Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:55 PM GMT

PDB ID	:	4JX8
Title	:	Crystal Structure of E.coli Enoyl Reductase in Complex with NAD and AEA16
Authors	:	Subramanya, H.; Rao, K.N.; Anirudha, L.
Deposited on	:	2013-03-28
Resolution	:	3.20 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:

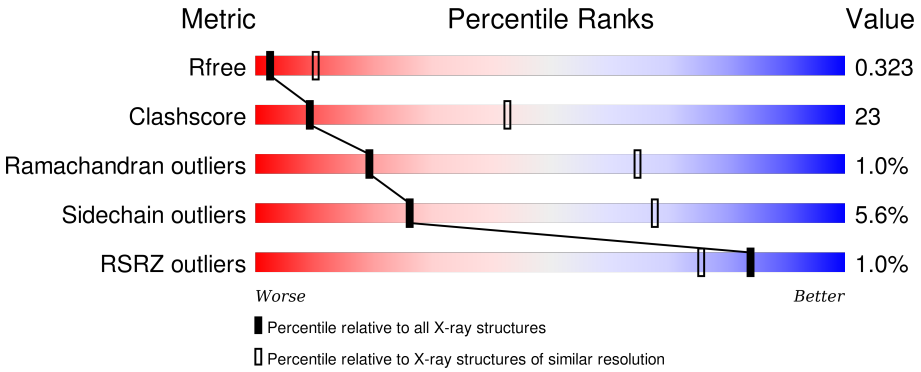
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	282	% 52% 33% • • 9%
1	B	282	57% 27% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3896 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 [NADH] FabI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1894	1191	326	364	13			
1	B	244	Total	C	N	O	S	0	0	0
			1802	1135	307	348	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P0AEK4
A	-18	GLY	-	EXPRESSION TAG	UNP P0AEK4
A	-17	SER	-	EXPRESSION TAG	UNP P0AEK4
A	-16	SER	-	EXPRESSION TAG	UNP P0AEK4
A	-15	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	-14	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	-13	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	-12	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	-11	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	-10	HIS	-	EXPRESSION TAG	UNP P0AEK4
A	-9	SER	-	EXPRESSION TAG	UNP P0AEK4
A	-8	SER	-	EXPRESSION TAG	UNP P0AEK4
A	-7	GLY	-	EXPRESSION TAG	UNP P0AEK4
A	-6	LEU	-	EXPRESSION TAG	UNP P0AEK4
A	-5	VAL	-	EXPRESSION TAG	UNP P0AEK4
A	-4	PRO	-	EXPRESSION TAG	UNP P0AEK4
A	-3	ARG	-	EXPRESSION TAG	UNP P0AEK4
A	-2	GLY	-	EXPRESSION TAG	UNP P0AEK4
A	-1	SER	-	EXPRESSION TAG	UNP P0AEK4
A	0	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	-19	MET	-	EXPRESSION TAG	UNP P0AEK4
B	-18	GLY	-	EXPRESSION TAG	UNP P0AEK4
B	-17	SER	-	EXPRESSION TAG	UNP P0AEK4
B	-16	SER	-	EXPRESSION TAG	UNP P0AEK4
B	-15	HIS	-	EXPRESSION TAG	UNP P0AEK4

