



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:07 PM GMT

PDB ID : 4BGI
Title : Crystal structure of InhA(S94A) mutant in complex with OH-141
Authors : Pojer, F.; Hartkoorn, R.C.; Cole, S.T.
Deposited on : 2013-03-27
Resolution : 2.09 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

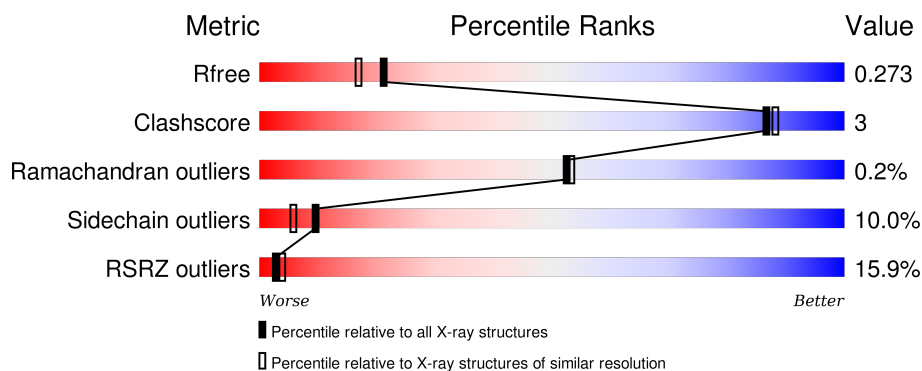
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. 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	281	<div> <div>7%</div> <div>83% 12% • 5%</div> </div>
1	B	281	<div> <div>9%</div> <div>85% 9% • 5%</div> </div>
1	C	281	<div> <div>18%</div> <div>78% 10% • 10%</div> </div>
1	D	281	<div> <div>15%</div> <div>79% 10% • 10%</div> </div>
1	E	281	<div> <div>16%</div> <div>76% 12% • 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	281	<div><div></div><div>22%</div><div></div><div>81%</div><div></div><div>12%</div><div></div><div>5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12372 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].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			
1	B	267	Total	C	N	O	S	0	1	0
			1993	1265	347	371	10			
1	C	254	Total	C	N	O	S	0	0	0
			1909	1210	334	356	9			
1	D	252	Total	C	N	O	S	0	0	0
			1889	1199	329	352	9			
1	E	251	Total	C	N	O	S	0	0	0
			1889	1199	331	350	9			
1	F	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	EXPRESSION TAG	UNP P0A5Y6
A	-2	ASP	-	EXPRESSION TAG	UNP P0A5Y6
A	-1	ILE	-	EXPRESSION TAG	UNP P0A5Y6
A	0	GLU	-	EXPRESSION TAG	UNP P0A5Y6
A	1	PHE	-	EXPRESSION TAG	UNP P0A5Y6
A	270	GLY	-	EXPRESSION TAG	UNP P0A5Y6
A	271	SER	-	EXPRESSION TAG	UNP P0A5Y6
A	272	HIS	-	EXPRESSION TAG	UNP P0A5Y6
A	273	HIS	-	EXPRESSION TAG	UNP P0A5Y6
A	274	HIS	-	EXPRESSION TAG	UNP P0A5Y6
A	275	HIS	-	EXPRESSION TAG	UNP P0A5Y6
A	276	HIS	-	EXPRESSION TAG	UNP P0A5Y6
A	277	HIS	-	EXPRESSION TAG	UNP P0A5Y6
A	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
B	-3	MET	-	EXPRESSION TAG	UNP P0A5Y6
B	-2	ASP	-	EXPRESSION TAG	UNP P0A5Y6

