Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:48 PM GMT

PDB ID	:	3S2G
Title	:	Crystal Structure of FurX NADH+:Furfuryl alcohol I
Authors	:	Hayes, R.; Sanchez, E.J.; Webb, B.N.; Hooper, T.; Nissen, M.S.; Li, Q.; Xun, L.
Deposited on	:	2011-05-16
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

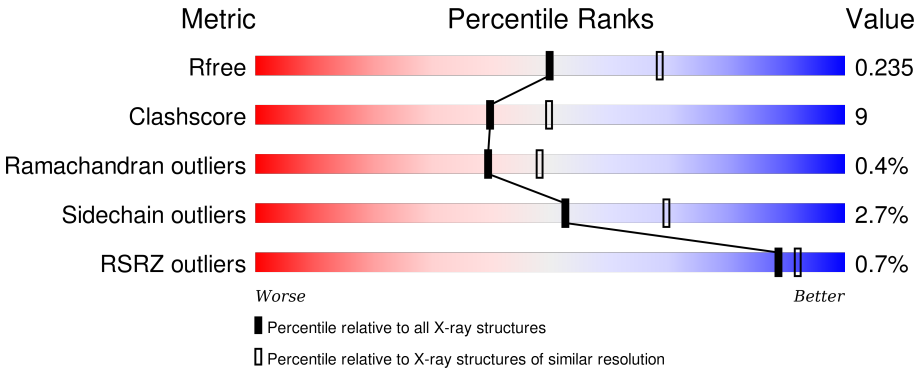
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	340	84% 16%
1	B	340	% 86% 14%
1	C	340	83% 16%
1	D	340	84% 15%
1	E	340	% 72% 26%

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Mol	Chain	Length	Quality of chain
1	F	340	
1	G	340	
1	H	340	

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	ZN	H	500	-	-	-	X
2	ZN	H	501	-	-	-	X
3	FU2	B	600	-	-	-	X
3	FU2	C	600	-	-	-	X
3	FU2	G	600	-	-	X	X
4	SO4	A	701	-	-	X	-
4	SO4	B	701	-	-	-	X
4	SO4	C	701	-	-	-	X
5	NAD	E	1250	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21825 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 Zinc-containing alcohol dehydrogenase superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	B	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	C	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	D	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	E	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	F	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	G	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			
1	H	340	Total	C	N	O	S	0	0	0
			2515	1593	443	469	10			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

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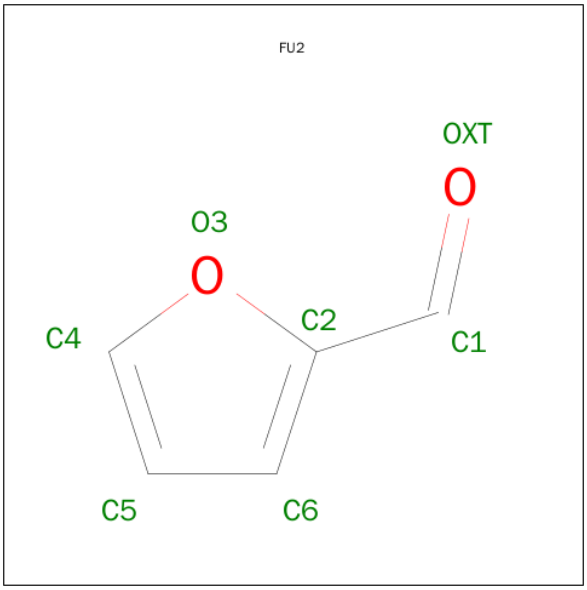
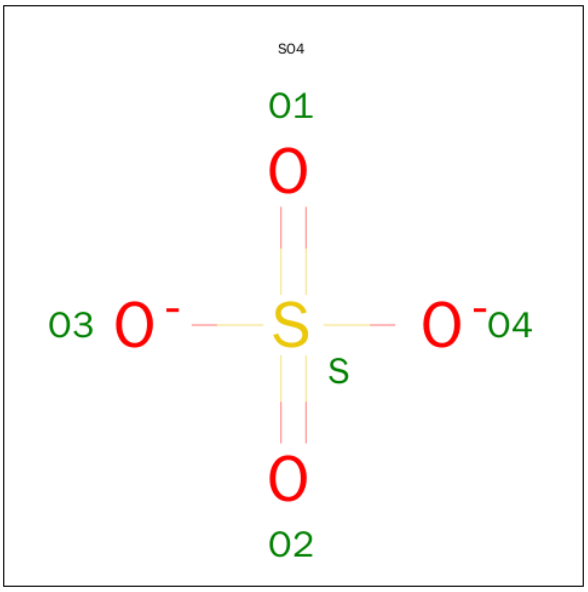
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is FURFURAL (three-letter code: FU2) (formula: $C_5H_4O_2$).