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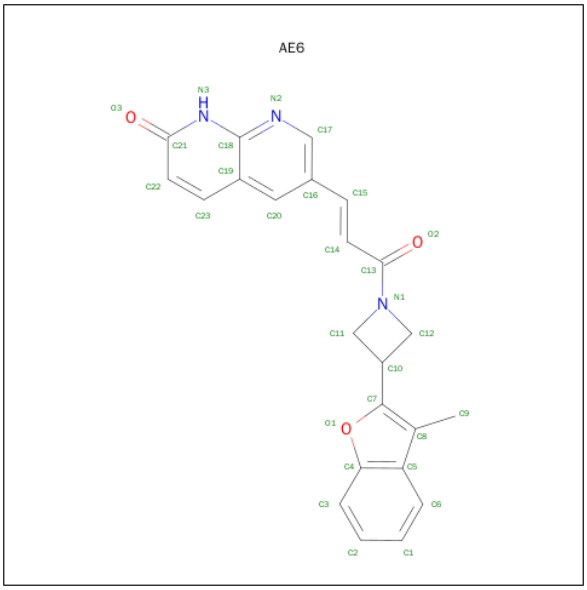
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	-13	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	-12	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	-11	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	-10	HIS	-	EXPRESSION TAG	UNP P0AEK4
B	-9	SER	-	EXPRESSION TAG	UNP P0AEK4
B	-8	SER	-	EXPRESSION TAG	UNP P0AEK4
B	-7	GLY	-	EXPRESSION TAG	UNP P0AEK4
B	-6	LEU	-	EXPRESSION TAG	UNP P0AEK4
B	-5	VAL	-	EXPRESSION TAG	UNP P0AEK4
B	-4	PRO	-	EXPRESSION TAG	UNP P0AEK4
B	-3	ARG	-	EXPRESSION TAG	UNP P0AEK4
B	-2	GLY	-	EXPRESSION TAG	UNP P0AEK4
B	-1	SER	-	EXPRESSION TAG	UNP P0AEK4
B	0	HIS	-	EXPRESSION TAG	UNP P0AEK4

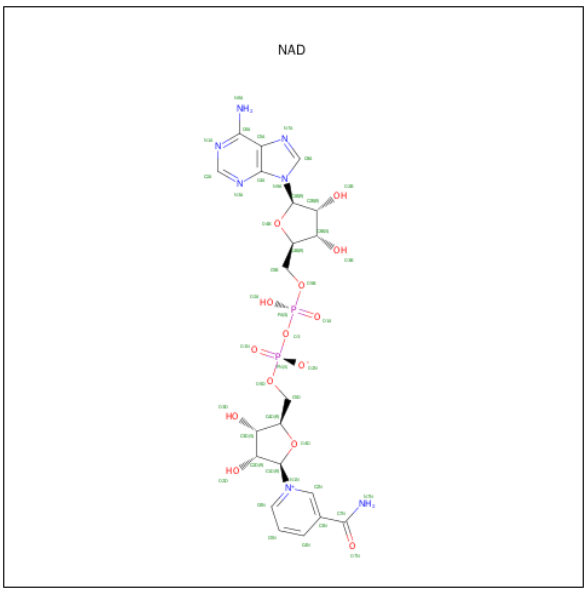
- Molecule 2 is 6-{(1E)-3-[3-(3-METHYL-1-BENZOFURAN-2-YL)AZETIDIN-1-YL]-3-OXO PROP-1-EN-1-YL}-1,8-NAPHTHYRIDIN-2(1H)-ONE (three-letter code: AE6) (formula: $C_{23}H_{19}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	23	3	3		
2	B	1	Total	C	N	O	0	0
			29	23	3	3		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)

(formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is water.

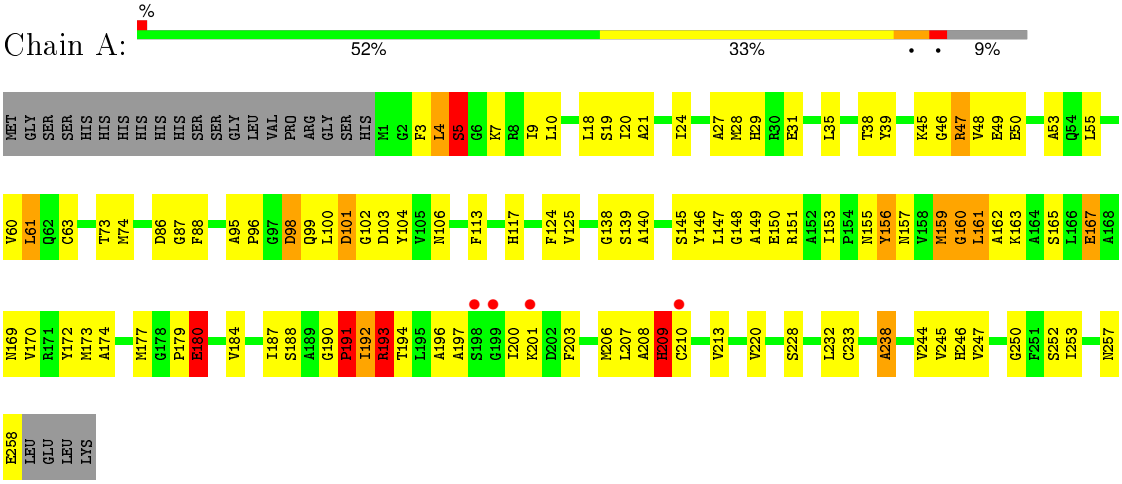
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	28	Total	O	0	0
			28	28		

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.

