Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2016 – 02:24 AM EDT

PDB ID	:	5KLO
Title	:	Crystal structure of thioacyl intermediate in 2-aminomuconate 6-semialdehyde dehydrogenase N169A
Authors	:	Yang, Y.; Davis, I.; Ha, U.; Wang, Y.; Shin, I.; Liu, A.
Deposited on	:	2016-06-24
Resolution	:	1.79 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:

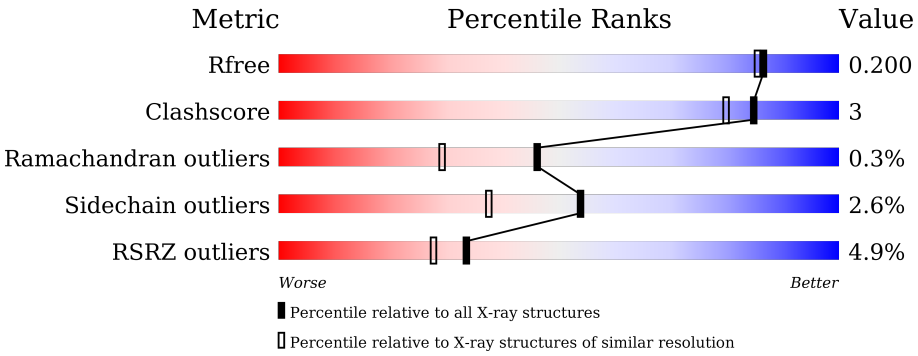
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	520	4% 86% 6% • 7%
1	B	520	4% 87% 5% • 7%
1	C	520	4% 86% 7% 7%
1	D	520	6% 87% 6% • 7%

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	2VS	A	601	-	-	X	-
2	2VS	B	601	-	-	X	-
2	2VS	D	601	-	-	X	-
3	NA	D	602	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16368 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-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3675	2325	637	701	12			
1	B	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			
1	C	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			
1	D	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q83V33
A	-18	GLY	-	expression tag	UNP Q83V33
A	-17	SER	-	expression tag	UNP Q83V33
A	-16	SER	-	expression tag	UNP Q83V33
A	-15	HIS	-	expression tag	UNP Q83V33
A	-14	HIS	-	expression tag	UNP Q83V33
A	-13	HIS	-	expression tag	UNP Q83V33
A	-12	HIS	-	expression tag	UNP Q83V33
A	-11	HIS	-	expression tag	UNP Q83V33
A	-10	HIS	-	expression tag	UNP Q83V33
A	-9	SER	-	expression tag	UNP Q83V33
A	-8	SER	-	expression tag	UNP Q83V33
A	-7	GLY	-	expression tag	UNP Q83V33
A	-6	LEU	-	expression tag	UNP Q83V33
A	-5	VAL	-	expression tag	UNP Q83V33
A	-4	PRO	-	expression tag	UNP Q83V33
A	-3	ARG	-	expression tag	UNP Q83V33
A	-2	GLY	-	expression tag	UNP Q83V33
A	-1	SER	-	expression tag	UNP Q83V33
A	0	HIS	-	expression tag	UNP Q83V33
A	169	ALA	ASN	engineered mutation	UNP Q83V33

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression tag	UNP Q83V33
B	-12	HIS	-	expression tag	UNP Q83V33
B	-11	HIS	-	expression tag	UNP Q83V33
B	-10	HIS	-	expression tag	UNP Q83V33
B	-9	SER	-	expression tag	UNP Q83V33
B	-8	SER	-	expression tag	UNP Q83V33
B	-7	GLY	-	expression tag	UNP Q83V33
B	-6	LEU	-	expression tag	UNP Q83V33
B	-5	VAL	-	expression tag	UNP Q83V33
B	-4	PRO	-	expression tag	UNP Q83V33
B	-3	ARG	-	expression tag	UNP Q83V33
B	-2	GLY	-	expression tag	UNP Q83V33
B	-1	SER	-	expression tag	UNP Q83V33
B	0	HIS	-	expression tag	UNP Q83V33
B	169	ALA	ASN	engineered mutation	UNP Q83V33
C	-19	MET	-	initiating methionine	UNP Q83V33
C	-18	GLY	-	expression tag	UNP Q83V33
C	-17	SER	-	expression tag	UNP Q83V33
C	-16	SER	-	expression tag	UNP Q83V33
C	-15	HIS	-	expression tag	UNP Q83V33
C	-14	HIS	-	expression tag	UNP Q83V33
C	-13	HIS	-	expression tag	UNP Q83V33
C	-12	HIS	-	expression tag	UNP Q83V33
C	-11	HIS	-	expression tag	UNP Q83V33
C	-10	HIS	-	expression tag	UNP Q83V33
C	-9	SER	-	expression tag	UNP Q83V33
C	-8	SER	-	expression tag	UNP Q83V33
C	-7	GLY	-	expression tag	UNP Q83V33
C	-6	LEU	-	expression tag	UNP Q83V33
C	-5	VAL	-	expression tag	UNP Q83V33
C	-4	PRO	-	expression tag	UNP Q83V33
C	-3	ARG	-	expression tag	UNP Q83V33
C	-2	GLY	-	expression tag	UNP Q83V33
C	-1	SER	-	expression tag	UNP Q83V33
C	0	HIS	-	expression tag	UNP Q83V33
C	169	ALA	ASN	engineered mutation	UNP Q83V33

