Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:31 PM GMT

PDB ID	:	4ZUK
Title	:	Structure ALDH7A1 complexed with NAD+
Authors	:	Luo, M.; Tanner, J.J.
Deposited on	:	2015-05-16
Resolution	:	2.00 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:

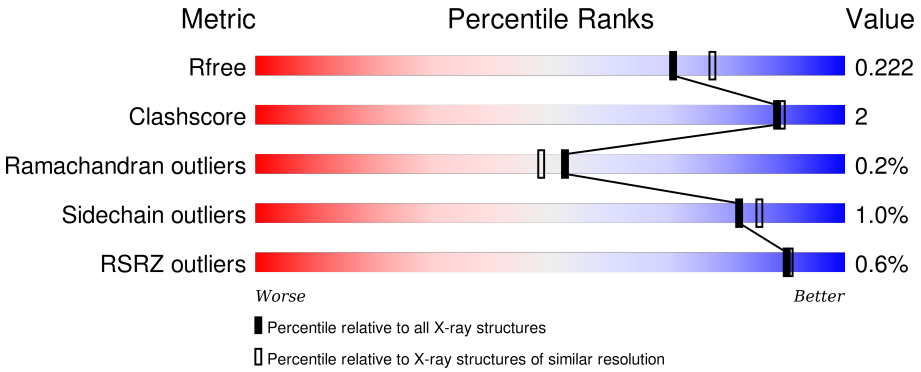
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	513	94% 5%
1	B	513	% 92% 8%
1	C	513	% 93% 6%
1	D	513	94% 5%
1	E	513	% 94% 6%

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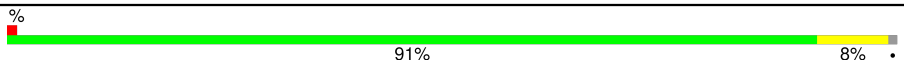
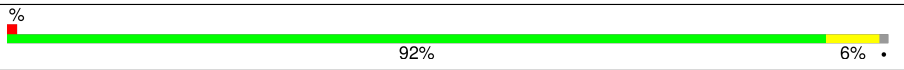
Mol	Chain	Length	Quality of chain
1	F	513	
1	G	513	
1	H	513	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	A	601	-	-	-	X
2	PG4	D	601	-	-	-	X
2	PG4	E	601	-	-	-	X
2	PG4	F	601	-	-	-	X
2	PG4	H	601	-	-	-	X
3	NAD	A	602	-	-	-	X
3	NAD	D	602	-	-	-	X
3	NAD	E	602	-	-	-	X
3	NAD	G	602	-	-	-	X
3	NAD	H	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32089 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3811	2423	661	710	17			
1	B	509	Total	C	N	O	S	0	0	0
			3818	2429	660	712	17			
1	C	509	Total	C	N	O	S	0	0	0
			3809	2422	659	711	17			
1	D	509	Total	C	N	O	S	0	0	0
			3788	2410	656	705	17			
1	E	509	Total	C	N	O	S	0	2	0
			3826	2434	662	712	18			
1	F	509	Total	C	N	O	S	0	0	0
			3819	2424	663	715	17			
1	G	499	Total	C	N	O	S	0	0	0
			3745	2377	650	701	17			
1	H	509	Total	C	N	O	S	0	0	0
			3824	2429	663	715	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419
E	0	HIS	-	expression tag	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419

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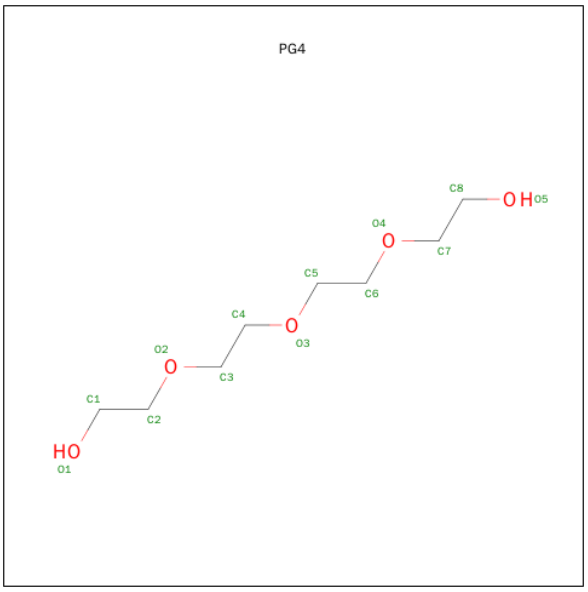
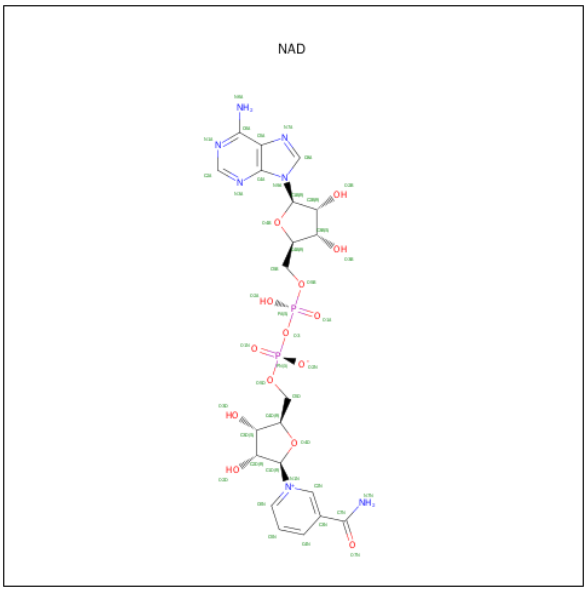
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0
2	B	1	Total C O 13 8 5	0	0
2	C	1	Total C O 13 8 5	0	0
2	D	1	Total C O 13 8 5	0	0
2	E	1	Total C O 13 8 5	0	0
2	F	1	Total C O 13 8 5	0	0
2	G	1	Total C O 13 8 5	0	0
2	H	1	Total C O 13 8 5	0	0