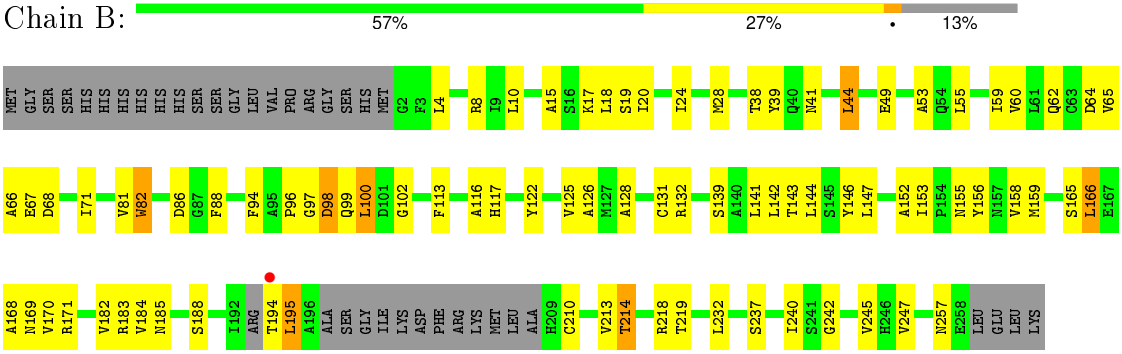
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain A:



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	79.63Å 79.63Å 323.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.24 – 3.20 29.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	77.0 (29.24-3.20) 77.2 (29.05-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	16.87 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.326 0.227 , 0.323	Depositor DCC
R_{free} test set	522 reflections (6.57%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 8344 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	3896	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: NAD, AE6

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	0.57	0/1926	1.03	14/2606 (0.5%)
1	B	0.55	1/1830 (0.1%)	0.82	3/2473 (0.1%)
All	All	0.56	1/3756 (0.0%)	0.94	17/5079 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	TRP	CD2-CE2	5.54	1.48	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ARG	CB-CA-C	-14.83	80.74	110.40
1	A	209	HIS	C-N-CA	-12.08	91.49	121.70
1	B	195	LEU	CB-CA-C	11.28	131.63	110.20
1	A	180	GLU	CB-CA-C	-10.53	89.34	110.40
1	B	100	LEU	N-CA-CB	-10.42	89.56	110.40
1	A	193	ARG	N-CA-C	10.36	138.96	111.00
1	A	4	LEU	CB-CA-C	-10.11	91.00	110.20
1	A	155	ASN	CB-CA-C	-8.97	92.45	110.40
1	A	238	ALA	CB-CA-C	-8.21	97.79	110.10
1	A	161	LEU	N-CA-C	-8.02	89.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	MET	CB-CA-C	7.76	125.93	110.40
1	A	101	ASP	N-CA-C	6.91	129.64	111.00
1	A	156	TYR	N-CA-C	-6.59	93.20	111.00
1	A	102	GLY	N-CA-C	-6.04	97.99	113.10
1	A	5	SER	N-CA-C	-5.77	95.43	111.00
1	B	53	ALA	CB-CA-C	-5.54	101.78	110.10
1	A	180	GLU	N-CA-C	5.27	125.22	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Peptide
1	A	180	GLU	Peptide
1	A	191	PRO	Peptide
1	A	208	ALA	Mainchain,Peptide
1	A	209	HIS	Peptide

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	1894	0	1849	115	0
1	B	1802	0	1777	64	1
2	A	29	0	19	5	0
2	B	29	0	19	8	0
3	A	44	0	26	2	0
3	B	44	0	26	3	0
4	A	26	0	0	2	1
4	B	28	0	0	5	0
All	All	3896	0	3716	173	1

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 23.