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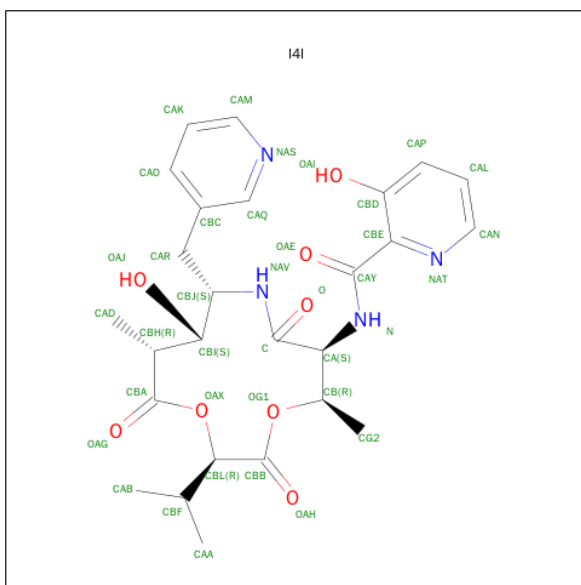
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ILE	-	EXPRESSION TAG	UNP P0A5Y6
B	0	GLU	-	EXPRESSION TAG	UNP P0A5Y6
B	1	PHE	-	EXPRESSION TAG	UNP P0A5Y6
B	270	GLY	-	EXPRESSION TAG	UNP P0A5Y6
B	271	SER	-	EXPRESSION TAG	UNP P0A5Y6
B	272	HIS	-	EXPRESSION TAG	UNP P0A5Y6
B	273	HIS	-	EXPRESSION TAG	UNP P0A5Y6
B	274	HIS	-	EXPRESSION TAG	UNP P0A5Y6
B	275	HIS	-	EXPRESSION TAG	UNP P0A5Y6
B	276	HIS	-	EXPRESSION TAG	UNP P0A5Y6
B	277	HIS	-	EXPRESSION TAG	UNP P0A5Y6
B	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
C	-3	MET	-	EXPRESSION TAG	UNP P0A5Y6
C	-2	ASP	-	EXPRESSION TAG	UNP P0A5Y6
C	-1	ILE	-	EXPRESSION TAG	UNP P0A5Y6
C	0	GLU	-	EXPRESSION TAG	UNP P0A5Y6
C	1	PHE	-	EXPRESSION TAG	UNP P0A5Y6
C	270	GLY	-	EXPRESSION TAG	UNP P0A5Y6
C	271	SER	-	EXPRESSION TAG	UNP P0A5Y6
C	272	HIS	-	EXPRESSION TAG	UNP P0A5Y6
C	273	HIS	-	EXPRESSION TAG	UNP P0A5Y6
C	274	HIS	-	EXPRESSION TAG	UNP P0A5Y6
C	275	HIS	-	EXPRESSION TAG	UNP P0A5Y6
C	276	HIS	-	EXPRESSION TAG	UNP P0A5Y6
C	277	HIS	-	EXPRESSION TAG	UNP P0A5Y6
C	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
D	-3	MET	-	EXPRESSION TAG	UNP P0A5Y6
D	-2	ASP	-	EXPRESSION TAG	UNP P0A5Y6
D	-1	ILE	-	EXPRESSION TAG	UNP P0A5Y6
D	0	GLU	-	EXPRESSION TAG	UNP P0A5Y6
D	1	PHE	-	EXPRESSION TAG	UNP P0A5Y6
D	270	GLY	-	EXPRESSION TAG	UNP P0A5Y6
D	271	SER	-	EXPRESSION TAG	UNP P0A5Y6
D	272	HIS	-	EXPRESSION TAG	UNP P0A5Y6
D	273	HIS	-	EXPRESSION TAG	UNP P0A5Y6
D	274	HIS	-	EXPRESSION TAG	UNP P0A5Y6
D	275	HIS	-	EXPRESSION TAG	UNP P0A5Y6
D	276	HIS	-	EXPRESSION TAG	UNP P0A5Y6
D	277	HIS	-	EXPRESSION TAG	UNP P0A5Y6
D	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
E	-3	MET	-	EXPRESSION TAG	UNP P0A5Y6
E	-2	ASP	-	EXPRESSION TAG	UNP P0A5Y6

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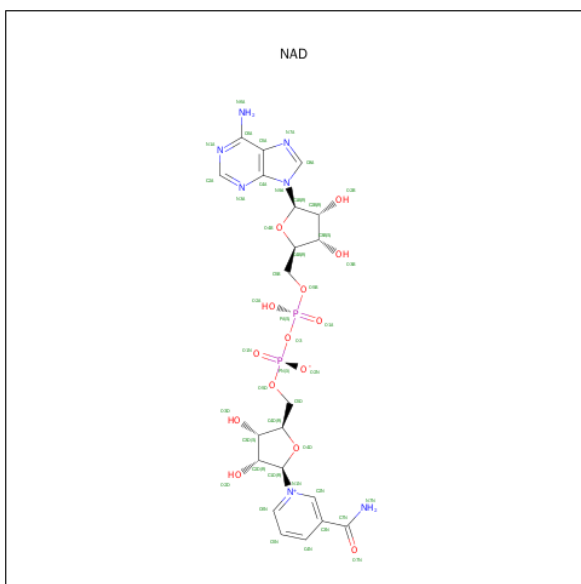
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ILE	-	EXPRESSION TAG	UNP P0A5Y6
E	0	GLU	-	EXPRESSION TAG	UNP P0A5Y6
E	1	PHE	-	EXPRESSION TAG	UNP P0A5Y6
E	270	GLY	-	EXPRESSION TAG	UNP P0A5Y6
E	271	SER	-	EXPRESSION TAG	UNP P0A5Y6
E	272	HIS	-	EXPRESSION TAG	UNP P0A5Y6
E	273	HIS	-	EXPRESSION TAG	UNP P0A5Y6
E	274	HIS	-	EXPRESSION TAG	UNP P0A5Y6
E	275	HIS	-	EXPRESSION TAG	UNP P0A5Y6
E	276	HIS	-	EXPRESSION TAG	UNP P0A5Y6
E	277	HIS	-	EXPRESSION TAG	UNP P0A5Y6
E	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
F	-3	MET	-	EXPRESSION TAG	UNP P0A5Y6
F	-2	ASP	-	EXPRESSION TAG	UNP P0A5Y6
F	-1	ILE	-	EXPRESSION TAG	UNP P0A5Y6
F	0	GLU	-	EXPRESSION TAG	UNP P0A5Y6
F	1	PHE	-	EXPRESSION TAG	UNP P0A5Y6
F	270	GLY	-	EXPRESSION TAG	UNP P0A5Y6
F	271	SER	-	EXPRESSION TAG	UNP P0A5Y6
F	272	HIS	-	EXPRESSION TAG	UNP P0A5Y6
F	273	HIS	-	EXPRESSION TAG	UNP P0A5Y6
F	274	HIS	-	EXPRESSION TAG	UNP P0A5Y6
F	275	HIS	-	EXPRESSION TAG	UNP P0A5Y6
F	276	HIS	-	EXPRESSION TAG	UNP P0A5Y6
F	277	HIS	-	EXPRESSION TAG	UNP P0A5Y6
F	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6

