
1:B:277:GLU:O	1:B:312:HIS:HE1	2.03	0.42
1:C:230:ALA:O	1:C:234:HIS:HB2	2.20	0.42
1:B:48:LEU:HD13	1:B:198:LEU:CD1	2.49	0.42
1:D:306:VAL:HG12	1:D:403:VAL:CG2	2.50	0.42
1:B:9:LYS:HB2	1:B:12:VAL:HG13	2.02	0.42
1:B:135:THR:HG22	1:B:183:ALA:HA	2.02	0.42
1:D:492:ASN:C	1:D:492:ASN:HD22	2.23	0.42
1:D:260:ILE:O	1:D:260:ILE:HG22	2.19	0.42
1:B:167:TRP:CE3	1:B:343:VAL:HG11	2.54	0.42
1:A:26:GLY:HA3	1:A:214:ASN:ND2	2.35	0.42
1:C:433:ASN:HD22	1:C:436:THR:H	1.66	0.42
1:B:393:ILE:HD12	1:B:404:VAL:CG2	2.49	0.41
1:A:124:THR:HG22	1:A:172:VAL:HB	2.01	0.41
1:C:292:ILE:HG21	1:C:403:VAL:HB	2.02	0.41
1:C:272:PRO:HG3	1:C:418:ALA:HB1	2.03	0.41
1:C:224:GLY:N	1:C:225:PRO:CD	2.83	0.41
1:B:260:ILE:O	1:B:260:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:O	1:A:407:PRO:HA	2.21	0.41
1:C:107:LEU:HD13	1:C:333:MET:HG3	2.03	0.41
1:C:364:THR:CG2	1:C:386:ASP:OD2	2.69	0.41
1:A:22:MET:CE	1:A:24:ILE:HD11	2.51	0.41
1:B:70:PHE:CE1	1:B:159:GLY:HA2	2.55	0.41
1:A:462:PRO:HG3	1:A:478:TYR:CD2	2.56	0.41
1:A:474:GLU:O	1:A:475:LEU:HB2	2.21	0.41
1:A:163:GLN:CD	1:A:177:LYS:HB3	2.41	0.41
1:C:59:ILE:HD12	1:C:231:ILE:CG1	2.48	0.40
1:A:156:GLU:OE2	1:A:487:LYS:HE3	2.22	0.40
1:C:75:TRP:CH2	1:C:83:ARG:HD2	2.57	0.40
1:B:272:PRO:HG3	1:B:418:ALA:HB1	2.04	0.40
1:A:75:TRP:HB2	1:A:213:PRO:HG2	2.02	0.40
1:D:447:GLY:HA3	1:D:464:GLY:O	2.22	0.40
1:C:8:LEU:HD11	1:C:107:LEU:HD21	2.04	0.40
1:A:444:LEU:O	1:D:487:LYS:NZ	2.51	0.40
1:A:459:ALA:HA	1:A:475:LEU:HD22	2.04	0.40
1:D:347:GLN:O	1:D:351:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	489/494 (99%)	468 (96%)	20 (4%)	1 (0%)	52 77
1	B	487/494 (99%)	463 (95%)	23 (5%)	1 (0%)	52 77
1	C	485/494 (98%)	471 (97%)	13 (3%)	1 (0%)	52 77
1	D	489/494 (99%)	463 (95%)	26 (5%)	0	100 100
All	All	1950/1976 (99%)	1865 (96%)	82 (4%)	3 (0%)	52 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	PRO
1	A	424	GLY
1	C	424	GLY

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	398/401 (99%)	358 (90%)	40 (10%)	9 17
1	B	396/401 (99%)	350 (88%)	46 (12%)	7 12
1	C	394/401 (98%)	349 (89%)	45 (11%)	7 12
1	D	398/401 (99%)	347 (87%)	51 (13%)	5 10
All	All	1586/1604 (99%)	1404 (88%)	182 (12%)	7 12

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	57	GLU
1	A	60	ASP
1	A	77	GLU
1	A	104	LEU
1	A	105	GLU
1	A	107	LEU
1	A	109	ASN
1	A	115	VAL
1	A	121	ILE
1	A	124	THR
1	A	146	SER
1	A	158	VAL
1	A	171	LEU
1	A	172	VAL
1	A	187	THR
1	A	191	LYS
1	A	217	VAL
1	A	283	GLU

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Mol	Chain	Res	Type
1	A	290	GLN
1	A	301	SER
1	A	311	LYS
1	A	322	LYS
1	A	329	LEU
1	A	342	LEU
1	A	343	VAL
1	A	360	LYS
1	A	364	THR
1	A	365	VAL
1	A	371	ARG
1	A	375	LYS
1	A	387	VAL
1	A	399	PHE
1	A	405	VAL
1	A	434	ILE
1	A	435	LYS
1	A	436	THR
1	A	457	GLU
1	A	484	THR
1	A	492	ASN
1	B	9	LYS
1	B	13	GLU
1	B	27	GLU
1	B	48	LEU
1	B	50	VAL
1	B	57	GLU
1	B	80	THR
1	B	104	LEU
1	B	105	GLU
1	B	109	ASN
1	B	115	VAL
1	B	120	ASP
1	B	124	THR
1	B	147	LYS
1	B	158	VAL
1	B	161	VAL
1	B	166	PRO
1	B	171	LEU
1	B	172	VAL
1	B	173	MET
1	B	187	THR