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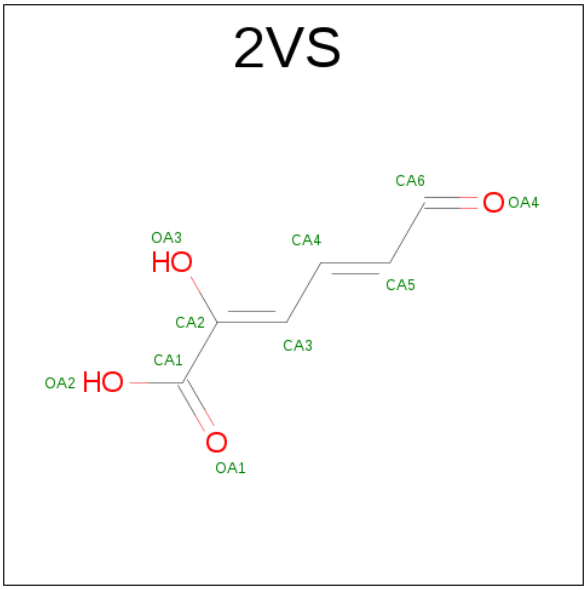
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q83V33
D	-18	GLY	-	expression tag	UNP Q83V33
D	-17	SER	-	expression tag	UNP Q83V33
D	-16	SER	-	expression tag	UNP Q83V33
D	-15	HIS	-	expression tag	UNP Q83V33
D	-14	HIS	-	expression tag	UNP Q83V33
D	-13	HIS	-	expression tag	UNP Q83V33
D	-12	HIS	-	expression tag	UNP Q83V33
D	-11	HIS	-	expression tag	UNP Q83V33
D	-10	HIS	-	expression tag	UNP Q83V33
D	-9	SER	-	expression tag	UNP Q83V33
D	-8	SER	-	expression tag	UNP Q83V33
D	-7	GLY	-	expression tag	UNP Q83V33
D	-6	LEU	-	expression tag	UNP Q83V33
D	-5	VAL	-	expression tag	UNP Q83V33
D	-4	PRO	-	expression tag	UNP Q83V33
D	-3	ARG	-	expression tag	UNP Q83V33
D	-2	GLY	-	expression tag	UNP Q83V33
D	-1	SER	-	expression tag	UNP Q83V33
D	0	HIS	-	expression tag	UNP Q83V33
D	169	ALA	ASN	engineered mutation	UNP Q83V33

- Molecule 2 is (2Z,4E)-2-hydroxy-6-oxohexa-2,4-dienoic acid (three-letter code: 2VS) (formula: $C_6H_6O_4$).

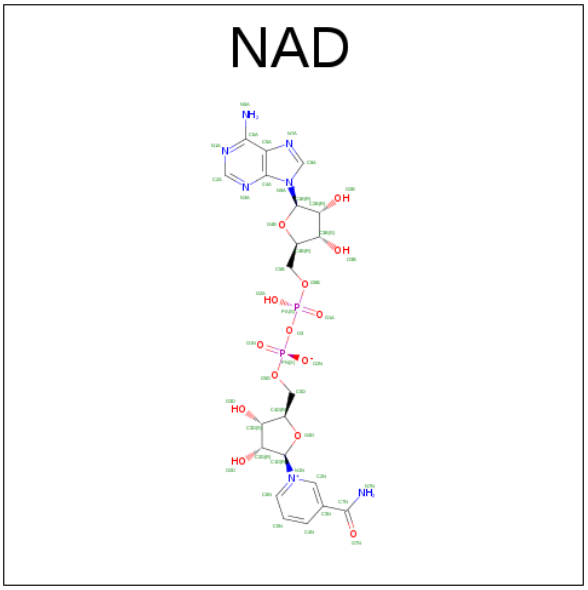


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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

- Molecule 5 is water.