- 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
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	B	170	Total	O	0	0
			170	170		
4	C	171	Total	O	0	0
			171	171		
4	D	139	Total	O	0	0
			139	139		

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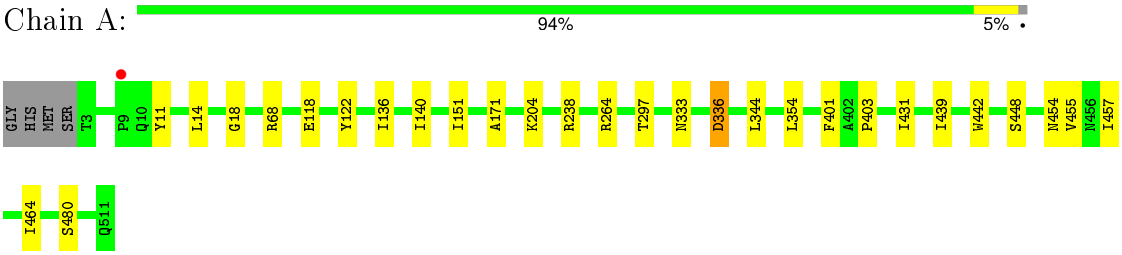
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	173	Total O 173 173	0	0
4	F	165	Total O 165 165	0	0
4	G	165	Total O 165 165	0	0
4	H	174	Total O 174 174	0	0

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.

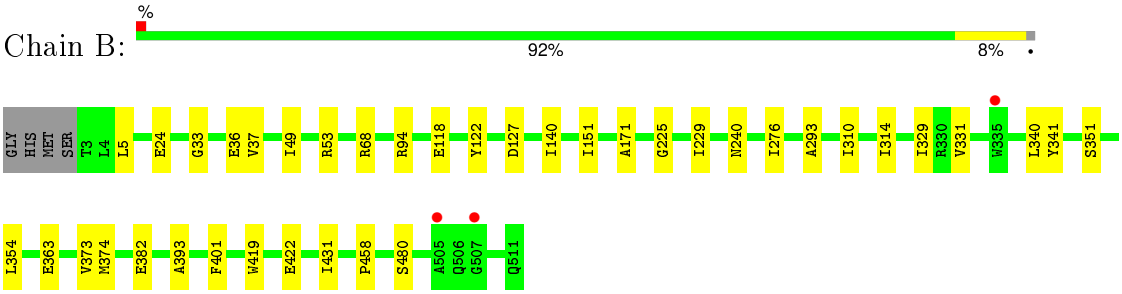
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain A:



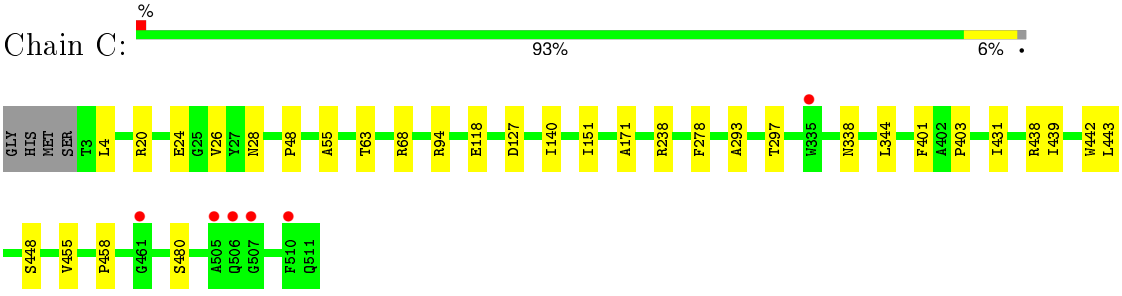
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain B:



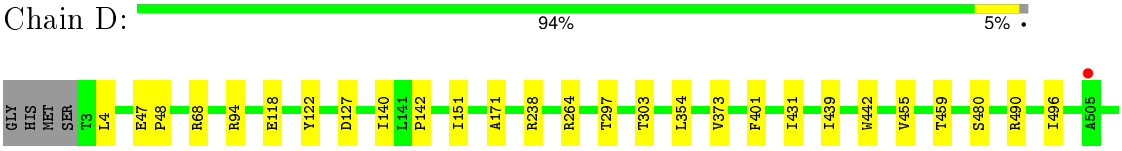
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain C:

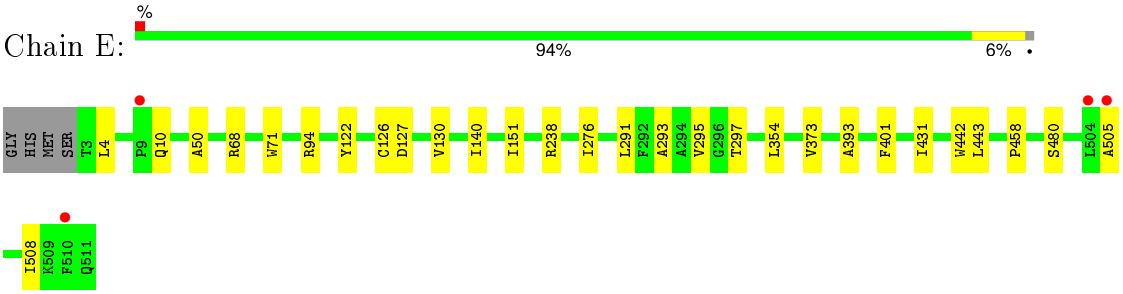


- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

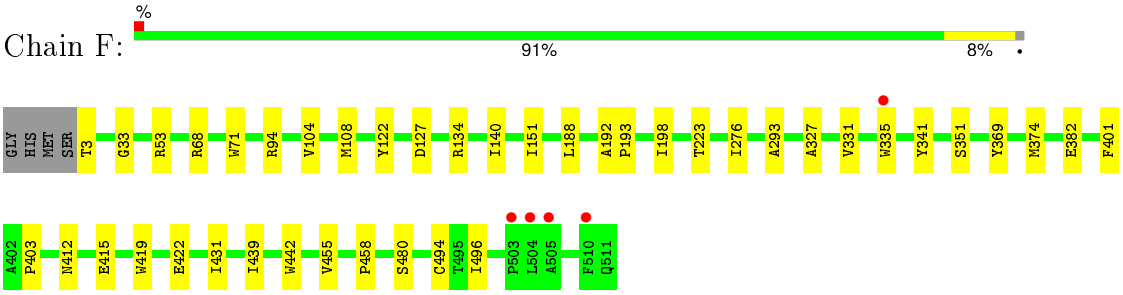
Chain D:



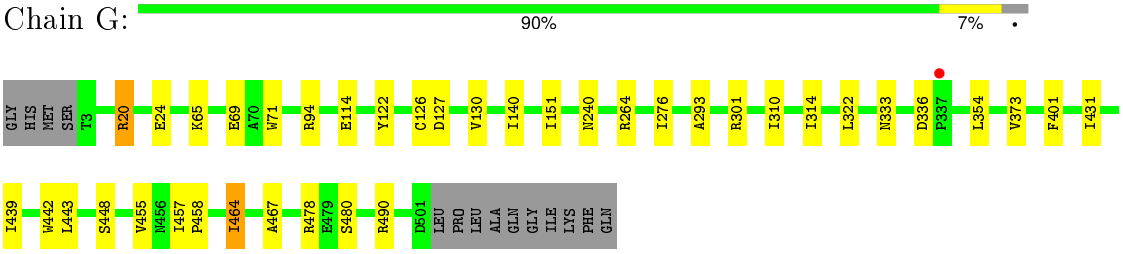
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



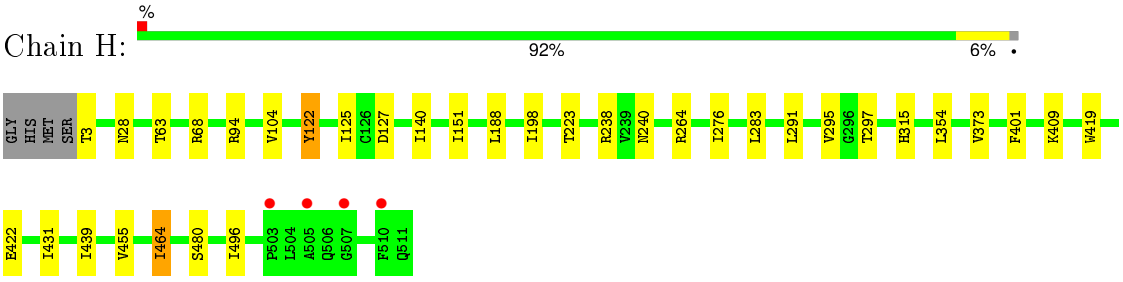
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.67Å 161.58Å 158.93Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	62.89 – 2.00 62.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (62.89-2.00) 99.4 (62.89-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.171 , 0.218 0.178 , 0.222	Depositor DCC
R_{free} test set	12917 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 261349 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32089	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.86% 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: PG4, 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	0/3890	0.51	0/5287
1	B	0.37	0/3897	0.50	0/5294
1	C	0.38	0/3888	0.50	0/5285
1	D	0.35	0/3867	0.49	0/5260
1	E	0.37	0/3911	0.51	0/5314
1	F	0.38	0/3897	0.51	0/5296
1	G	0.37	0/3822	0.50	0/5195
1	H	0.37	0/3903	0.49	0/5304
All	All	0.37	0/31075	0.50	0/42235