- Molecule 2 is 3-HYDROXY-N-[(2R,5R,6S,9S,10S,11R)-10-HYDROXY-5,11-DIMETHYL-3,7,12-TRIOXO-2-(PROPAN-2-YL)-9-(PYRIDIN-3-YLMETHYL)-1,4-DIOXA-8-AZACYCLODODECAN-6-YL]PYRIDINE-2-CARBOXAMIDE (three-letter code: I4I) (formula: C₂₆H₃₂N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 38	C 26	N 4	O 8	0	0
2	B	1	Total 38	C 26	N 4	O 8	0	0
2	F	1	Total 38	C 26	N 4	O 8	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

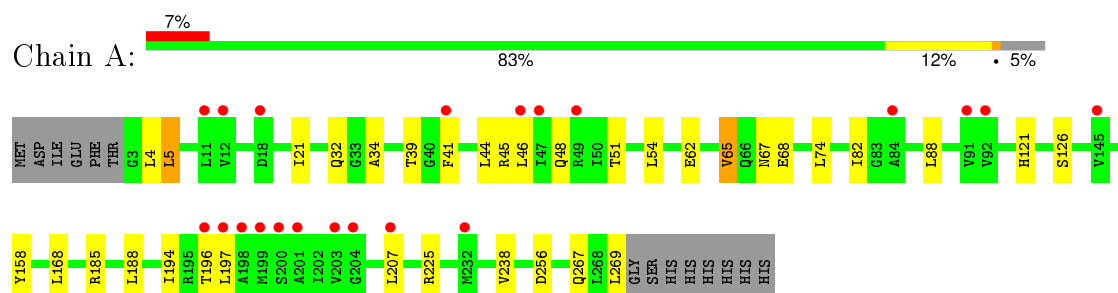
- Molecule 4 is water.

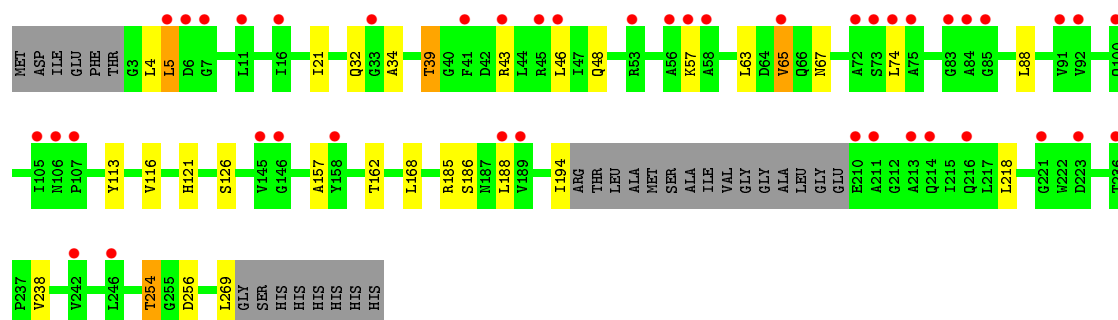
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	78	Total	O	0	0
			78	78		
4	C	67	Total	O	0	0
			67	67		
4	D	60	Total	O	0	0
			60	60		
4	E	46	Total	O	0	0
			46	46		
4	F	100	Total	O	0	0
			100	100		

3 Residue-property plots [i](#)

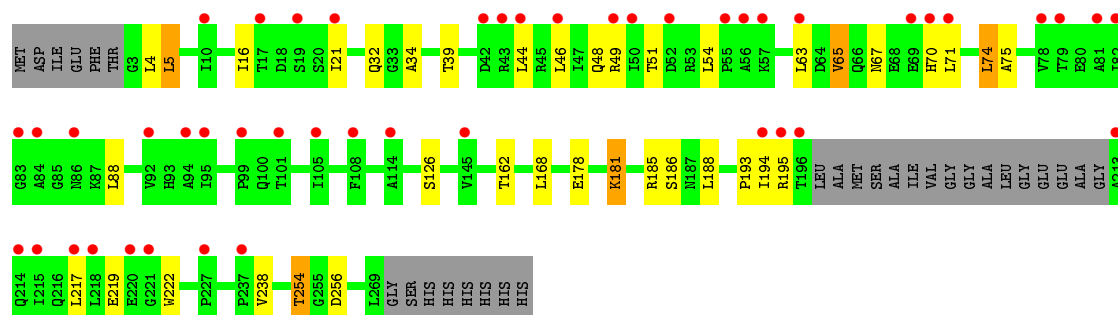
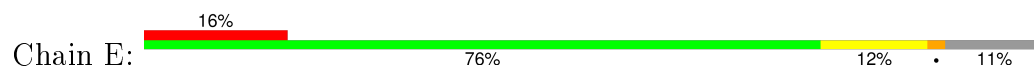
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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]