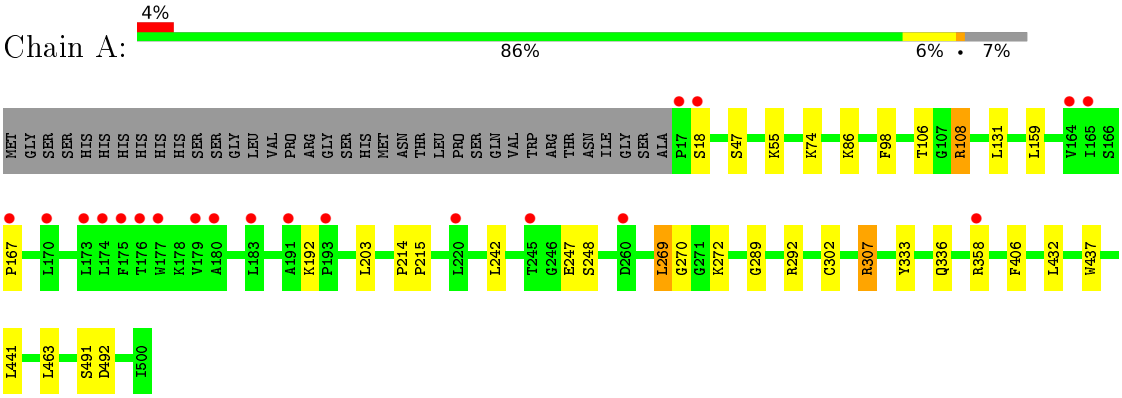
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	410	Total	O	0	0
			410	410		
5	B	364	Total	O	0	0
			364	364		
5	C	370	Total	O	0	0
			370	370		
5	D	325	Total	O	0	0
			325	325		

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.

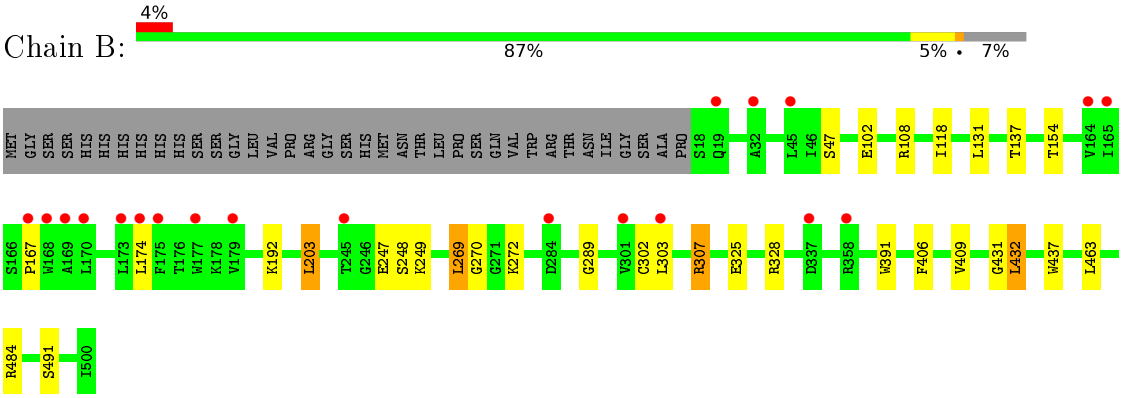
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain A:



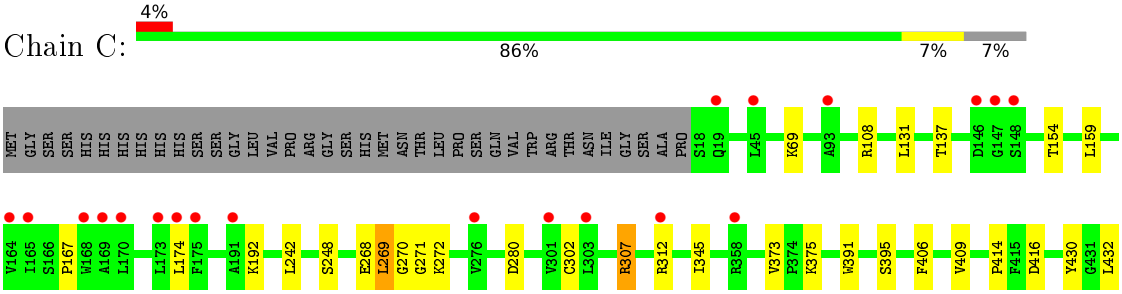
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

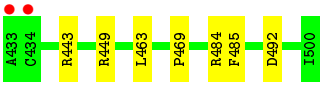
Chain B:



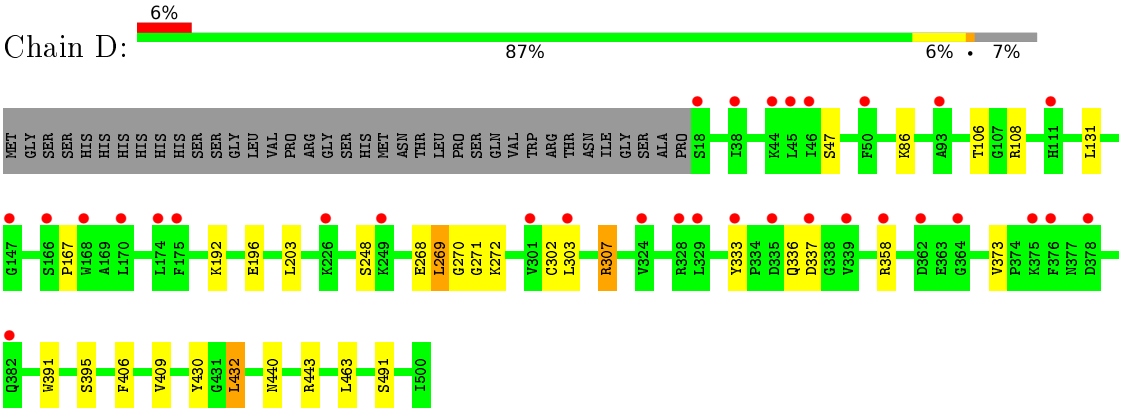
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain C:





• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.11Å 141.72Å 171.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 1.79 34.90 – 1.79	Depositor EDS
% Data completeness (in resolution range)	95.0 (34.90-1.79) 92.4 (34.90-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.203 0.172 , 0.200	Depositor DCC
R_{free} test set	1927 reflections (1.03%)	DCC
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16368	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 2VS, NA, 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	0.38	0/3755	0.61	3/5105 (0.1%)
1	B	0.36	0/3747	0.57	2/5094 (0.0%)
1	C	0.38	0/3747	0.59	2/5094 (0.0%)
1	D	0.34	0/3747	0.54	1/5094 (0.0%)
All	All	0.36	0/14996	0.58	8/20387 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	307	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	307	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	C	307	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	307	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	307	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	307	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	108	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3675	0	3612	22	0
1	B	3668	0	3603	20	0
1	C	3668	0	3604	20	0
1	D	3668	0	3604	17	0
2	A	10	0	4	4	0
2	B	10	0	3	5	0
2	C	10	0	4	3	0
2	D	10	0	4	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	2	0
4	C	44	0	26	2	0
4	D	44	0	26	2	0
5	A	410	0	0	6	0
5	B	364	0	0	3	0
5	C	370	0	0	5	0
5	D	325	0	0	4	0
All	All	16368	0	14542	85	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 3.