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

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	3811	0	3752	17	0
1	B	3818	0	3769	24	0
1	C	3809	0	3744	19	0
1	D	3788	0	3714	16	0
1	E	3826	0	3781	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3819	0	3766	25	0
1	G	3745	0	3684	26	0
1	H	3824	0	3767	24	0
2	A	13	0	18	0	0
2	B	13	0	18	4	0
2	C	13	0	18	0	0
2	D	13	0	18	2	0
2	E	13	0	18	2	0
2	F	13	0	18	4	0
2	G	13	0	18	3	0
2	H	13	0	18	5	0
3	A	27	0	12	0	0
3	B	23	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	23	0	12	0	0
3	G	23	0	12	0	0
3	H	23	0	12	0	0
4	A	188	0	0	1	0
4	B	170	0	0	0	0
4	C	171	0	0	0	0
4	D	139	0	0	0	0
4	E	173	0	0	0	0
4	F	165	0	0	0	0
4	G	165	0	0	1	0
4	H	174	0	0	2	0
All	All	32089	0	30217	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (152) 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:H:240:ASN:HD21	2:H:601:PG4:H11	1.42	0.85
1:F:140:ILE:HD11	1:G:151:ILE:HB	1.62	0.80
1:B:240:ASN:HD21	2:B:601:PG4:H81	1.48	0.78
1:A:151:ILE:HB	1:D:140:ILE:HD11	1.64	0.77
1:H:68:ARG:HH22	2:H:601:PG4:H12	1.49	0.76
1:B:151:ILE:HB	1:C:140:ILE:HD11	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HH22	2:B:601:PG4:H61	1.51	0.75
1:E:151:ILE:HB	1:H:140:ILE:HD11	1.67	0.75
1:A:140:ILE:HD11	1:D:151:ILE:HB	1.69	0.74
1:E:94:ARG:NH2	1:E:127:ASP:OD2	2.24	0.70
1:F:151:ILE:HB	1:G:140:ILE:HD11	1.76	0.67
1:E:140:ILE:HD11	1:H:151:ILE:HB	1.75	0.67
1:F:331:VAL:HG13	1:F:341:TYR:HD2	1.61	0.65
1:H:68:ARG:NH2	2:H:601:PG4:H12	2.10	0.65
1:B:140:ILE:HD11	1:C:151:ILE:HB	1.77	0.64
1:G:443:LEU:HD11	1:H:496:ILE:HD11	1.81	0.62
1:C:94:ARG:NH2	1:C:127:ASP:OD2	2.28	0.62
1:D:94:ARG:NH2	1:D:127:ASP:OD2	2.33	0.60
1:G:240:ASN:HD21	2:G:601:PG4:H81	1.65	0.60
1:E:354:LEU:HD21	1:E:373:VAL:HG23	1.82	0.60
1:H:240:ASN:ND2	2:H:601:PG4:H11	2.14	0.60
1:B:118:GLU:HG3	1:B:171:ALA:HB2	1.83	0.59
1:D:118:GLU:HG3	1:D:171:ALA:HB2	1.85	0.58
1:C:20:ARG:NH2	1:C:24:GLU:OE1	2.35	0.58
1:G:443:LEU:HD13	1:H:151:ILE:HD11	1.85	0.57
1:D:140:ILE:HG23	1:D:151:ILE:HG22	1.86	0.57
1:H:94:ARG:NH2	1:H:127:ASP:OD2	2.34	0.56
1:C:293:ALA:HB2	1:C:458:PRO:HB2	1.87	0.56
1:F:134:ARG:HD2	1:H:464:ILE:HD11	1.87	0.56
1:B:94:ARG:NH2	1:B:127:ASP:OD2	2.35	0.55
1:A:354:LEU:HD12	1:F:351:SER:HB2	1.89	0.55
1:G:293:ALA:HB2	1:G:458:PRO:HB2	1.88	0.55
1:C:140:ILE:HG23	1:C:151:ILE:HG22	1.89	0.54
1:H:28:ASN:HB3	1:H:63:THR:HG23	1.89	0.54
1:E:293:ALA:HB2	1:E:458:PRO:HB2	1.89	0.54
1:F:33:GLY:O	1:F:53:ARG:HG2	2.07	0.54
1:A:140:ILE:HG23	1:A:151:ILE:HG22	1.88	0.54
1:F:104:VAL:HA	1:F:198:ILE:HD11	1.90	0.54
1:F:374:MET:HE3	1:F:382:GLU:HA	1.91	0.53
1:B:293:ALA:HB2	1:B:458:PRO:HB2	1.91	0.53
1:G:457:ILE:HG12	1:G:458:PRO:HD2	1.91	0.53
1:A:344:LEU:HD21	1:A:403:PRO:HD3	1.90	0.53
1:B:374:MET:HE3	1:B:382:GLU:HA	1.90	0.53
1:E:71:TRP:CE3	2:E:601:PG4:H52	2.43	0.52
1:B:24:GLU:HG3	1:B:53:ARG:NH1	2.24	0.52
1:G:71:TRP:CE3	2:G:601:PG4:H42	2.45	0.52
1:C:443:LEU:HD11	1:D:496:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ARG:HB3	2:E:601:PG4:H62	1.91	0.52
1:G:94:ARG:NH2	1:G:127:ASP:OD2	2.43	0.52
1:B:68:ARG:NH2	2:B:601:PG4:H61	2.20	0.52
1:C:442:TRP:CH2	1:C:448:SER:HB2	2.45	0.51
1:H:354:LEU:HD21	1:H:373:VAL:HG23	1.93	0.51
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.92	0.51
1:A:118:GLU:HG2	1:A:171:ALA:HB2	1.93	0.51
1:F:94:ARG:NH2	1:F:127:ASP:OD2	2.38	0.51
1:B:276:ILE:HB	1:B:431:ILE:HG22	1.93	0.50
1:G:20:ARG:NH2	1:G:24:GLU:OE1	2.44	0.49
1:F:68:ARG:NH2	2:F:601:PG4:H52	2.27	0.49
1:D:264:ARG:HH22	1:D:490:ARG:HA	1.78	0.49
1:A:264:ARG:NH2	4:A:703:HOH:O	2.42	0.49
1:C:118:GLU:HG3	1:C:171:ALA:HB2	1.94	0.49
1:C:4:LEU:HD23	1:C:48:PRO:HB2	1.94	0.49
1:D:68:ARG:CZ	2:D:601:PG4:H41	2.43	0.49
1:G:126:CYS:O	1:G:130:VAL:HG23	2.11	0.49
1:F:293:ALA:HB2	1:F:458:PRO:HB2	1.95	0.49
1:F:341:TYR:OH	1:F:403:PRO:HG3	2.13	0.49
1:E:443:LEU:HD11	1:F:496:ILE:HD11	1.95	0.48
1:G:439:ILE:HG23	1:G:455:VAL:HG21	1.95	0.48
1:C:28:ASN:HB3	1:C:63:THR:HG23	1.96	0.48
1:B:310:ILE:HG22	1:B:314:ILE:HG13	1.96	0.48
1:H:276:ILE:HB	1:H:431:ILE:HG22	1.94	0.47
1:G:442:TRP:CH2	1:G:448:SER:HB2	2.49	0.47
1:F:68:ARG:CZ	2:F:601:PG4:H52	2.44	0.47
1:C:439:ILE:HG23	1:C:455:VAL:HG21	1.96	0.47