All (173) 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:209:HIS:O	1:A:209:HIS:CD2	1.67	1.44
1:A:46:GLY:HA3	1:A:47:ARG:CB	1.36	1.42
1:A:19:SER:O	1:A:20:ILE:HG22	1.25	1.30
1:A:46:GLY:CA	1:A:47:ARG:HB2	1.73	1.16
1:A:46:GLY:CA	1:A:47:ARG:CB	2.20	1.15
1:A:209:HIS:O	1:A:209:HIS:CG	2.01	1.09
1:A:180:GLU:O	4:A:417:HOH:O	1.70	1.09
1:B:97:GLY:HA2	1:B:99:GLN:H	1.12	1.08
1:A:193:ARG:CG	1:A:193:ARG:O	1.89	1.07
1:A:19:SER:O	1:A:20:ILE:CG2	2.10	0.97
1:A:196:ALA:HB2	3:A:302:NAD:O2N	1.71	0.91
1:B:97:GLY:CA	1:B:99:GLN:H	1.85	0.90
1:A:101:ASP:O	1:A:201:LYS:HE3	1.73	0.89
1:A:46:GLY:HA3	1:A:47:ARG:HB3	1.53	0.88
1:B:94:PHE:CD1	2:B:302:AE6:H13	2.08	0.88
1:A:193:ARG:O	1:A:193:ARG:HG3	1.71	0.87
1:A:193:ARG:O	1:A:193:ARG:HG2	1.74	0.86
1:A:46:GLY:CA	1:A:47:ARG:HB3	2.06	0.86
1:A:18:LEU:O	1:A:194:THR:HG22	1.76	0.85
1:A:209:HIS:O	1:A:209:HIS:HD2	1.58	0.84
1:A:160:GLY:HA2	1:A:163:LYS:H	1.45	0.82
1:A:190:GLY:O	1:A:192:ILE:HB	1.78	0.82
1:B:97:GLY:HA2	1:B:99:GLN:N	1.93	0.81
1:A:125:VAL:HB	1:A:173:MET:HE2	1.62	0.80
1:B:86:ASP:HB2	4:B:415:HOH:O	1.80	0.80
1:A:191:PRO:HA	1:A:192:ILE:HB	1.64	0.79
1:A:159:MET:O	1:A:162:ALA:HB3	1.81	0.79
1:A:161:LEU:HD11	1:B:169:ASN:HA	1.65	0.78
1:A:20:ILE:HG23	1:A:21:ALA:N	1.97	0.77
1:A:46:GLY:HA3	1:A:47:ARG:HB2	0.76	0.76
1:A:192:ILE:CG2	1:A:192:ILE:O	2.34	0.75
1:B:213:VAL:HG13	1:B:257:ASN:HB2	1.70	0.74
1:B:68:ASP:HB2	4:B:403:HOH:O	1.88	0.73
1:A:145:SER:HA	1:A:163:LYS:HE3	1.68	0.73
1:B:8:ARG:HD2	4:B:412:HOH:O	1.90	0.71
1:B:94:PHE:O	1:B:116:ALA:HA	1.91	0.70
1:A:117:HIS:NE2	1:A:161:LEU:O	2.25	0.69
1:A:20:ILE:CG2	1:A:21:ALA:N	2.57	0.67
1:A:161:LEU:HD11	1:B:169:ASN:CA	2.24	0.67
1:A:250:GLY:O	1:A:253:ILE:HG12	1.95	0.66
1:A:192:ILE:HG22	1:A:192:ILE:O	1.94	0.66
1:A:113:PHE:CE1	1:A:161:LEU:HD23	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:SER:C	1:A:20:ILE:HG22	2.11	0.66
1:A:193:ARG:HB3	1:A:203:PHE:HZ	1.61	0.65
1:B:96:PRO:O	1:B:98:ASP:HB2	1.98	0.64
1:A:4:LEU:C	1:A:5:SER:O	2.28	0.64
1:A:113:PHE:HE1	1:A:161:LEU:HD23	1.65	0.62
1:A:245:VAL:HA	4:A:416:HOH:O	1.99	0.62
1:A:160:GLY:HA2	1:A:163:LYS:N	2.16	0.61
1:A:3:PHE:O	1:A:4:LEU:HB2	2.00	0.60
1:A:149:ALA:HB2	1:A:163:LYS:HB2	1.83	0.59
1:A:167:GLU:HG3	1:A:244:VAL:HG21	1.83	0.59
1:A:149:ALA:HB2	1:A:163:LYS:CB	2.32	0.59
1:A:20:ILE:CG2	1:A:21:ALA:H	2.16	0.58
1:B:94:PHE:CE1	2:B:302:AE6:H14	2.38	0.58
1:A:7:LYS:NZ	1:A:138:GLY:O	2.35	0.58
1:B:102:GLY:H	1:B:155:ASN:ND2	2.01	0.58
1:A:160:GLY:C	1:A:162:ALA:H	2.01	0.57