All (85) 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:B:302:CYS:SG	2:B:601:2VS:CA6	2.03	1.46
1:C:302:CYS:SG	2:C:601:2VS:H1	1.55	1.44
1:D:302:CYS:SG	2:D:601:2VS:CA6	2.06	1.43
1:A:302:CYS:SG	2:A:601:2VS:CA6	2.14	1.36
1:C:302:CYS:SG	2:C:601:2VS:CA6	2.15	1.34
1:D:302:CYS:SG	2:D:601:2VS:H1	1.64	1.33
1:A:302:CYS:SG	2:A:601:2VS:H1	1.71	1.30
1:B:302:CYS:SG	2:B:601:2VS:CA5	2.46	1.04
1:D:302:CYS:HG	2:D:601:2VS:H1	1.24	1.00
1:C:302:CYS:HG	2:C:601:2VS:H1	1.15	0.95
1:A:302:CYS:HG	2:A:601:2VS:H1	1.32	0.90
1:C:248:SER:HA	1:C:269:LEU:HG	1.58	0.85
1:D:248:SER:HA	1:D:269:LEU:HG	1.62	0.80
1:B:248:SER:HA	1:B:269:LEU:HG	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:CYS:SG	2:D:601:2VS:CA5	2.71	0.77
4:B:603:NAD:H52N	4:B:603:NAD:H6N	1.67	0.77
1:B:174:LEU:HD21	2:B:601:2VS:H5	1.67	0.77
1:A:248:SER:HA	1:A:269:LEU:HG	1.68	0.76
4:C:603:NAD:H52N	4:C:603:NAD:H6N	1.67	0.76
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.69	0.74
1:A:292:ARG:NH2	5:A:703:HOH:O	2.19	0.74
1:C:108:ARG:NH2	5:C:702:HOH:O	2.22	0.71
4:D:603:NAD:H52N	4:D:603:NAD:H6N	1.74	0.69
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.73	0.69
1:A:302:CYS:SG	2:A:601:2VS:CA5	2.80	0.68
1:B:108:ARG:NH2	5:B:704:HOH:O	2.28	0.67
1:D:196:GLU:OE1	5:D:701:HOH:O	2.12	0.66
1:C:312:ARG:HG2	1:C:414:PRO:HB2	1.77	0.65
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.79	0.65
1:C:375:LYS:NZ	5:C:707:HOH:O	2.30	0.64
1:D:358:ARG:NH2	5:D:705:HOH:O	2.30	0.64
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.81	0.63
1:C:69:LYS:NZ	5:C:710:HOH:O	2.34	0.61
1:A:270:GLY:HA2	1:A:302:CYS:HB2	1.83	0.59
1:A:358:ARG:NH2	5:A:701:HOH:O	2.15	0.59
1:A:491:SER:O	5:A:702:HOH:O	2.17	0.57
1:B:391:TRP:CH2	1:B:409:VAL:HG21	2.42	0.55
1:A:108:ARG:NH2	5:A:711:HOH:O	2.40	0.54
1:C:280:ASP:OD2	1:C:443:ARG:NH1	2.40	0.54
4:D:603:NAD:C5D	4:D:603:NAD:H6N	2.38	0.53
1:D:491:SER:O	5:D:702:HOH:O	2.19	0.53
4:C:603:NAD:C5D	4:C:603:NAD:H6N	2.39	0.53
1:C:270:GLY:HA2	1:C:302:CYS:HB2	1.91	0.52
1:B:270:GLY:HA2	1:B:302:CYS:HB2	1.92	0.51
4:B:603:NAD:H6N	4:B:603:NAD:C5D	2.39	0.51
1:D:333:TYR:HB2	1:D:336:GLN:HB2	1.93	0.50
1:D:270:GLY:HA2	1:D:302:CYS:HB2	1.93	0.50
1:D:108:ARG:NH2	5:D:713:HOH:O	2.45	0.49
1:D:271:GLY:HA2	1:D:430:TYR:CD1	2.48	0.49
1:C:484:ARG:NH2	5:C:712:HOH:O	2.35	0.48
1:A:86:LYS:HE3	5:A:1046:HOH:O	2.13	0.48
1:A:333:TYR:HB2	1:A:336:GLN:HB2	1.96	0.48
1:B:303:LEU:HD23	1:B:432:LEU:HD13	1.96	0.47
1:C:345:ILE:O	5:C:701:HOH:O	2.20	0.47
1:B:491:SER:O	5:B:702:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD21	2:B:601:2VS:CA4	2.40	0.46
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.51	0.45
1:A:86:LYS:HB3	1:A:86:LYS:HE2	1.66	0.45
1:B:247:GLU:HG2	1:B:249:LYS:HG2	1.98	0.45
1:D:303:LEU:HD23	1:D:432:LEU:HD13	1.98	0.45
1:C:159:LEU:HD12	1:C:492:ASP:OD1	2.15	0.45
1:B:289:GLY:HA3	1:B:437:TRP:CZ2	2.52	0.44
1:A:289:GLY:HA3	1:A:437:TRP:CZ2	2.53	0.44
1:B:102:GLU:HG3	1:B:118:ILE:HD11	1.99	0.44
1:C:174:LEU:HA	1:C:174:LEU:HD23	1.88	0.44
1:B:137:THR:HB	1:B:154:THR:OG1	2.19	0.43
1:D:106:THR:HG21	1:D:108:ARG:HH21	1.83	0.43
1:A:98:PHE:CE1	1:A:203:LEU:HB3	2.54	0.43
1:B:302:CYS:SG	2:B:601:2VS:H4	2.50	0.43
1:A:247:GLU:HB2	4:A:603:NAD:O4D	2.18	0.43
1:A:106:THR:HG21	1:A:108:ARG:HH21	1.84	0.42
1:C:137:THR:HB	1:C:154:THR:OG1	2.19	0.42
1:C:391:TRP:CH2	1:C:409:VAL:HG21	2.54	0.42
1:D:440:ASN:HB3	1:D:443:ARG:HB3	2.01	0.42
1:A:55:LYS:HD3	5:A:1003:HOH:O	2.20	0.42
1:C:469:PRO:HB3	1:C:485:PHE:CE1	2.55	0.42
1:C:312:ARG:HG3	1:C:416:ASP:OD1	2.20	0.42
1:A:18:SER:OG	1:A:47:SER:HB3	2.19	0.42
1:B:484:ARG:NH2	5:B:722:HOH:O	2.51	0.42
1:A:159:LEU:HD12	1:A:492:ASP:OD1	2.19	0.41
1:C:271:GLY:HA2	1:C:430:TYR:CD1	2.54	0.41
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.91	0.41
1:B:325:GLU:OE2	1:B:328:ARG:NH1	2.54	0.41
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.91	0.40
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.94	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	482/520 (93%)	469 (97%)	12 (2%)	1 (0%)	52	35
1	B	481/520 (92%)	467 (97%)	12 (2%)	2 (0%)	39	23
1	C	481/520 (92%)	466 (97%)	14 (3%)	1 (0%)	52	35
1	D	481/520 (92%)	467 (97%)	13 (3%)	1 (0%)	52	35
All	All	1925/2080 (92%)	1869 (97%)	51 (3%)	5 (0%)	46	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	PRO
1	A	167	PRO
1	D	167	PRO
1	B	431	GLY
1	C	167	PRO