1:G:264:ARG:HH22	1:G:490:ARG:HA	1.79	0.47
1:A:431:ILE:HG23	1:A:442:TRP:CE2	2.50	0.47
1:B:37:VAL:HG22	1:B:53:ARG:HG2	1.96	0.47
1:H:439:ILE:HG23	1:H:455:VAL:HG21	1.96	0.46
1:B:363:GLU:OE1	1:B:393:ALA:HB1	2.16	0.46
1:E:126:CYS:O	1:E:130:VAL:HG23	2.15	0.46
1:D:354:LEU:HD21	1:D:373:VAL:HG23	1.97	0.46
1:A:442:TRP:CH2	1:A:448:SER:HB2	2.51	0.46
1:E:431:ILE:HG23	1:E:442:TRP:CE2	2.50	0.46
1:H:291:LEU:O	1:H:295:VAL:HG22	2.16	0.45
1:B:329:ILE:HG23	1:B:340:LEU:HD23	1.98	0.45
1:G:310:ILE:HG22	1:G:314:ILE:HG13	1.99	0.45
1:H:315:HIS:CD2	1:H:409:LYS:HG2	2.51	0.45
1:B:5:LEU:HB2	1:B:49:ILE:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:TRP:CE3	2:F:601:PG4:H62	2.52	0.45
1:B:33:GLY:O	1:B:53:ARG:NH2	2.49	0.45
1:G:464:ILE:HG23	4:H:763:HOH:O	2.16	0.45
1:G:467:ALA:HB1	1:G:478:ARG:HB3	1.98	0.44
1:A:333:ASN:O	1:A:336:ASP:HB2	2.18	0.44
1:H:419:TRP:O	1:H:422:GLU:HG2	2.18	0.44
1:G:114:GLU:OE2	1:G:301:ARG:NH1	2.51	0.44
1:B:351:SER:HB2	1:E:354:LEU:HD12	1.99	0.44
1:F:419:TRP:O	1:F:422:GLU:HG2	2.18	0.44
1:D:439:ILE:HG23	1:D:455:VAL:HG21	2.00	0.44
1:F:188:LEU:HD11	1:F:223:THR:HG23	2.00	0.44
1:F:431:ILE:HG23	1:F:442:TRP:CE2	2.53	0.44
1:C:68:ARG:HD2	1:C:238:ARG:HB3	1.99	0.44
1:C:278:PHE:CE2	1:C:438:ARG:HD3	2.53	0.43
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.84	0.43
1:B:225:GLY:HA3	1:B:229:ILE:HG13	2.00	0.43
1:F:151:ILE:HG12	1:F:494:CYS:HB2	2.01	0.43
1:D:68:ARG:HD2	1:D:238:ARG:HB3	2.00	0.43
1:D:431:ILE:HG23	1:D:442:TRP:CE2	2.53	0.43
1:B:151:ILE:HB	1:C:140:ILE:CD1	2.43	0.43
1:H:104:VAL:HA	1:H:198:ILE:HD11	2.00	0.43
1:E:4:LEU:HD22	1:E:50:ALA:HA	2.01	0.43
1:A:439:ILE:HG23	1:A:455:VAL:HG21	2.00	0.43
1:E:68:ARG:HD2	1:E:238:ARG:HB3	2.01	0.42
1:E:276:ILE:HB	1:E:431:ILE:HG22	2.00	0.42
1:H:188:LEU:HD11	1:H:223:THR:HG23	2.00	0.42
1:A:454:ASN:HB3	1:A:457:ILE:HG23	2.01	0.42
1:C:431:ILE:HG23	1:C:442:TRP:CE2	2.54	0.42
1:E:291:LEU:O	1:E:295:VAL:HG22	2.20	0.42
1:B:419:TRP:O	1:B:422:GLU:HG2	2.19	0.42
1:E:505:ALA:HB1	1:E:508:ILE:O	2.19	0.42
1:E:431:ILE:HG23	1:E:442:TRP:CZ2	2.54	0.42
1:D:4:LEU:HD23	1:D:48:PRO:HB2	2.01	0.42
1:G:354:LEU:HD21	1:G:373:VAL:HG23	2.02	0.42
1:B:331:VAL:HG22	1:B:341:TYR:CD2	2.54	0.42
2:D:601:PG4:H32	2:D:601:PG4:H52	1.83	0.42
1:D:303:THR:HB	1:D:459:THR:O	2.20	0.42
1:G:65:LYS:O	1:G:69:GLU:HG2	2.19	0.42
1:G:240:ASN:ND2	2:G:601:PG4:H81	2.34	0.41
1:C:344:LEU:HD21	1:C:403:PRO:HD3	2.01	0.41
1:G:322:LEU:HA	1:G:322:LEU:HD12	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:ILE:HB	1:G:431:ILE:HG22	2.02	0.41
1:B:36:GLU:OE2	1:E:393:ALA:HA	2.20	0.41
1:H:264:ARG:NH2	4:H:710:HOH:O	2.52	0.41
2:B:601:PG4:H42	2:B:601:PG4:H22	1.86	0.41
1:A:11:TYR:HB3	1:A:14:LEU:HD12	2.02	0.41
1:F:276:ILE:HB	1:F:431:ILE:HG22	2.03	0.41
1:A:136:ILE:O	1:D:142:PRO:HD3	2.20	0.41
1:G:333:ASN:O	1:G:336:ASP:HB2	2.21	0.41
1:C:443:LEU:HD13	1:D:151:ILE:HD11	2.03	0.41
1:A:18:GLY:O	1:A:204:LYS:HE3	2.21	0.41
1:B:354:LEU:HD21	1:B:373:VAL:HG23	2.03	0.41
1:H:68:ARG:HD2	1:H:238:ARG:HB3	2.03	0.41
1:H:122:TYR:O	1:H:125:ILE:HG22	2.21	0.41
1:F:327:ALA:HA	1:F:369:TYR:OH	2.21	0.41
1:H:240:ASN:HD21	2:H:601:PG4:C1	2.22	0.40
1:G:293:ALA:HB2	1:G:458:PRO:CB	2.51	0.40
1:F:68:ARG:HH22	2:F:601:PG4:H31	1.86	0.40
1:H:283:LEU:HD23	1:H:283:LEU:HA	1.85	0.40
1:F:439:ILE:HG23	1:F:455:VAL:HG21	2.03	0.40
1:G:264:ARG:NH2	4:G:706:HOH:O	2.53	0.40
1:F:412:ASN:O	1:F:415:GLU:HG2	2.21	0.40
1:C:26:VAL:HG22	1:C:55:ALA:HB2	2.04	0.40
1:F:192:ALA:HA	1:F:193:PRO:HD3	1.92	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	507/513 (99%)	493 (97%)	13 (3%)	1 (0%)	52	48
1	B	507/513 (99%)	493 (97%)	13 (3%)	1 (0%)	52	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	52	48
1	D	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	52	48
1	E	509/513 (99%)	490 (96%)	18 (4%)	1 (0%)	52	48
1	F	507/513 (99%)	495 (98%)	11 (2%)	1 (0%)	52	48
1	G	497/513 (97%)	480 (97%)	16 (3%)	1 (0%)	52	48
1	H	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	52	48
All	All	4048/4104 (99%)	3923 (97%)	117 (3%)	8 (0%)	52	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	C	480	SER
1	B	480	SER
1	E	480	SER
1	F	480	SER
1	D	480	SER
1	G	480	SER
1	H	480	SER