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Mol	Chain	Res	Type
1	B	199	SER
1	B	217	VAL
1	B	232	VAL
1	B	239	LYS
1	B	282	GLU
1	B	290	GLN
1	B	296	HIS
1	B	327	VAL
1	B	329	LEU
1	B	342	LEU
1	B	360	LYS
1	B	364	THR
1	B	371	ARG
1	B	375	LYS
1	B	385	THR
1	B	387	VAL
1	B	388	THR
1	B	390	ASP
1	B	399	PHE
1	B	404	VAL
1	B	405	VAL
1	B	429	VAL
1	B	436	THR
1	B	484	THR
1	B	492	ASN
1	C	9	LYS
1	C	12	VAL
1	C	18	GLU
1	C	27	GLU
1	C	48	LEU
1	C	104	LEU
1	C	105	GLU
1	C	107	LEU
1	C	120	ASP
1	C	147	LYS
1	C	158	VAL
1	C	161	VAL
1	C	171	LEU
1	C	173	MET
1	C	187	THR
1	C	188	ILE
1	C	190	LEU

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Mol	Chain	Res	Type
1	C	191	LYS
1	C	205	LYS
1	C	208	LYS
1	C	217	VAL
1	C	220	VAL
1	C	232	VAL
1	C	243	THR
1	C	258	GLU
1	C	290	GLN
1	C	311	LYS
1	C	316	VAL
1	C	335	LYS
1	C	343	VAL
1	C	351	VAL
1	C	364	THR
1	C	365	VAL
1	C	371	ARG
1	C	375	LYS
1	C	380	LYS
1	C	394	VAL
1	C	399	PHE
1	C	414	VAL
1	C	431	THR
1	C	435	LYS
1	C	436	THR
1	C	448	THR
1	C	484	THR
1	C	492	ASN
1	D	4	THR
1	D	7	GLU
1	D	9	LYS
1	D	12	VAL
1	D	18	GLU
1	D	27	GLU
1	D	48	LEU
1	D	50	VAL
1	D	57	GLU
1	D	71	GLU
1	D	77	GLU
1	D	104	LEU
1	D	105	GLU
1	D	107	LEU

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Mol	Chain	Res	Type
1	D	109	ASN
1	D	115	VAL
1	D	120	ASP
1	D	122	SER
1	D	124	THR
1	D	146	SER
1	D	158	VAL
1	D	171	LEU
1	D	172	VAL
1	D	187	THR
1	D	188	ILE
1	D	190	LEU
1	D	199	SER
1	D	208	LYS
1	D	232	VAL
1	D	239	LYS
1	D	283	GLU
1	D	296	HIS
1	D	311	LYS
1	D	327	VAL
1	D	342	LEU
1	D	353	ASN
1	D	360	LYS
1	D	364	THR
1	D	371	ARG
1	D	375	LYS
1	D	379	VAL
1	D	394	VAL
1	D	399	PHE
1	D	405	VAL
1	D	416	GLU
1	D	429	VAL
1	D	435	LYS
1	D	443	LYS
1	D	453	ASP
1	D	484	THR
1	D	492	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN

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Mol	Chain	Res	Type
1	A	214	ASN
1	A	262	HIS
1	A	290	GLN
1	A	325	ASN
1	A	326	ASN
1	A	433	ASN
1	A	438	HIS
1	A	442	ASN
1	A	482	ASN
1	A	492	ASN
1	B	214	ASN
1	B	262	HIS
1	B	312	HIS
1	B	325	ASN
1	B	326	ASN
1	B	433	ASN
1	B	438	HIS
1	B	442	ASN
1	B	482	ASN
1	B	492	ASN
1	C	85	HIS
1	C	103	GLN
1	C	114	GLN
1	C	214	ASN
1	C	262	HIS
1	C	290	GLN
1	C	312	HIS
1	C	326	ASN
1	C	433	ASN
1	C	438	HIS
1	C	442	ASN
1	C	482	ASN
1	C	492	ASN
1	D	103	GLN
1	D	214	ASN
1	D	262	HIS
1	D	312	HIS
1	D	325	ASN
1	D	433	ASN
1	D	438	HIS
1	D	442	ASN
1	D	492	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	491/494 (99%)	-0.50	0 100 100	10, 17, 31, 45	0
1	B	489/494 (98%)	-0.56	1 (0%) 95 95	9, 17, 31, 58	0
1	C	487/494 (98%)	-0.55	0 100 100	9, 18, 31, 43	0
1	D	491/494 (99%)	-0.43	0 100 100	10, 19, 34, 54	0
All	All	1958/1976 (99%)	-0.51	1 (0%) 95 95	9, 18, 32, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	GLU	2.4

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
2	NA	A	501	1/1	0.81	0.19	3.96	28,28,28,28	0
2	NA	B	501	1/1	0.74	0.20	2.16	34,34,34,34	0
2	NA	D	501	1/1	0.93	0.12	-0.54	31,31,31,31	0
2	NA	C	501	1/1	0.95	0.11	-1.53	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.