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	392/423 (93%)	383 (98%)	9 (2%)	58	42
1	B	391/423 (92%)	383 (98%)	8 (2%)	63	49
1	C	391/423 (92%)	380 (97%)	11 (3%)	51	35
1	D	391/423 (92%)	378 (97%)	13 (3%)	45	27
All	All	1565/1692 (92%)	1524 (97%)	41 (3%)	54	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	131	LEU
1	A	192	LYS

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	269	LEU
1	A	406	PHE
1	A	432	LEU
1	A	441	LEU
1	A	463	LEU
1	B	47	SER
1	B	131	LEU
1	B	192	LYS
1	B	203	LEU
1	B	269	LEU
1	B	406	PHE
1	B	432	LEU
1	B	463	LEU
1	C	131	LEU
1	C	192	LYS
1	C	242	LEU
1	C	268	GLU
1	C	269	LEU
1	C	373	VAL
1	C	395	SER
1	C	406	PHE
1	C	432	LEU
1	C	449	ARG
1	C	463	LEU
1	D	47	SER
1	D	86	LYS
1	D	131	LEU
1	D	192	LYS
1	D	203	LEU
1	D	268	GLU
1	D	269	LEU
1	D	337	ASP
1	D	373	VAL
1	D	395	SER
1	D	406	PHE
1	D	432	LEU
1	D	463	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	2VS	A	601	-	5,9,9	3.30	2 (40%)	4,10,10	3.16	2 (50%)
4	NAD	A	603	-	42,48,48	1.95	8 (19%)	46,73,73	2.25	8 (17%)
2	2VS	B	601	-	5,9,9	3.29	4 (80%)	4,10,10	2.46	1 (25%)
4	NAD	B	603	-	42,48,48	1.95	9 (21%)	46,73,73	2.25	6 (13%)
2	2VS	C	601	-	5,9,9	3.29	3 (60%)	4,10,10	3.02	2 (50%)
4	NAD	C	603	-	42,48,48	1.90	10 (23%)	46,73,73	2.18	6 (13%)
2	2VS	D	601	-	5,9,9	3.26	3 (60%)	4,10,10	2.37	1 (25%)
4	NAD	D	603	-	42,48,48	1.96	10 (23%)	46,73,73	2.37	7 (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	2VS	A	601	-	-	0/3/9/9	0/0/0/0
4	NAD	A	603	-	-	0/22/62/62	0/5/5/5
2	2VS	B	601	-	-	0/3/9/9	0/0/0/0
4	NAD	B	603	-	-	0/22/62/62	0/5/5/5
2	2VS	C	601	-	-	0/3/9/9	0/0/0/0
4	NAD	C	603	-	-	0/22/62/62	0/5/5/5
2	2VS	D	601	-	-	0/3/9/9	0/0/0/0
4	NAD	D	603	-	-	0/22/62/62	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	NAD	C2B-C1B	-4.81	1.46	1.53
4	A	603	NAD	C2B-C1B	-4.63	1.46	1.53
4	B	603	NAD	C2B-C1B	-4.48	1.46	1.53
4	C	603	NAD	C2B-C1B	-4.16	1.47	1.53
2	A	601	2VS	OA3-CA2	-3.98	1.23	1.32
2	C	601	2VS	OA3-CA2	-3.95	1.23	1.32
2	D	601	2VS	OA3-CA2	-3.88	1.23	1.32
2	B	601	2VS	OA3-CA2	-3.71	1.23	1.32
4	D	603	NAD	C2B-C3B	-3.59	1.43	1.53
4	B	603	NAD	C2B-C3B	-3.47	1.44	1.53
4	C	603	NAD	C2B-C3B	-3.39	1.44	1.53
4	A	603	NAD	C2B-C3B	-3.34	1.44	1.53
4	D	603	NAD	C2D-C1D	-2.97	1.48	1.53
4	C	603	NAD	C2D-C1D	-2.71	1.49	1.53
4	B	603	NAD	C2D-C1D	-2.65	1.49	1.53
4	A	603	NAD	C2D-C1D	-2.55	1.49	1.53
4	D	603	NAD	O4B-C4B	-2.49	1.39	1.45
4	C	603	NAD	O2D-C2D	-2.40	1.37	1.43
4	A	603	NAD	O3D-C3D	-2.32	1.37	1.43
4	C	603	NAD	O4B-C4B	-2.29	1.39	1.45
4	B	603	NAD	O3D-C3D	-2.27	1.37	1.43
4	D	603	NAD	O2D-C2D	-2.26	1.37	1.43
4	B	603	NAD	O4B-C4B	-2.22	1.39	1.45
4	C	603	NAD	O5D-C5D	-2.21	1.36	1.44
4	A	603	NAD	O4B-C4B	-2.16	1.40	1.45