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	388/410 (95%)	383 (99%)	5 (1%)	76	79
1	B	390/410 (95%)	388 (100%)	2 (0%)	92	94
1	C	387/410 (94%)	384 (99%)	3 (1%)	86	89
1	D	383/410 (93%)	379 (99%)	4 (1%)	82	85
1	E	392/410 (96%)	388 (99%)	4 (1%)	82	85
1	F	391/410 (95%)	386 (99%)	5 (1%)	76	79
1	G	383/410 (93%)	379 (99%)	4 (1%)	82	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	391/410 (95%)	386 (99%)	5 (1%)	76 79
All	All	3105/3280 (95%)	3073 (99%)	32 (1%)	82 85

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	TYR
1	A	297	THR
1	A	336	ASP
1	A	401	PHE
1	A	464	ILE
1	B	122	TYR
1	B	401	PHE
1	C	297	THR
1	C	338	ASN
1	C	401	PHE
1	D	47	GLU
1	D	122	TYR
1	D	297	THR
1	D	401	PHE
1	E	10	GLN
1	E	122	TYR
1	E	297	THR
1	E	401	PHE
1	F	3	THR
1	F	108	MET
1	F	122	TYR
1	F	335	TRP
1	F	401	PHE
1	G	20	ARG
1	G	122	TYR
1	G	401	PHE
1	G	464	ILE
1	H	3	THR
1	H	122	TYR
1	H	297	THR
1	H	401	PHE
1	H	464	ILE

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

16 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	PG4	A	601	-	12,12,12	0.69	0	11,11,11	0.32	0
3	NAD	A	602	-	25,29,48	1.45	7 (28%)	26,45,73	2.34	4 (15%)
2	PG4	B	601	-	12,12,12	0.65	0	11,11,11	0.33	0
3	NAD	B	602	-	22,25,48	1.60	6 (27%)	22,38,73	2.95	7 (31%)
2	PG4	C	601	-	12,12,12	0.70	0	11,11,11	0.38	0
3	NAD	C	602	-	25,29,48	1.42	5 (20%)	26,45,73	2.27	4 (15%)
2	PG4	D	601	-	12,12,12	0.67	0	11,11,11	0.23	0
3	NAD	D	602	-	25,29,48	1.46	6 (24%)	26,45,73	2.52	6 (23%)
2	PG4	E	601	-	12,12,12	0.69	0	11,11,11	0.29	0
3	NAD	E	602	-	25,29,48	1.44	6 (24%)	26,45,73	2.33	5 (19%)
2	PG4	F	601	-	12,12,12	0.65	0	11,11,11	0.23	0
3	NAD	F	602	-	22,25,48	1.61	7 (31%)	22,38,73	2.95	7 (31%)
2	PG4	G	601	-	12,12,12	0.72	0	11,11,11	0.28	0
3	NAD	G	602	-	22,25,48	1.64	5 (22%)	22,38,73	3.31	9 (40%)
2	PG4	H	601	-	12,12,12	0.69	0	11,11,11	0.30	0
3	NAD	H	602	-	22,25,48	1.69	5 (22%)	22,38,73	2.82	7 (31%)