1:A:193:ARG:HE	1:A:207:LEU:HD11	1.69	0.57
1:A:86:ASP:C	1:A:139:SER:HB2	2.23	0.57
1:B:94:PHE:HD1	2:B:302:AE6:H13	1.68	0.57
1:A:39:TYR:HB3	1:A:48:VAL:HG21	1.87	0.56
1:B:39:TYR:CE2	1:B:62:GLN:HG2	2.40	0.56
1:B:194:THR:N	3:B:301:NAD:O2A	2.38	0.56
1:A:38:THR:HA	1:A:61:LEU:O	2.06	0.55
1:B:113:PHE:HA	1:B:158:VAL:HG21	1.87	0.55
1:A:86:ASP:HA	1:A:139:SER:HB3	1.89	0.55
1:B:156:TYR:CD2	2:B:302:AE6:H2	2.42	0.55
1:A:160:GLY:CA	1:A:162:ALA:H	2.20	0.54
1:A:191:PRO:HB3	2:A:301:AE6:C9	2.38	0.54
1:A:63:CYS:HB2	1:A:74:MET:HG3	1.89	0.54
1:A:191:PRO:CA	1:A:192:ILE:HB	2.37	0.54
1:A:50:GLU:O	1:A:53:ALA:HB3	2.07	0.54
1:B:232:LEU:HD11	1:B:245:VAL:HG11	1.88	0.54
1:B:139:SER:HB2	1:B:182:VAL:HG22	1.90	0.54
1:A:49:GLU:HG3	1:A:60:VAL:HG21	1.90	0.54
1:A:125:VAL:HB	1:A:173:MET:CE	2.35	0.54
1:B:210:CYS:O	1:B:214:THR:OG1	2.25	0.52
1:A:20:ILE:HG23	1:A:21:ALA:H	1.73	0.52
1:B:100:LEU:HD21	1:B:159:MET:HG2	1.92	0.51
1:B:67:GLU:HB3	4:B:407:HOH:O	2.09	0.51
1:A:173:MET:HB3	1:A:184:VAL:HG21	1.92	0.51
1:B:153:ILE:HG21	2:B:302:AE6:N3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:CG	1:B:147:LEU:N	2.79	0.51
1:A:86:ASP:O	1:A:139:SER:HB2	2.10	0.51
1:A:46:GLY:N	1:A:47:ARG:HB3	2.26	0.51
1:A:187:ILE:HG23	1:A:247:VAL:HG12	1.93	0.51
1:B:156:TYR:CE2	2:B:302:AE6:H2	2.46	0.50
1:B:19:SER:HG	1:B:194:THR:N	2.10	0.49
1:B:210:CYS:SG	1:B:219:THR:HG22	2.52	0.49
1:B:247:VAL:HG12	1:B:247:VAL:O	2.13	0.49
1:A:165:SER:HB2	1:B:165:SER:HB2	1.93	0.49
1:B:10:LEU:HD11	1:B:38:THR:HG23	1.93	0.49
1:B:49:GLU:HG2	1:B:60:VAL:HG11	1.95	0.49
1:B:142:LEU:HD12	1:B:185:ASN:O	2.12	0.49
1:A:124:PHE:CD2	1:A:173:MET:HE3	2.48	0.49
1:B:166:LEU:O	1:B:170:VAL:HG23	2.13	0.49
1:A:45:LYS:O	1:A:46:GLY:C	2.49	0.49
1:A:191:PRO:HA	1:A:192:ILE:CB	2.38	0.49
1:B:213:VAL:CG1	1:B:257:ASN:HB2	2.41	0.49
1:A:192:ILE:HG12	1:A:220:VAL:O	2.13	0.48
1:B:15:ALA:HB2	3:B:301:NAD:O3B	2.13	0.48
1:A:117:HIS:CE1	1:A:161:LEU:HB3	2.48	0.48
1:A:104:TYR:HD2	1:A:157:ASN:HB3	1.79	0.48
1:A:47:ARG:H	1:A:50:GLU:HG3	1.78	0.48
1:A:196:ALA:HB1	2:A:301:AE6:H7	1.94	0.48
1:A:100:LEU:HD12	1:A:100:LEU:N	2.29	0.48
1:B:20:ILE:HG21	1:B:144:LEU:HG	1.95	0.48
1:B:183:ARG:HD2	1:B:240:ILE:O	2.13	0.48
1:A:257:ASN:OD1	1:A:257:ASN:N	2.47	0.47
1:B:237:SER:HB2	1:B:240:ILE:HD12	1.96	0.47
1:A:29:HIS:CD2	1:A:55:LEU:O	2.66	0.47
1:A:124:PHE:CD2	1:A:173:MET:CE	2.97	0.47
1:B:153:ILE:HG21	2:B:302:AE6:H1	1.80	0.47
1:A:213:VAL:HG21	1:A:257:ASN:O	2.15	0.46
1:A:192:ILE:HG23	1:A:192:ILE:O	2.16	0.46