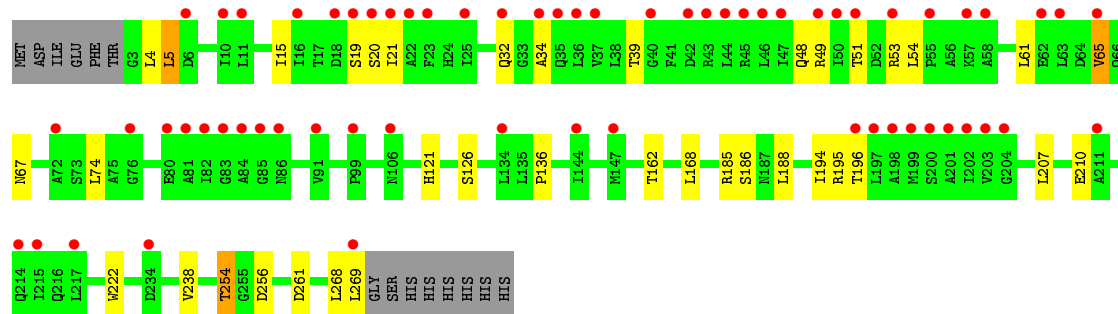
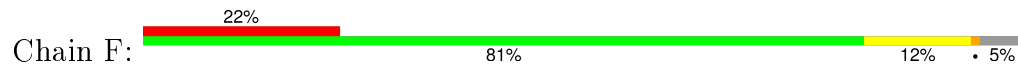




- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.44Å 82.45Å 189.65Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	30.60 – 2.09 30.18 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.60-2.09) 99.4 (30.18-2.09)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.211 , 0.238 0.242 , 0.273	Depositor DCC
R_{free} test set	4530 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 90347 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12372	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, I4I

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	0.53	0/2026	0.68	0/2750
1	B	0.53	0/2034	0.68	0/2761
1	C	0.47	0/1946	0.66	0/2640
1	D	0.47	0/1926	0.66	0/2614
1	E	0.47	0/1926	0.68	0/2614
1	F	0.46	0/2026	0.66	0/2750
All	All	0.49	0/11884	0.67	0/16129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1988	0	2006	10	0
1	B	1993	0	2017	9	0
1	C	1909	0	1918	14	0
1	D	1889	0	1899	11	0
1	E	1889	0	1905	14	0
1	F	1988	0	2006	11	0
2	A	38	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	38	0	31	0	0
2	F	38	0	31	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
3	E	44	0	26	0	0
4	A	119	0	0	1	0
4	B	78	0	0	1	0
4	C	67	0	0	0	0
4	D	60	0	0	0	0
4	E	46	0	0	1	0
4	F	100	0	0	1	0
All	All	12372	0	11922	65	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 (65) 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:254:THR:HG21	4:B:2052:HOH:O	1.61	1.00
1:D:4:LEU:H	1:D:32:GLN:HE21	1.39	0.71
1:A:4:LEU:H	1:A:32:GLN:HE21	1.38	0.71
1:F:4:LEU:H	1:F:32:GLN:HE21	1.38	0.71
1:C:140:PRO:HG2	1:E:195:ARG:HH12	1.57	0.70
1:E:254:THR:HG21	4:E:2037:HOH:O	1.92	0.70
1:C:4:LEU:H	1:C:32:GLN:HE21	1.39	0.69
1:E:4:LEU:H	1:E:32:GLN:HE21	1.39	0.68
1:B:45:ARG:HB3	1:F:136:PRO:HB3	1.85	0.58
1:F:21:ILE:HD11	1:F:194:ILE:HG13	1.85	0.58
1:B:21:ILE:HD11	1:B:194:ILE:HG13	1.86	0.57
1:C:74:LEU:HD22	1:C:134:LEU:HD21	1.85	0.57
1:E:21:ILE:HD11	1:E:194:ILE:HG13	1.87	0.57
1:C:21:ILE:HD11	1:C:194:ILE:HG13	1.88	0.56
1:A:21:ILE:HD11	1:A:194:ILE:HG13	1.87	0.55
1:D:21:ILE:HD11	1:D:194:ILE:HG13	1.90	0.52
1:F:222:TRP:HE1	1:F:261:ASP:HB2	1.74	0.52
1:E:70:HIS:O	1:E:74:LEU:HB2	2.10	0.52
1:C:16:ILE:HD12	1:C:47:ILE:HD11	1.92	0.52
1:A:44:LEU:HD11	1:A:62:GLU:HB2	1.92	0.51
1:D:185:ARG:HA	1:D:254:THR:HG23	1.93	0.51
1:C:185:ARG:HA	1:C:254:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ARG:HA	1:E:254:THR:HG23	1.94	0.50
1:B:185:ARG:HA	1:B:254:THR:HG23	1.94	0.50
1:F:185:ARG:HA	1:F:254:THR:HG23	1.94	0.49
1:C:45:ARG:HE	1:C:46:LEU:HG	1.78	0.48
1:F:15:ILE:HA	4:F:2002:HOH:O	2.16	0.45
1:B:65:VAL:CG2	1:B:126:SER:HB2	2.47	0.44
1:C:65:VAL:CG2	1:C:126:SER:HB2	2.47	0.44
1:A:5:LEU:HB3	1:A:34:ALA:HB2	2.00	0.44
1:B:186:SER:H	1:B:254:THR:HG23	1.81	0.44
1:A:51:THR:O	1:A:54:LEU:HB2	2.18	0.43
1:F:5:LEU:HB3	1:F:34:ALA:HB2	2.00	0.43
1:A:225:ARG:HD2	1:A:267:GLN:O	2.18	0.43
1:C:195:ARG:HD3	1:C:232:MET:HG3	1.99	0.43
1:E:193:PRO:HB2	1:E:219:GLU:HG2	2.01	0.43
1:F:186:SER:H	1:F:254:THR:HG23	1.83	0.43
1:C:124:ALA:HA	1:C:168:LEU:HD13	2.01	0.43
1:D:63:LEU:HD13	1:D:74:LEU:HD13	2.00	0.43
1:D:65:VAL:CG2	1:D:126:SER:HB2	2.49	0.43
1:E:178:GLU:O	1:E:181:LYS:HG2	2.18	0.43
1:E:5:LEU:HB3	1:E:34:ALA:HB2	2.01	0.43
1:B:51:THR:O	1:B:54:LEU:HB2	2.18	0.43
1:F:51:THR:O	1:F:54:LEU:HB2	2.19	0.43
1:B:5:LEU:HB3	1:B:34:ALA:HB2	2.01	0.43
1:D:5:LEU:HB3	1:D:34:ALA:HB2	2.01	0.43
1:E:65:VAL:CG2	1:E:126:SER:HB2	2.49	0.42
1:D:43:ARG:HB3	1:D:46:LEU:HB3	2.01	0.42
1:A:158:TYR:HD1	2:A:1270:I4I:HAB	1.84	0.42
1:C:61:LEU:HD22	1:C:77:ARG:HB3	2.01	0.42
1:F:65:VAL:CG2	1:F:126:SER:HB2	2.50	0.42
1:A:21:ILE:HD12	2:A:1270:I4I:CAK	2.49	0.41
1:E:51:THR:O	1:E:54:LEU:HB2	2.19	0.41
1:C:140:PRO:HG2	1:E:195:ARG:NH1	2.29	0.41
1:D:218:LEU:HD11	1:F:268:LEU:HD23	2.03	0.41
1:D:39:THR:HG23	1:D:63:LEU:HB3	2.03	0.41
1:D:113:TYR:HA	1:D:116:VAL:HG22	2.03	0.41
1:E:63:LEU:HD11	1:E:71:LEU:HD12	2.02	0.41
1:A:65:VAL:CG2	1:A:126:SER:HB2	2.51	0.41
1:C:5:LEU:HB3	1:C:34:ALA:HB2	2.01	0.41
1:E:186:SER:H	1:E:254:THR:HG23	1.86	0.41
1:A:185:ARG:HD2	4:A:2106:HOH:O	2.21	0.40
1:D:186:SER:H	1:D:254:THR:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:SER:H	1:C:254:THR:HG23	1.85	0.40
1:B:43:ARG:H	1:B:43:ARG:HG2	1.75	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	265/281 (94%)	252 (95%)	13 (5%)	0	100	100
1	B	266/281 (95%)	257 (97%)	9 (3%)	0	100	100
1	C	250/281 (89%)	238 (95%)	11 (4%)	1 (0%)	39	37
1	D	248/281 (88%)	238 (96%)	9 (4%)	1 (0%)	39	37
1	E	247/281 (88%)	233 (94%)	13 (5%)	1 (0%)	39	37
1	F	265/281 (94%)	251 (95%)	14 (5%)	0	100	100
All	All	1541/1686 (91%)	1469 (95%)	69 (4%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	75	ALA
1	C	74	LEU
1	D	157	ALA