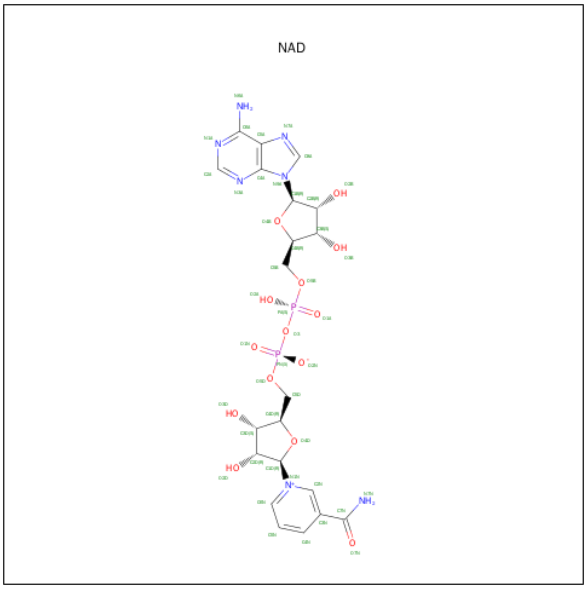
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 5 2	0	0
3	B	1	Total C O 7 5 2	0	0
3	C	1	Total C O 7 5 2	0	0
3	D	1	Total C O 7 5 2	0	0
3	E	1	Total C O 7 5 2	0	0
3	F	1	Total C O 7 5 2	0	0
3	G	1	Total C O 7 5 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	204	Total	O	0	0
			204	204		
6	B	214	Total	O	0	0
			214	214		
6	C	156	Total	O	0	0
			156	156		
6	D	170	Total	O	0	0
			170	170		
6	E	127	Total	O	0	0
			127	127		
6	F	122	Total	O	0	0
			122	122		

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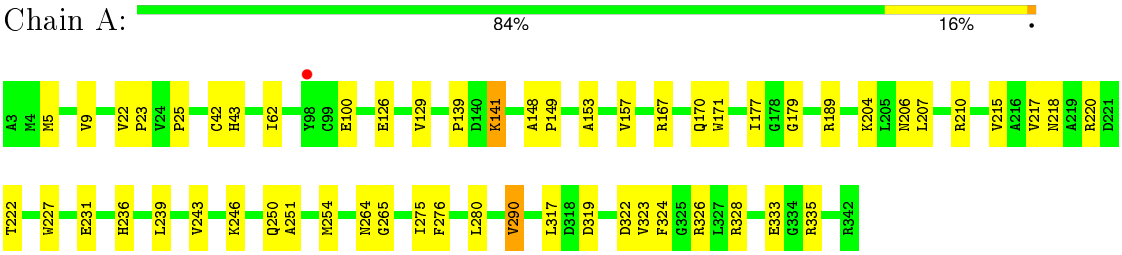
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	194	Total O 194 194	0	0
6	H	207	Total O 207 207	0	0

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.

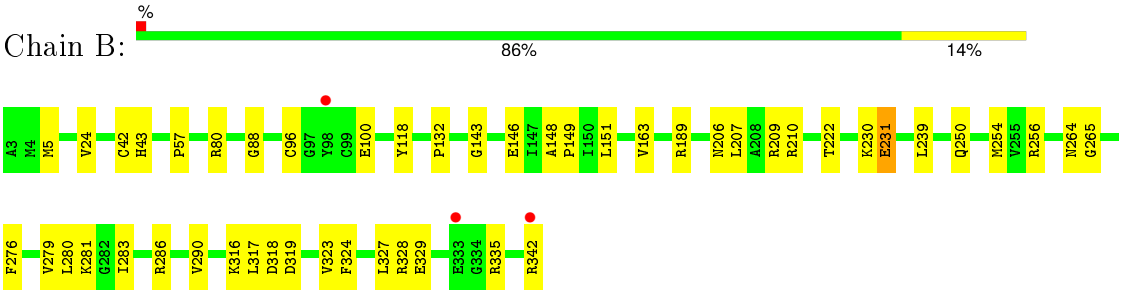
- Molecule 1: Zinc-containing alcohol dehydrogenase superfamily