1:A:156:TYR:CD2	2:A:301:AE6:H13	2.51	0.45
1:B:170:VAL:HG13	1:B:184:VAL:HG12	1.97	0.45
1:B:171:ARG:HD3	4:B:426:HOH:O	2.16	0.45
1:A:174:ALA:HB2	1:A:184:VAL:HB	1.99	0.45
1:A:3:PHE:C	1:A:5:SER:H	2.20	0.45
1:A:247:VAL:O	1:A:247:VAL:HG13	2.16	0.45
1:B:122:TYR:CE2	1:B:126:ALA:HB2	2.51	0.45
1:A:95:ALA:HB3	1:A:100:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ILE:O	1:B:28:MET:HG3	2.16	0.45
1:B:194:THR:OG1	1:B:195:LEU:N	2.49	0.45
1:A:24:ILE:O	1:A:28:MET:HG3	2.18	0.44
1:A:19:SER:O	1:A:21:ALA:N	2.43	0.44
1:A:196:ALA:CB	3:A:302:NAD:O2N	2.54	0.44
1:A:45:LYS:C	1:A:47:ARG:HB3	2.38	0.44
1:B:41:ASN:HB2	1:B:44:LEU:HD22	1.99	0.44
1:A:170:VAL:HG13	1:A:184:VAL:HG12	2.00	0.44
1:A:169:ASN:O	1:A:173:MET:HG3	2.18	0.44
1:B:168:ALA:HA	1:B:171:ARG:NH2	2.32	0.43
1:A:95:ALA:N	2:A:301:AE6:N2	2.61	0.43
1:A:96:PRO:O	1:A:99:GLN:HB2	2.19	0.43
1:A:18:LEU:O	1:A:194:THR:CG2	2.57	0.43
1:B:166:LEU:O	1:B:169:ASN:HB3	2.18	0.43
1:A:103:ASP:HB3	1:A:106:ASN:HD22	1.82	0.43
1:B:184:VAL:O	1:B:242:GLY:N	2.48	0.43
1:A:148:GLY:HA2	1:A:153:ILE:HD12	2.01	0.43
1:A:156:TYR:HD2	2:A:301:AE6:H13	1.83	0.42
1:A:160:GLY:C	1:A:162:ALA:N	2.56	0.42
1:A:167:GLU:CG	1:A:244:VAL:HG21	2.50	0.42
1:A:161:LEU:HD11	1:B:169:ASN:CB	2.49	0.42
1:A:209:HIS:HA	1:A:210:CYS:HA	1.80	0.42
1:B:125:VAL:O	1:B:128:ALA:HB3	2.19	0.42
1:A:258:GLU:OE1	1:A:258:GLU:HA	2.20	0.42
1:B:131:CYS:O	1:B:132:ARG:C	2.56	0.42
1:A:197:ALA:HA	1:A:200:ILE:HB	2.01	0.42
1:A:117:HIS:CD2	1:B:117:HIS:CD2	3.08	0.42
1:A:172:TYR:CZ	1:B:152:ALA:HA	2.55	0.42
1:B:64:ASP:OD2	1:B:66:ALA:HB3	2.19	0.42
1:B:143:THR:HG21	1:B:166:LEU:CD2	2.50	0.41
1:A:28:MET:HE2	1:A:233:CYS:HB2	2.01	0.41
1:A:87:GLY:HA3	1:A:140:ALA:O	2.20	0.41
1:A:187:ILE:CG2	1:A:247:VAL:HG12	2.50	0.41
1:A:10:LEU:O	1:A:88:PHE:HA	2.20	0.41
1:B:8:ARG:HD3	1:B:82:TRP:CD1	2.56	0.41
1:A:151:ARG:NH2	1:A:252:SER:O	2.54	0.41
1:B:156:TYR:CZ	1:B:159:MET:HB3	2.56	0.41
1:A:228:SER:O	1:A:232:LEU:HD23	2.20	0.41
1:A:147:LEU:HD12	1:A:150:GLU:HB2	2.03	0.41
1:A:9:ILE:O	1:A:35:LEU:HA	2.21	0.41
1:B:59:ILE:HG12	1:B:81:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG22	3:B:301:NAD:N1A	2.36	0.41
1:B:88:PHE:CE1	1:B:141:LEU:HD22	2.56	0.41
1:B:65:VAL:HA	1:B:71:ILE:HD11	2.03	0.40
2:B:302:AE6:H7	2:B:302:AE6:H2	1.87	0.40
1:A:161:LEU:CD1	1:B:169:ASN:HA	2.44	0.40
1:A:146:TYR:CG	1:A:147:LEU:N	2.89	0.40
1:A:150:GLU:CD	1:A:246:HIS:HE2	2.24	0.40
1:A:27:ALA:O	1:A:31:GLU:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:ND2	4:A:406:HOH:O[8_567]	2.16	0.04