4	C	603	NAD	O3D-C3D	-2.12	1.38	1.43
4	D	603	NAD	O3D-C3D	-2.11	1.38	1.43
4	B	603	NAD	O5D-C5D	-2.01	1.36	1.44
4	D	603	NAD	O5D-C5D	-2.01	1.36	1.44
2	B	601	2VS	CA4-CA3	2.03	1.49	1.43
2	C	601	2VS	CA4-CA3	2.03	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	2VS	CA5-CA6	2.05	1.50	1.44
2	D	601	2VS	CA4-CA3	2.06	1.49	1.43
4	C	603	NAD	C6A-N6A	2.20	1.43	1.34
4	D	603	NAD	C6A-N6A	2.34	1.43	1.34
4	A	603	NAD	C6A-N6A	2.36	1.43	1.34
4	B	603	NAD	C6A-N6A	2.38	1.43	1.34
4	C	603	NAD	C7N-N7N	4.79	1.42	1.33
4	D	603	NAD	C7N-N7N	5.06	1.43	1.33
4	B	603	NAD	C7N-N7N	5.23	1.43	1.33
2	D	601	2VS	OA4-CA6	5.47	1.39	1.22
4	A	603	NAD	C7N-N7N	5.49	1.44	1.33
2	C	601	2VS	OA4-CA6	5.53	1.39	1.22
2	A	601	2VS	OA4-CA6	5.56	1.39	1.22
2	B	601	2VS	OA4-CA6	5.65	1.39	1.22
4	A	603	NAD	O4D-C1D	6.33	1.50	1.41
4	C	603	NAD	O4D-C1D	6.39	1.50	1.41
4	D	603	NAD	O4D-C1D	6.44	1.50	1.41
4	B	603	NAD	O4D-C1D	6.56	1.50	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	NAD	N3A-C2A-N1A	-11.12	120.14	128.87
4	D	603	NAD	N3A-C2A-N1A	-10.89	120.32	128.87
4	C	603	NAD	N3A-C2A-N1A	-10.80	120.39	128.87
4	B	603	NAD	N3A-C2A-N1A	-10.70	120.47	128.87
2	A	601	2VS	OA4-CA6-CA5	-5.70	116.29	125.77
2	C	601	2VS	OA4-CA6-CA5	-5.47	116.67	125.77
2	B	601	2VS	OA4-CA6-CA5	-4.64	118.04	125.77
2	D	601	2VS	OA4-CA6-CA5	-3.96	119.19	125.77
4	B	603	NAD	C1B-N9A-C4A	-3.58	122.81	126.81
4	D	603	NAD	C1B-N9A-C4A	-3.48	122.92	126.81
4	A	603	NAD	O7N-C7N-C3N	-3.45	115.77	119.60
4	A	603	NAD	C1B-N9A-C4A	-3.05	123.40	126.81
2	C	601	2VS	CA5-CA4-CA3	-2.45	117.94	123.23
2	A	601	2VS	CA5-CA4-CA3	-2.38	118.09	123.23
4	C	603	NAD	C1B-N9A-C4A	-2.25	124.30	126.81
4	A	603	NAD	O5B-C5B-C4B	2.04	116.44	109.09
4	D	603	NAD	O5B-C5B-C4B	2.06	116.52	109.09
4	A	603	NAD	C2N-C3N-C4N	2.13	120.68	118.27
4	C	603	NAD	C2N-C3N-C4N	2.14	120.70	118.27
4	D	603	NAD	C2D-C3D-C4D	2.14	107.02	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	NAD	C2D-C3D-C4D	2.19	107.11	102.64
4	C	603	NAD	O5D-C5D-C4D	2.74	118.99	109.09
4	A	603	NAD	O5D-C5D-C4D	2.92	119.63	109.09
4	C	603	NAD	C3N-C7N-N7N	2.92	121.13	117.82
4	D	603	NAD	O5D-C5D-C4D	3.05	120.08	109.09
4	B	603	NAD	C3N-C7N-N7N	3.13	121.37	117.82
4	D	603	NAD	C3N-C7N-N7N	3.33	121.59	117.82
4	B	603	NAD	O5D-C5D-C4D	3.41	121.41	109.09
4	A	603	NAD	C3N-C7N-N7N	3.72	122.02	117.82
4	A	603	NAD	O4D-C1D-N1N	5.80	114.36	108.10
4	C	603	NAD	O4D-C1D-N1N	6.30	114.91	108.10
4	B	603	NAD	O4D-C1D-N1N	6.73	115.37	108.10
4	D	603	NAD	O4D-C1D-N1N	8.13	116.88	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	2VS	4	0
4	A	603	NAD	1	0
2	B	601	2VS	5	0
4	B	603	NAD	2	0
2	C	601	2VS	3	0
4	C	603	NAD	2	0
2	D	601	2VS	4	0
4	D	603	NAD	2	0