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	202/215 (94%)	181 (90%)	21 (10%)	9	5
1	B	203/215 (94%)	183 (90%)	20 (10%)	10	6
1	C	195/215 (91%)	175 (90%)	20 (10%)	9	5
1	D	193/215 (90%)	178 (92%)	15 (8%)	16	11
1	E	194/215 (90%)	174 (90%)	20 (10%)	9	5
1	F	202/215 (94%)	179 (89%)	23 (11%)	7	4
All	All	1189/1290 (92%)	1070 (90%)	119 (10%)	9	6

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	39	THR
1	A	41	PHE
1	A	45	ARG
1	A	46	LEU
1	A	48	GLN
1	A	65	VAL
1	A	67	ASN
1	A	68	GLU
1	A	74	LEU
1	A	82	ILE
1	A	88	LEU
1	A	121	HIS
1	A	168	LEU
1	A	188	LEU
1	A	196	THR
1	A	197	LEU
1	A	207	LEU
1	A	238	VAL
1	A	256	ASP
1	A	269	LEU
1	B	5	LEU
1	B	39	THR
1	B	44	LEU
1	B	45	ARG
1	B	48	GLN
1	B	65	VAL
1	B	67	ASN

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Mol	Chain	Res	Type
1	B	74	LEU
1	B	88	LEU
1	B	121	HIS
1	B	162	THR
1	B	168	LEU
1	B	188	LEU
1	B	196	THR
1	B	199	MET
1	B	207	LEU
1	B	238	VAL
1	B	254	THR
1	B	256	ASP
1	B	269	LEU
1	C	5	LEU
1	C	16	ILE
1	C	44	LEU
1	C	45	ARG
1	C	46	LEU
1	C	48	GLN
1	C	54	LEU
1	C	60	LEU
1	C	65	VAL
1	C	74	LEU
1	C	88	LEU
1	C	121	HIS
1	C	162	THR
1	C	188	LEU
1	C	195	ARG
1	C	216	GLN
1	C	238	VAL
1	C	254	THR
1	C	256	ASP
1	C	269	LEU
1	D	5	LEU
1	D	39	THR
1	D	48	GLN
1	D	57	LYS
1	D	65	VAL
1	D	67	ASN
1	D	88	LEU
1	D	121	HIS
1	D	162	THR