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	256/282 (91%)	216 (84%)	35 (14%)	5 (2%)	9 48
1	B	238/282 (84%)	213 (90%)	25 (10%)	0	100 100
All	All	494/564 (88%)	429 (87%)	60 (12%)	5 (1%)	19 65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	98	ASP
1	A	191	PRO
1	A	238	ALA
1	A	192	ILE

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	190/218 (87%)	179 (94%)	11 (6%)	25	66
1	B	185/218 (85%)	175 (95%)	10 (5%)	27	68
All	All	375/436 (86%)	354 (94%)	21 (6%)	26	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	61	LEU
1	A	73	THR
1	A	98	ASP
1	A	167	GLU
1	A	177	MET
1	A	179	PRO
1	A	180	GLU
1	A	188	SER
1	A	193	ARG
1	A	206	MET
1	B	4	LEU
1	B	17	LYS
1	B	18	LEU
1	B	44	LEU
1	B	55	LEU
1	B	98	ASP
1	B	166	LEU
1	B	188	SER
1	B	214	THR
1	B	218	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	209	HIS
1	B	54	GLN
1	B	155	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

4 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	AE6	A	301	-	26,33,33	2.54	4 (15%)	27,48,48	2.27	11 (40%)
3	NAD	A	302	-	38,48,48	0.99	2 (5%)	47,73,73	1.88	8 (17%)
3	NAD	B	301	-	38,48,48	0.91	2 (5%)	47,73,73	1.70	6 (12%)
2	AE6	B	302	-	26,33,33	2.70	4 (15%)	27,48,48	2.01	8 (29%)

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	AE6	A	301	-	-	0/7/21/21	0/4/5/5
3	NAD	A	302	-	-	0/22/62/62	0/5/5/5
3	NAD	B	301	-	-	0/22/62/62	0/5/5/5
2	AE6	B	302	-	-	0/7/21/21	0/4/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	AE6	C14-C13	-9.01	1.34	1.48
2	A	301	AE6	C14-C13	-7.73	1.36	1.48
3	B	301	NAD	C5A-C4A	2.57	1.46	1.40
3	A	302	NAD	O4D-C1D	2.65	1.44	1.41
3	B	301	NAD	O4D-C1D	2.70	1.44	1.41
2	A	301	AE6	C13-N1	3.16	1.43	1.35
2	B	302	AE6	C13-N1	3.23	1.43	1.35
3	A	302	NAD	C5A-C4A	3.45	1.48	1.40
2	A	301	AE6	C23-C19	3.82	1.51	1.41
2	B	302	AE6	C23-C19	4.01	1.51	1.41
2	A	301	AE6	C23-C22	7.92	1.53	1.36
2	B	302	AE6	C23-C22	8.02	1.53	1.36