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	484/520 (93%)	0.12	20 (4%)	41	35	23, 30, 40, 58	0
1	B	483/520 (92%)	0.16	20 (4%)	41	35	24, 32, 42, 51	0
1	C	483/520 (92%)	0.24	22 (4%)	36	30	23, 32, 43, 55	0
1	D	483/520 (92%)	0.30	32 (6%)	22	17	23, 35, 47, 61	0
All	All	1933/2080 (92%)	0.21	94 (4%)	33	27	23, 32, 44, 61	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	PRO	5.0
1	B	174	LEU	4.9
1	D	45	LEU	4.8
1	B	169	ALA	4.3
1	D	174	LEU	4.3
1	A	164	VAL	4.3
1	C	170	LEU	4.2
1	B	337	ASP	4.1
1	A	174	LEU	4.0
1	B	168	TRP	3.8
1	D	324	VAL	3.6
1	D	382	GLN	3.5
1	D	337	ASP	3.4
1	C	169	ALA	3.2
1	D	333	TYR	3.2
1	B	303	LEU	3.2
1	B	173	LEU	3.2
1	C	164	VAL	3.2
1	A	179	VAL	3.2
1	A	175	PHE	3.0
1	C	174	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	339	VAL	3.0
1	A	170	LEU	2.9
1	D	376	PHE	2.9
1	C	168	TRP	2.9
1	C	433	ALA	2.9
1	A	176	THR	2.8
1	D	301	VAL	2.8
1	C	146	ASP	2.8
1	C	175	PHE	2.8
1	A	165	ILE	2.8
1	D	303	LEU	2.8
1	D	328	ARG	2.7
1	B	165	ILE	2.7
1	A	193	PRO	2.7
1	C	434	CYS	2.7
1	D	18	SER	2.7
1	D	93	ALA	2.7
1	A	167	PRO	2.7
1	A	191	ALA	2.6
1	B	175	PHE	2.6
1	D	44	LYS	2.6
1	C	19	GLN	2.6
1	D	362	ASP	2.6
1	C	191	ALA	2.5
1	B	170	LEU	2.5
1	B	32	ALA	2.5
1	D	175	PHE	2.5
1	B	177	TRP	2.5
1	D	335	ASP	2.5
1	C	358	ARG	2.4
1	C	312	ARG	2.4
1	C	303	LEU	2.4
1	D	38	ILE	2.4
1	D	50	PHE	2.4
1	D	166	SER	2.4
1	B	301	VAL	2.3
1	C	301	VAL	2.3
1	B	45	LEU	2.3
1	D	170	LEU	2.3
1	A	180	ALA	2.3
1	C	93	ALA	2.3
1	D	375	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	18	SER	2.2
1	A	173	LEU	2.2
1	A	358	ARG	2.2
1	C	147	GLY	2.2
1	B	179	VAL	2.2
1	B	167	PRO	2.2
1	D	364	GLY	2.2
1	D	46	ILE	2.2
1	D	147	GLY	2.2
1	A	183	LEU	2.1
1	C	45	LEU	2.1
1	B	358	ARG	2.1
1	A	177	TRP	2.1
1	C	173	LEU	2.1
1	D	358	ARG	2.1
1	A	220	LEU	2.1
1	C	165	ILE	2.1
1	D	378	ASP	2.1
1	B	245	THR	2.1
1	B	164	VAL	2.1
1	D	168	TRP	2.1
1	D	249	LYS	2.1
1	C	148	SER	2.1
1	D	111	HIS	2.1
1	B	284	ASP	2.0
1	D	329	LEU	2.0
1	B	19	GLN	2.0
1	A	260	ASP	2.0
1	D	226	LYS	2.0
1	C	276	VAL	2.0
1	A	245	THR	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, 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
3	NA	D	602	1/1	0.92	0.24	3.49	37,37,37,37	0
3	NA	B	602	1/1	0.96	0.14	1.78	30,30,30,30	0
2	2VS	D	601	10/10	0.95	0.20	0.99	33,34,40,40	0
2	2VS	A	601	10/10	0.98	0.15	0.18	27,30,34,35	0
3	NA	A	602	1/1	0.96	0.10	-0.14	27,27,27,27	0
2	2VS	C	601	10/10	0.97	0.15	-0.16	28,32,36,37	0
4	NAD	B	603	44/44	0.91	0.11	-0.32	31,39,48,57	0
4	NAD	A	603	44/44	0.92	0.11	-0.37	31,38,47,51	0
2	2VS	B	601	10/10	0.97	0.14	-0.45	30,32,37,38	0
4	NAD	D	603	44/44	0.93	0.10	-0.61	33,40,48,57	0
4	NAD	C	603	44/44	0.94	0.10	-0.85	29,36,45,56	0
3	NA	C	602	1/1	0.94	0.08	-1.28	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.