Chain A:



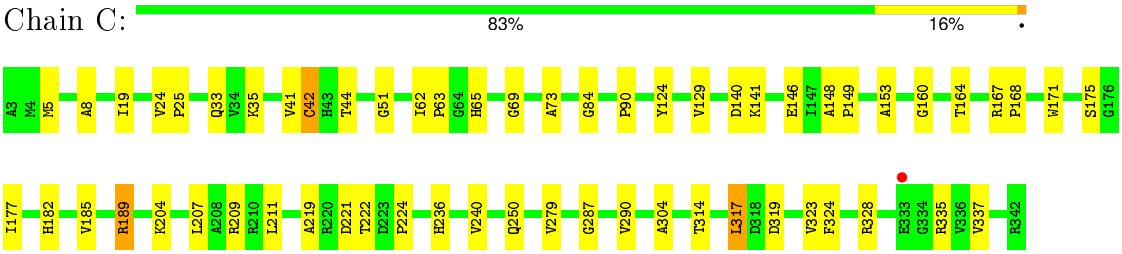
- Molecule 1: Zinc-containing alcohol dehydrogenase superfamily

Chain B:



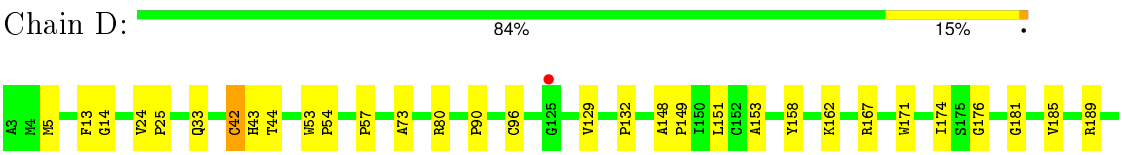
- Molecule 1: Zinc-containing alcohol dehydrogenase superfamily

Chain C:

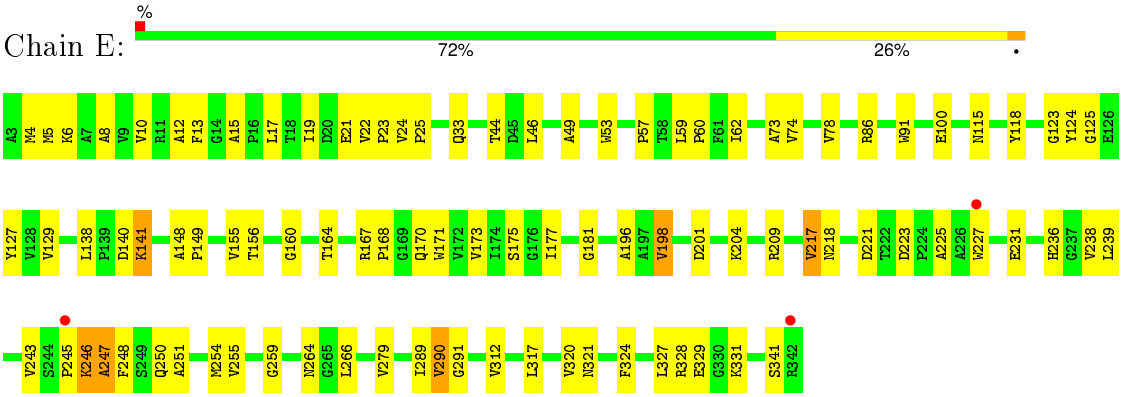


- Molecule 1: Zinc-containing alcohol dehydrogenase superfamily

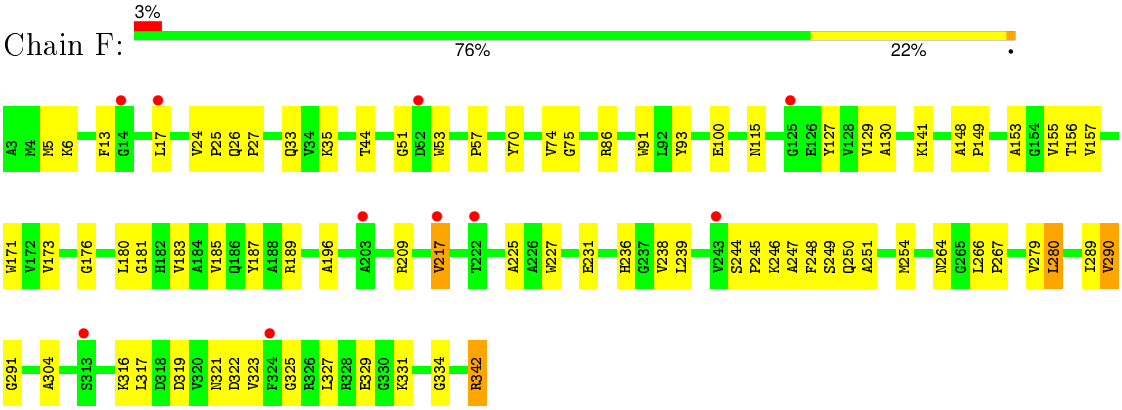
Chain D:



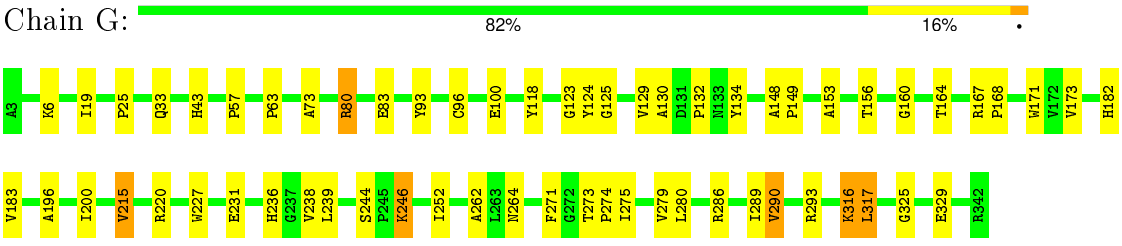
• Molecule 1: Zinc-containing alcohol dehydrogenase superfamily



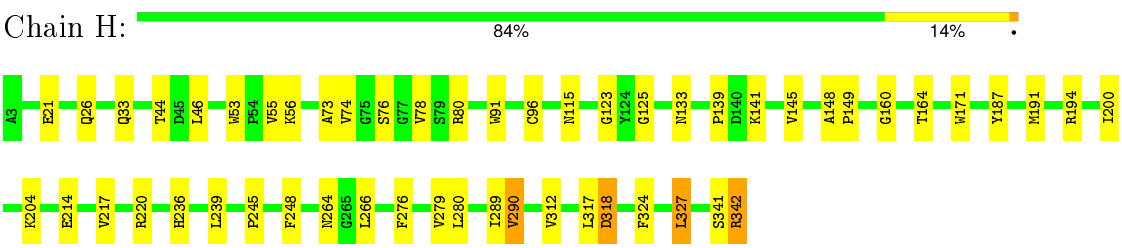
• Molecule 1: Zinc-containing alcohol dehydrogenase superfamily



• Molecule 1: Zinc-containing alcohol dehydrogenase superfamily



• Molecule 1: Zinc-containing alcohol dehydrogenase superfamily



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.08Å 92.47Å 116.86Å 106.28° 90.00° 89.97°	Depositor
Resolution (Å)	45.91 – 2.30 45.91 – 1.88	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.91-2.30) 74.0 (45.91-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.63 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.198 , 0.230 0.197 , 0.235	Depositor DCC
R_{free} test set	1227 reflections (1.09%)	DCC
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.1	EDS
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 196744 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21825	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: ZN, FU2, SO4, 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	0.21	0/2568	0.40	0/3496
1	B	0.21	0/2568	0.40	0/3496
1	C	0.21	0/2568	0.40	0/3496
1	D	0.21	0/2568	0.41	0/3496
1	E	0.21	0/2568	0.41	0/3496
1	F	0.21	0/2568	0.41	0/3496
1	G	0.21	0/2568	0.41	0/3496
1	H	0.21	0/2568	0.41	0/3496
All	All	0.21	0/20544	0.41	0/27968