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	NAD	N3A-C2A-N1A	-7.70	123.00	128.89
3	A	302	NAD	N3A-C2A-N1A	-7.40	123.23	128.89
3	A	302	NAD	C4B-O4B-C1B	-5.25	103.95	109.72
3	A	302	NAD	PN-O3-PA	-4.62	119.74	132.73
2	B	302	AE6	C22-C23-C19	-4.54	113.78	120.83
3	B	301	NAD	C4B-O4B-C1B	-3.97	105.36	109.72
2	A	301	AE6	C22-C23-C19	-3.55	115.33	120.83
2	A	301	AE6	C11-N1-C12	-3.52	90.53	94.88
2	B	302	AE6	C11-N1-C12	-3.48	90.58	94.88
3	A	302	NAD	C4A-C5A-N7A	-3.26	106.48	109.48
3	A	302	NAD	C1B-N9A-C4A	-3.18	122.14	126.94
3	B	301	NAD	C4A-C5A-N7A	-3.11	106.61	109.48
2	A	301	AE6	C19-C18-N2	-2.63	119.52	122.32
2	A	301	AE6	C23-C22-C21	-2.59	115.70	120.03
2	B	302	AE6	C23-C22-C21	-2.54	115.80	120.03
2	A	301	AE6	O2-C13-N1	-2.51	116.40	120.79
2	B	302	AE6	C16-C15-C14	-2.43	120.44	126.91
2	B	302	AE6	C19-C18-N2	-2.39	119.77	122.32
3	B	301	NAD	C1B-N9A-C4A	-2.19	123.63	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	AE6	C16-C17-N2	-2.17	121.67	124.26
3	A	302	NAD	C2A-N1A-C6A	2.02	122.38	118.77
3	B	301	NAD	O2A-PA-O3	2.14	114.79	105.09
2	A	301	AE6	C6-C5-C4	2.30	121.63	120.33
2	B	302	AE6	C23-C19-C18	2.43	119.92	117.79
3	A	302	NAD	O4B-C1B-N9A	2.50	113.33	108.10
3	B	301	NAD	O4D-C1D-N1N	2.75	111.15	108.13
2	A	301	AE6	C23-C19-C18	2.82	120.26	117.79
3	A	302	NAD	O4D-C1D-N1N	3.19	111.64	108.13
2	A	301	AE6	C20-C16-C15	3.67	125.62	119.70
2	B	302	AE6	C17-N2-C18	3.70	121.29	116.93
2	B	302	AE6	C14-C13-N1	4.05	122.33	118.04
2	A	301	AE6	C17-N2-C18	4.10	121.76	116.93
2	A	301	AE6	C14-C13-N1	5.70	124.08	118.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AE6	5	0
3	A	302	NAD	2	0
3	B	301	NAD	3	0
2	B	302	AE6	8	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, 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	258/282 (91%)	-0.59	4 (1%)	74	62	13, 22, 58, 87	0
1	B	244/282 (86%)	-0.73	1 (0%)	93	90	12, 18, 38, 101	0
All	All	502/564 (89%)	-0.66	5 (0%)	84	75	12, 20, 44, 101	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	THR	3.4
1	A	198	SER	3.3
1	A	199	GLY	3.0
1	A	210	CYS	2.9
1	A	201	LYS	2.1

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	AE6	B	302	29/29	0.88	0.30	1.98	43,44,44,45	0
2	AE6	A	301	29/29	0.93	0.21	-0.06	26,27,28,28	0
3	NAD	B	301	44/44	0.96	0.15	-0.26	27,33,40,43	0
3	NAD	A	302	44/44	0.96	0.14	-0.46	36,48,62,70	0

6.5 Other polymers (i)

There are no such residues in this entry.