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	PG4	A	601	-	-	0/10/10/10	0/0/0/0
3	NAD	A	602	-	-	0/12/32/62	0/3/3/5
2	PG4	B	601	-	-	0/10/10/10	0/0/0/0
3	NAD	B	602	-	-	0/6/26/62	0/3/3/5
2	PG4	C	601	-	-	0/10/10/10	0/0/0/0
3	NAD	C	602	-	-	0/12/32/62	0/3/3/5
2	PG4	D	601	-	-	0/10/10/10	0/0/0/0
3	NAD	D	602	-	-	0/12/32/62	0/3/3/5
2	PG4	E	601	-	-	0/10/10/10	0/0/0/0
3	NAD	E	602	-	-	0/12/32/62	0/3/3/5
2	PG4	F	601	-	-	0/10/10/10	0/0/0/0
3	NAD	F	602	-	-	0/6/26/62	0/3/3/5
2	PG4	G	601	-	-	0/10/10/10	0/0/0/0
3	NAD	G	602	-	-	0/6/26/62	0/3/3/5
2	PG4	H	601	-	-	0/10/10/10	0/0/0/0
3	NAD	H	602	-	-	0/6/26/62	0/3/3/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	602	NAD	PA-O5B	-3.97	1.48	1.59
3	F	602	NAD	PA-O5B	-3.76	1.49	1.59
3	G	602	NAD	PA-O5B	-3.63	1.49	1.59
3	B	602	NAD	PA-O5B	-3.61	1.49	1.59
3	H	602	NAD	C2B-C1B	-3.33	1.48	1.53
3	G	602	NAD	C2B-C1B	-3.13	1.48	1.53
3	C	602	NAD	C2B-C1B	-2.92	1.49	1.53
3	D	602	NAD	C2B-C1B	-2.78	1.49	1.53
3	A	602	NAD	C2B-C1B	-2.75	1.49	1.53
3	E	602	NAD	C2B-C1B	-2.67	1.49	1.53
3	G	602	NAD	PA-O2A	-2.65	1.45	1.54
3	F	602	NAD	C2B-C1B	-2.61	1.49	1.53
3	D	602	NAD	O3B-C3B	-2.36	1.37	1.43
3	E	602	NAD	PA-O5B	-2.31	1.49	1.59
3	C	602	NAD	PA-O5B	-2.25	1.49	1.59
3	B	602	NAD	C2B-C1B	-2.25	1.50	1.53
3	B	602	NAD	O3B-C3B	-2.24	1.37	1.43
3	C	602	NAD	PA-O2A	-2.21	1.45	1.55
3	D	602	NAD	PA-O5B	-2.20	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAD	PA-O2A	-2.19	1.45	1.55
3	B	602	NAD	PA-O3	-2.16	1.47	1.54
3	A	602	NAD	O3B-C3B	-2.16	1.37	1.43
3	A	602	NAD	PA-O5B	-2.15	1.50	1.59
3	A	602	NAD	C2B-C3B	-2.13	1.47	1.53
3	F	602	NAD	O3B-C3B	-2.06	1.38	1.43
3	H	602	NAD	PA-O3	-2.04	1.47	1.54
3	F	602	NAD	PA-O3	-2.03	1.47	1.54
3	F	602	NAD	C2B-C3B	-2.02	1.48	1.53
3	E	602	NAD	C2B-C3B	-2.00	1.48	1.53
3	E	602	NAD	O3B-C3B	-2.00	1.38	1.43
3	D	602	NAD	C2A-N3A	2.32	1.36	1.32
3	C	602	NAD	C6A-N6A	2.34	1.43	1.34
3	G	602	NAD	C6A-N6A	2.34	1.43	1.34
3	H	602	NAD	C6A-N6A	2.34	1.43	1.34
3	F	602	NAD	C2A-N3A	2.40	1.36	1.32
3	G	602	NAD	C2A-N3A	2.41	1.36	1.32
3	F	602	NAD	C6A-N6A	2.42	1.44	1.34
3	D	602	NAD	C6A-N6A	2.44	1.44	1.34
3	D	602	NAD	PN-O1N	2.47	1.57	1.50
3	E	602	NAD	C6A-N6A	2.47	1.44	1.34
3	B	602	NAD	C6A-N6A	2.48	1.44	1.34
3	A	602	NAD	C6A-N6A	2.48	1.44	1.34
3	H	602	NAD	C2A-N3A	2.49	1.36	1.32
3	C	602	NAD	C2A-N3A	2.56	1.36	1.32
3	A	602	NAD	C2A-N3A	2.66	1.36	1.32
3	B	602	NAD	C2A-N3A	2.79	1.37	1.32
3	E	602	NAD	C2A-N3A	2.83	1.37	1.32