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	2515	0	2512	39	0
1	B	2515	0	2512	25	1
1	C	2515	0	2512	34	0
1	D	2515	0	2512	36	0
1	E	2515	0	2512	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2515	0	2512	71	0
1	G	2515	0	2512	48	0
1	H	2515	0	2512	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	7	0	4	1	0
3	B	7	0	4	0	0
3	C	7	0	4	0	0
3	D	7	0	4	0	0
3	E	7	0	4	2	0
3	F	7	0	4	1	0
3	G	7	0	4	6	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
5	E	44	0	25	3	0
5	F	44	0	25	6	0
5	G	44	0	25	5	0
5	H	44	0	25	4	0
6	A	204	0	0	5	0
6	B	214	0	0	5	0
6	C	156	0	0	6	1
6	D	170	0	0	4	0
6	E	127	0	0	3	0
6	F	122	0	0	3	0
6	G	194	0	0	3	0
6	H	207	0	0	4	0
All	All	21825	0	20224	358	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (358) 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:341:SER:HB3	1:H:342:ARG:HA	1.23	1.16
1:H:141:LYS:HD2	1:H:141:LYS:H	1.20	1.02
1:H:341:SER:HB3	1:H:342:ARG:CA	1.91	1.00
1:G:246:LYS:H	1:G:246:LYS:HE2	1.27	0.98
1:H:289:ILE:HD12	5:H:1250:NAD:H72N	1.32	0.93
1:F:289:ILE:HA	5:F:1250:NAD:H72N	1.39	0.86
1:E:246:LYS:H	1:E:246:LYS:HD3	1.43	0.82
1:D:189:ARG:HH11	1:D:189:ARG:HG3	1.43	0.82
1:E:5:MET:HE1	1:E:127:TYR:HB2	1.64	0.79
1:D:227:TRP:O	1:D:231:GLU:HG2	1.83	0.78
1:G:63:PRO:HG2	1:G:124:TYR:CD1	2.19	0.77
1:H:341:SER:CB	1:H:342:ARG:HA	2.10	0.77
1:G:289:ILE:CD1	3:G:600:FU2:H5	2.15	0.77
1:G:246:LYS:HE2	1:G:246:LYS:N	2.00	0.76
1:F:27:PRO:HG3	1:F:33:GLN:HB2	1.67	0.76
1:E:245:PRO:O	1:E:248:PHE:HB2	1.85	0.76
1:F:5:MET:HE1	1:F:127:TYR:HB2	1.70	0.74
1:F:245:PRO:O	1:F:248:PHE:HB2	1.88	0.74
1:H:141:LYS:HD2	1:H:141:LYS:N	2.02	0.72
1:F:5:MET:HE3	1:F:24:VAL:HA	1.71	0.71
1:A:43:HIS:HD2	4:A:701:SO4:O2	1.74	0.71
1:G:290:VAL:HG13	3:G:600:FU2:H6	1.73	0.70
1:G:19:ILE:HD12	1:G:317:LEU:HD22	1.74	0.70
1:D:207:LEU:HD22	1:D:211:LEU:HD22	1.73	0.70
1:E:141:LYS:CE	1:E:141:LYS:H	2.05	0.69
1:G:25:PRO:HB2	1:G:129:VAL:HG23	1.73	0.69
1:F:70:TYR:CE2	1:F:86:ARG:HG2	2.28	0.69
1:F:249:SER:O	6:F:1070:HOH:O	2.10	0.69
1:F:334:GLY:O	6:F:354:HOH:O	2.11	0.68
1:F:153:ALA:HA	1:F:180:LEU:HD22	1.75	0.68
1:E:5:MET:CE	1:E:127:TYR:HB2	2.23	0.68
1:B:209:ARG:NH1	6:B:486:HOH:O	2.27	0.68
1:F:171:TRP:H	1:F:236:HIS:HD2	1.42	0.65