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Mol	Chain	Res	Type
1	D	168	LEU
1	D	188	LEU
1	D	238	VAL
1	D	254	THR
1	D	256	ASP
1	D	269	LEU
1	E	5	LEU
1	E	16	ILE
1	E	39	THR
1	E	44	LEU
1	E	46	LEU
1	E	48	GLN
1	E	49	ARG
1	E	65	VAL
1	E	67	ASN
1	E	74	LEU
1	E	88	LEU
1	E	162	THR
1	E	168	LEU
1	E	181	LYS
1	E	188	LEU
1	E	217	LEU
1	E	222	TRP
1	E	238	VAL
1	E	254	THR
1	E	256	ASP
1	F	5	LEU
1	F	19	SER
1	F	20	SER
1	F	39	THR
1	F	48	GLN
1	F	49	ARG
1	F	53	ARG
1	F	61	LEU
1	F	65	VAL
1	F	67	ASN
1	F	74	LEU
1	F	121	HIS
1	F	162	THR
1	F	168	LEU
1	F	188	LEU
1	F	195	ARG

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Mol	Chain	Res	Type
1	F	196	THR
1	F	207	LEU
1	F	210	GLU
1	F	238	VAL
1	F	254	THR
1	F	256	ASP
1	F	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	66	GLN
1	A	67	ASN
1	A	86	ASN
1	A	106	ASN
1	A	121	HIS
1	A	187	ASN
1	B	67	ASN
1	B	187	ASN
1	C	32	GLN
1	C	67	ASN
1	C	187	ASN
1	D	32	GLN
1	D	67	ASN
1	D	187	ASN
1	D	216	GLN
1	E	32	GLN
1	E	67	ASN
1	E	187	ASN
1	F	32	GLN
1	F	48	GLN
1	F	66	GLN
1	F	67	ASN
1	F	121	HIS
1	F	187	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	I4I	A	1270	-	39,40,40	1.13	5 (12%)	52,56,56	1.38	6 (11%)
2	I4I	B	1270	-	39,40,40	1.30	3 (7%)	52,56,56	1.41	6 (11%)
3	NAD	C	1270	-	38,48,48	0.65	0	47,73,73	0.63	1 (2%)
3	NAD	D	1270	-	38,48,48	0.57	0	47,73,73	0.87	1 (2%)
3	NAD	E	1270	-	38,48,48	0.56	0	47,73,73	0.68	1 (2%)
2	I4I	F	1270	-	39,40,40	1.34	5 (12%)	52,56,56	1.33	5 (9%)