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	602	NAD	N3A-C2A-N1A	-12.02	119.43	128.87
3	B	602	NAD	N3A-C2A-N1A	-10.56	120.58	128.87
3	F	602	NAD	N3A-C2A-N1A	-10.44	120.67	128.87
3	D	602	NAD	N3A-C2A-N1A	-10.38	120.71	128.87
3	E	602	NAD	N3A-C2A-N1A	-10.07	120.96	128.87
3	A	602	NAD	N3A-C2A-N1A	-10.00	121.01	128.87
3	C	602	NAD	N3A-C2A-N1A	-9.87	121.12	128.87
3	H	602	NAD	N3A-C2A-N1A	-9.81	121.17	128.87
3	F	602	NAD	O3-PA-O1A	-4.43	96.18	110.63
3	G	602	NAD	O2A-PA-O1A	-4.38	96.34	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	602	NAD	O3-PA-O1A	-4.02	97.50	110.63
3	B	602	NAD	O3-PA-O1A	-3.84	98.10	110.63
3	B	602	NAD	O5B-PA-O1A	-3.75	97.66	107.08
3	G	602	NAD	C1B-N9A-C4A	-3.65	122.73	126.81
3	H	602	NAD	O5B-PA-O1A	-3.32	98.74	107.08
3	G	602	NAD	C4B-O4B-C1B	-3.21	106.24	109.64
3	F	602	NAD	C4B-O4B-C1B	-3.16	106.29	109.64
3	E	602	NAD	C4B-O4B-C1B	-3.05	106.41	109.64
3	F	602	NAD	O5B-PA-O1A	-3.04	99.45	107.08
3	A	602	NAD	C4B-O4B-C1B	-3.01	106.45	109.64
3	H	602	NAD	C4B-O4B-C1B	-2.96	106.50	109.64
3	D	602	NAD	O5B-PA-O1A	-2.89	97.40	109.21
3	C	602	NAD	O2A-PA-O3	-2.81	93.23	105.27
3	D	602	NAD	C4B-O4B-C1B	-2.74	106.74	109.64
3	C	602	NAD	C4B-O4B-C1B	-2.66	106.83	109.64
3	B	602	NAD	C4B-O4B-C1B	-2.55	106.94	109.64
3	G	602	NAD	O2A-PA-O5B	-2.54	99.31	106.72
3	E	602	NAD	C1B-N9A-C4A	-2.42	124.10	126.81
3	A	602	NAD	O2A-PA-O3	-2.39	95.01	105.27
3	G	602	NAD	O5B-PA-O1A	-2.38	101.09	107.08
3	E	602	NAD	O2A-PA-O3	-2.32	95.34	105.27
3	A	602	NAD	O2A-PA-O5B	-2.06	98.42	108.24
3	E	602	NAD	O5B-PA-O1A	2.11	117.86	109.21
3	C	602	NAD	O5B-PA-O1A	2.13	117.94	109.21
3	D	602	NAD	O4B-C1B-N9A	2.18	112.22	108.11
3	D	602	NAD	O2A-PA-O5B	2.23	118.87	108.24
3	B	602	NAD	O2A-PA-O1A	2.45	118.62	110.63
3	H	602	NAD	O2A-PA-O1A	2.70	119.43	110.63
3	G	602	NAD	O3-PA-O1A	2.73	119.54	110.63
3	F	602	NAD	O2A-PA-O1A	2.81	119.79	110.63
3	H	602	NAD	O2A-PA-O5B	2.90	115.20	106.72
3	B	602	NAD	O3-PA-O2A	3.08	118.73	107.44
3	F	602	NAD	O3-PA-O2A	3.17	119.06	107.44
3	G	602	NAD	O3-PA-O2A	3.29	119.52	107.44
3	D	602	NAD	O2A-PA-O3	3.32	119.50	105.27
3	F	602	NAD	O2A-PA-O5B	3.37	116.57	106.72
3	H	602	NAD	O3-PA-O2A	3.44	120.06	107.44
3	G	602	NAD	O3-PA-O5B	3.50	116.95	106.72
3	B	602	NAD	O2A-PA-O5B	3.95	118.26	106.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PG4	4	0
2	D	601	PG4	2	0
2	E	601	PG4	2	0
2	F	601	PG4	4	0
2	G	601	PG4	3	0
2	H	601	PG4	5	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	509/513 (99%)	-0.42	1 (0%)	95	95	15, 26, 44, 59	0
1	B	509/513 (99%)	-0.43	3 (0%)	90	90	17, 27, 46, 63	0
1	C	509/513 (99%)	-0.38	6 (1%)	81	81	17, 28, 50, 73	0
1	D	509/513 (99%)	-0.35	1 (0%)	95	95	15, 31, 50, 66	0
1	E	509/513 (99%)	-0.47	4 (0%)	87	88	18, 27, 44, 62	0
1	F	509/513 (99%)	-0.40	5 (0%)	84	84	19, 27, 44, 67	0
1	G	499/513 (97%)	-0.51	1 (0%)	95	95	18, 28, 42, 60	0
1	H	509/513 (99%)	-0.42	4 (0%)	87	88	17, 28, 46, 65	0
All	All	4062/4104 (98%)	-0.42	25 (0%)	90	90	15, 28, 47, 73	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	ALA	4.3
1	E	505	ALA	3.9
1	B	507	GLY	3.8
1	C	505	ALA	3.7
1	C	335	TRP	3.7
1	F	510	PHE	3.6
1	F	504	LEU	3.4
1	H	505	ALA	3.4
1	H	507	GLY	2.9
1	F	503	PRO	2.9
1	F	335	TRP	2.9
1	B	335	TRP	2.6
1	D	505	ALA	2.5
1	C	510	PHE	2.4
1	C	461	GLY	2.3
1	E	504	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	506	GLN	2.2
1	G	337	PRO	2.2
1	C	507	GLY	2.2
1	H	510	PHE	2.2
1	A	9	PRO	2.1
1	F	505	ALA	2.1
1	E	510	PHE	2.1
1	E	9	PRO	2.0
1	H	503	PRO	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
2	PG4	H	601	13/13	0.87	0.18	6.86	33,43,50,51	0
2	PG4	E	601	13/13	0.87	0.18	5.25	43,47,56,56	0
2	PG4	A	601	13/13	0.83	0.16	4.43	34,47,51,53	0
2	PG4	F	601	13/13	0.91	0.16	4.18	31,43,55,56	0
2	PG4	D	601	13/13	0.87	0.15	3.39	36,43,56,58	0
3	NAD	E	602	27/44	0.87	0.15	3.30	24,36,104,107	0
3	NAD	D	602	27/44	0.91	0.13	2.61	26,35,107,118	0
3	NAD	A	602	27/44	0.88	0.14	2.11	28,33,84,90	0
3	NAD	G	602	23/44	0.91	0.12	2.09	24,33,46,56	0
3	NAD	H	602	23/44	0.92	0.11	2.06	21,27,37,42	23
2	PG4	G	601	13/13	0.81	0.15	1.93	40,45,57,58	0
2	PG4	B	601	13/13	0.89	0.15	1.91	33,39,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAD	C	602	27/44	0.91	0.11	1.18	26,33,81,83	0
2	PG4	C	601	13/13	0.93	0.12	1.06	30,39,46,46	0
3	NAD	F	602	23/44	0.91	0.11	0.66	21,32,47,58	0
3	NAD	B	602	23/44	0.91	0.10	0.40	24,34,48,86	0

6.5 Other polymers (i)

There are no such residues in this entry.