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	I4I	A	1270	-	-	2/52/52/52	0/2/3/3
2	I4I	B	1270	-	-	3/52/52/52	0/2/3/3
3	NAD	C	1270	-	-	0/22/62/62	0/5/5/5
3	NAD	D	1270	-	-	0/22/62/62	0/5/5/5
3	NAD	E	1270	-	-	0/22/62/62	0/5/5/5
2	I4I	F	1270	-	-	1/52/52/52	0/2/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1270	I4I	CAQ-CBC	2.00	1.41	1.38
2	A	1270	I4I	C-NAV	2.02	1.38	1.34
2	F	1270	I4I	CBE-NAT	2.12	1.38	1.34
2	A	1270	I4I	CBD-CBE	2.23	1.43	1.40
2	A	1270	I4I	OAX-CBA	2.30	1.39	1.34
2	F	1270	I4I	CBD-CBE	2.51	1.44	1.40
2	A	1270	I4I	CBE-NAT	2.76	1.39	1.34
2	F	1270	I4I	CAY-N	2.79	1.40	1.34
2	B	1270	I4I	CBE-NAT	2.93	1.40	1.34
2	B	1270	I4I	CAQ-CBC	3.10	1.43	1.38
2	F	1270	I4I	CAQ-CBC	3.14	1.43	1.38
2	F	1270	I4I	CBL-CBB	3.19	1.57	1.52
2	B	1270	I4I	CBL-CBB	3.59	1.58	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1270	I4I	C-CA-N	-4.31	98.88	110.59
3	D	1270	NAD	C4B-O4B-C1B	-4.05	105.27	109.72
2	B	1270	I4I	C-CA-N	-4.05	99.59	110.59
2	F	1270	I4I	C-CA-N	-3.46	101.20	110.59
3	E	1270	NAD	C4B-O4B-C1B	-2.70	106.75	109.72
2	A	1270	I4I	OAX-CBA-OAG	-2.26	119.24	123.89
2	B	1270	I4I	OG1-CB-CA	-2.12	100.66	105.61
2	B	1270	I4I	CAY-CBE-NAT	-2.08	111.89	115.54
3	C	1270	NAD	O3-PA-O5B	2.05	108.38	102.94
2	F	1270	I4I	CBF-CBL-CBB	2.45	119.56	112.27
2	A	1270	I4I	CBH-CBI-CBJ	2.58	117.34	113.52
2	A	1270	I4I	CB-CA-C	2.73	116.10	110.44
2	B	1270	I4I	CB-CA-C	3.13	116.93	110.44
2	F	1270	I4I	CB-CA-C	3.14	116.94	110.44
2	A	1270	I4I	CB-OG1-CBB	3.21	122.37	117.44
2	B	1270	I4I	CA-N-CAY	3.28	128.18	121.43
2	F	1270	I4I	CA-N-CAY	3.46	128.57	121.43
2	A	1270	I4I	CA-N-CAY	3.79	129.24	121.43
2	F	1270	I4I	CB-OG1-CBB	4.85	124.89	117.44
2	B	1270	I4I	CB-OG1-CBB	4.89	124.95	117.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1270	I4I	NAT-CBE-CAY-N
2	A	1270	I4I	NAT-CBE-CAY-N
2	B	1270	I4I	OAE-CAY-CBE-CBD
2	F	1270	I4I	CBD-CBE-CAY-N
2	A	1270	I4I	CBD-CBE-CAY-N
2	B	1270	I4I	CBD-CBE-CAY-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1270	I4I	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/281 (95%)	0.47	21 (7%) 15 21	7, 22, 52, 65	0
1	B	267/281 (95%)	0.57	24 (8%) 12 16	7, 21, 54, 82	0
1	C	254/281 (90%)	1.22	50 (19%) 1 2	21, 40, 65, 85	0
1	D	252/281 (89%)	1.15	43 (17%) 2 3	21, 39, 63, 89	0
1	E	251/281 (89%)	1.19	46 (18%) 2 2	21, 40, 65, 85	0
1	F	267/281 (95%)	1.38	63 (23%) 1 1	24, 43, 74, 92	0
All	All	1558/1686 (92%)	0.99	247 (15%) 3 4	7, 35, 64, 92	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	ILE	9.3
1	B	197[A]	LEU	8.7
1	C	213	ALA	8.5
1	F	50	ILE	8.0
1	D	84	ALA	7.6
1	F	204	GLY	6.7
1	F	197	LEU	6.6
1	F	43	ARG	6.6
1	F	44	LEU	6.2
1	F	46	LEU	6.1
1	D	105	ILE	5.9
1	C	73	SER	5.7
1	E	217	LEU	5.5
1	F	202	ILE	5.5
1	E	196	THR	5.5
1	F	16	ILE	5.5
1	D	85	GLY	5.4
1	F	19	SER	5.3
1	E	82	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	203	VAL	5.0
1	C	41	PHE	5.0
1	C	105	ILE	4.9
1	B	204	GLY	4.9
1	A	198	ALA	4.8
1	F	82	ILE	4.7
1	C	44	LEU	4.6
1	D	100	GLN	4.6
1	C	81	ALA	4.4
1	D	58	ALA	4.4
1	E	105	ILE	4.4
1	E	43	ARG	4.3
1	B	203	VAL	4.3
1	E	19	SER	4.2
1	C	3	GLY	4.2
1	E	84	ALA	4.1
1	E	50	ILE	4.1
1	D	45	ARG	4.1
1	E	92	VAL	4.1
1	C	84	ALA	4.0
1	F	198	ALA	4.0
1	F	49	ARG	4.0
1	B	84	ALA	3.9
1	C	124	ALA	3.9
1	A	203	VAL	3.9
1	C	78	VAL	3.9
1	E	79	THR	3.8
1	F	21	ILE	3.8
1	F	196	THR	3.8
1	C	85	GLY	3.8
1	F	45	ARG	3.8
1	F	83	GLY	3.8
1	F	11	LEU	3.8
1	C	50	ILE	3.7
1	A	92	VAL	3.7
1	F	20	SER	3.7
1	C	58	ALA	3.7
1	B	50	ILE	3.7
1	B	46	LEU	3.7
1	E	46	LEU	3.7
1	A	84	ALA	3.6
1	E	218	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	199	MET	3.6
1	A	204	GLY	3.6
1	E	86	ASN	3.6
1	D	214	GLN	3.6
1	D	91	VAL	3.6
1	D	53	ARG	3.6
1	F	85	GLY	3.5
1	E	56	ALA	3.5
1	D	210	GLU	3.5
1	C	19	SER	3.4
1	A	196	THR	3.4
1	F	234	ASP	3.4
1	F	106	ASN	3.3
1	F	22	ALA	3.3
1	C	221	GLY	3.3
1	F	86	ASN	3.3
1	D	57	LYS	3.3
1	F	6	ASP	3.3
1	F	84	ALA	3.2
1	F	80	GLU	3.2
1	D	46	LEU	3.2
1	F	201	ALA	3.2
1	D	92	VAL	3.2
1	E	145	VAL	3.2
1	E	213	ALA	3.2
1	F	40	GLY	3.2
1	D	72	ALA	3.2
1	F	25	ILE	3.2
1	F	55	PRO	3.2
1	D	158	TYR	3.2
1	A	49	ARG	3.1
1	F	91	VAL	3.1
1	C	76	GLY	3.1
1	F	53	ARG	3.1
1	E	81	ALA	3.1
1	F	217	LEU	3.1
1	C	42	ASP	3.1
1	D	106	ASN	3.1
1	A	12	VAL	3.0
1	C	45	ARG	3.0
1	C	214	GLN	3.0
1	F	62	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	32	GLN	3.0
1	E	71	LEU	3.0
1	C	6	ASP	2.9
1	A	201	ALA	2.9
1	A	197	LEU	2.9
1	E	17	THR	2.9
1	A	46	LEU	2.8
1	D	83	GLY	2.8
1	F	57	LYS	2.8
1	A	145	VAL	2.8
1	D	7	GLY	2.8
1	B	43	ARG	2.8
1	D	145	VAL	2.8
1	C	232	MET	2.8
1	F	23	PHE	2.8
1	C	80	GLU	2.8
1	D	236	THR	2.8
1	E	221	GLY	2.8
1	F	51	THR	2.7
1	D	11	LEU	2.7
1	A	11	LEU	2.7
1	C	15	ILE	2.7
1	F	47	ILE	2.7
1	C	65	VAL	2.7
1	D	65	VAL	2.7
1	D	221	GLY	2.7
1	C	210	GLU	2.7
1	B	188	LEU	2.7
1	A	41	PHE	2.7
1	F	18	ASP	2.7
1	B	96	GLY	2.7
1	B	19	SER	2.7
1	D	41	PHE	2.7
1	E	194	ILE	2.6
1	F	144	ILE	2.6
1	F	211	ALA	2.6
1	D	223	ASP	2.6
1	B	92	VAL	2.6
1	F	37	VAL	2.6
1	B	45	ARG	2.6
1	C	211	ALA	2.6
1	D	73	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	11	LEU	2.6
1	C	135	LEU	2.6
1	C	212	GLY	2.6
1	C	88	LEU	2.5
1	C	79	THR	2.5
1	D	211	ALA	2.5
1	C	92	VAL	2.5
1	D	107	PRO	2.5
1	C	246	LEU	2.5
1	E	49	ARG	2.5
1	C	40	GLY	2.5
1	A	207	LEU	2.5
1	F	36	LEU	2.5
1	B	16	ILE	2.5
1	C	95	ILE	2.5
1	C	145	VAL	2.5
1	F	35	GLN	2.5
1	F	81	ALA	2.5
1	C	74	LEU	2.5
1	E	83	GLY	2.4
1	E	55	PRO	2.4
1	C	100	GLN	2.4
1	E	214	GLN	2.4
1	F	58	ALA	2.4
1	A	199	MET	2.4
1	B	124	ALA	2.4
1	D	213	ALA	2.4
1	B	196	THR	2.4
1	D	146	GLY	2.4
1	F	76	GLY	2.4
1	B	42	ASP	2.4
1	D	74	LEU	2.4
1	D	188	LEU	2.4
1	E	101	THR	2.4
1	C	179	ALA	2.3
1	F	34	ALA	2.3
1	A	91	VAL	2.3
1	C	55	PRO	2.3
1	E	237	PRO	2.3
1	C	43	ARG	2.3
1	B	91	VAL	2.3
1	D	242	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	63	LEU	2.3
1	E	44	LEU	2.3
1	E	63	LEU	2.3
1	F	63	LEU	2.3
1	C	128	ALA	2.3
1	D	33	GLY	2.3
1	F	214	GLN	2.3
1	B	15	ILE	2.3
1	E	10	ILE	2.3
1	C	12	VAL	2.3
1	E	21	ILE	2.3
1	F	215	ILE	2.3
1	D	6	ASP	2.3
1	F	42	ASP	2.3
1	D	75	ALA	2.3
1	E	94	ALA	2.3
1	C	218	LEU	2.3
1	D	246	LEU	2.3
1	F	269	LEU	2.3
1	E	99	PRO	2.2
1	E	70	HIS	2.2
1	E	114	ALA	2.2
1	F	134	LEU	2.2
1	E	69	GLU	2.2
1	A	18	ASP	2.2
1	E	52	ASP	2.2
1	C	112	PRO	2.2
1	B	69	GLU	2.2
1	E	220	GLU	2.2
1	F	65	VAL	2.2
1	B	47	ILE	2.2
1	E	57	LYS	2.2
1	D	216	GLN	2.2
1	C	127	TYR	2.2
1	E	42	ASP	2.2
1	F	72	ALA	2.2
1	D	43	ARG	2.1
1	F	147	MET	2.1
1	B	127	TYR	2.1
1	B	48	GLN	2.1
1	C	219	GLU	2.1
1	C	134	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	216	GLN	2.1
1	E	108	PHE	2.1
1	D	189	VAL	2.1
1	B	147	MET	2.1
1	B	234	ASP	2.1
1	A	47	ILE	2.1
1	A	200	SER	2.1
1	D	56	ALA	2.1
1	F	200	SER	2.1
1	F	99	PRO	2.1
1	D	16	ILE	2.1
1	D	5	LEU	2.1
1	E	227	PRO	2.1
1	F	10	ILE	2.0
1	E	78	VAL	2.0
1	E	195	ARG	2.0
1	A	232	MET	2.0
1	E	95	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAD	C	1270	44/44	0.78	0.20	0.26	42,53,64,68	0
2	I4I	F	1270	38/38	0.81	0.19	0.04	44,51,56,57	0
2	I4I	A	1270	38/38	0.92	0.14	-0.43	14,23,30,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAD	E	1270	44/44	0.87	0.16	-0.46	27,48,62,66	0
2	I4I	B	1270	38/38	0.93	0.14	-0.73	18,23,33,36	0
3	NAD	D	1270	44/44	0.88	0.13	-0.93	30,39,47,50	0

6.5 Other polymers

There are no such residues in this entry.