1:E:201:ASP:HB3	1:E:204:LYS:HG3	1.78	0.65
1:E:289:ILE:HA	5:E:1250:NAD:H72N	1.62	0.65
1:G:246:LYS:CE	1:G:246:LYS:H	2.06	0.64
1:H:141:LYS:CD	1:H:141:LYS:H	2.02	0.64
1:E:22:VAL:HB	1:E:23:PRO:HD2	1.80	0.64
1:E:33:GLN:HB3	1:E:73:ALA:HB3	1.81	0.63
1:F:5:MET:HE1	1:F:25:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:LYS:O	1:E:247:ALA:HB3	1.99	0.62
1:F:246:LYS:O	1:F:247:ALA:HB3	1.99	0.62
1:E:289:ILE:HD11	3:E:600:FU2:H5	1.81	0.62
1:G:215:VAL:HG22	1:G:227:TRP:HH2	1.64	0.62
1:E:289:ILE:HD11	3:E:600:FU2:C5	2.29	0.61
1:E:243:VAL:O	1:E:243:VAL:HG12	2.00	0.61
1:F:171:TRP:H	1:F:236:HIS:CD2	2.18	0.61
1:E:5:MET:HE3	1:E:24:VAL:HA	1.82	0.61
1:G:173:VAL:HB	1:G:238:VAL:HG22	1.82	0.61
1:H:194:ARG:HD2	1:H:214:GLU:OE1	2.01	0.61
1:F:5:MET:CE	1:F:127:TYR:HB2	2.31	0.60
1:A:276:PHE:CZ	1:A:280:LEU:HD22	2.37	0.60
1:H:289:ILE:HD12	5:H:1250:NAD:N7N	2.12	0.60
1:F:266:LEU:N	1:F:267:PRO:HD3	2.16	0.60
6:C:1344:HOH:O	1:D:206:ASN:HB3	2.02	0.60
1:D:220:ARG:HD3	6:D:585:HOH:O	2.03	0.59
1:E:209:ARG:NH2	6:E:1296:HOH:O	2.35	0.59
1:A:324:PHE:O	1:A:328:ARG:HG3	2.02	0.59
1:E:13:PHE:HA	1:E:49:ALA:O	2.02	0.59
1:D:189:ARG:HH11	1:D:189:ARG:CG	2.15	0.59
1:E:171:TRP:H	1:E:236:HIS:HD2	1.51	0.59
1:D:148:ALA:HB3	1:D:149:PRO:HD3	1.84	0.59
1:E:156:THR:OG1	5:E:1250:NAD:H4N	2.02	0.58
1:E:175:SER:HA	1:E:198:VAL:HG22	1.86	0.58
1:E:12:ALA:HB3	1:E:15:ALA:HB3	1.84	0.58
1:E:25:PRO:HB2	1:E:129:VAL:HG23	1.85	0.58
1:E:5:MET:HE3	1:E:24:VAL:HG22	1.86	0.58
1:G:274:PRO:HD3	6:G:858:HOH:O	2.04	0.58
1:A:141:LYS:H	1:A:141:LYS:CE	2.17	0.57
1:E:324:PHE:O	1:E:328:ARG:HG3	2.05	0.57
1:H:289:ILE:CD1	5:H:1250:NAD:H72N	2.10	0.57
1:E:141:LYS:H	1:E:141:LYS:HE3	1.68	0.57
1:A:141:LYS:H	1:A:141:LYS:HE2	1.69	0.56
1:E:255:VAL:CG2	1:E:259:GLY:HA3	2.36	0.56
1:A:333:GLU:O	6:A:1050:HOH:O	2.18	0.56
1:F:180:LEU:HD11	5:F:1250:NAD:H6N	1.87	0.56
1:G:33:GLN:HB3	1:G:73:ALA:HB3	1.87	0.56
1:D:287:GLY:HA3	1:F:279:VAL:HA	1.87	0.56
1:C:182:HIS:HB2	1:C:207:LEU:HD11	1.88	0.56
1:F:244:SER:O	1:F:248:PHE:HD2	1.89	0.56
1:E:289:ILE:HG13	1:E:290:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:PRO:HD3	1:E:118:TYR:CZ	2.41	0.55
1:C:25:PRO:HB2	1:C:129:VAL:HG23	1.88	0.55
1:F:27:PRO:CG	1:F:33:GLN:HB2	2.34	0.55
1:H:33:GLN:HB3	1:H:73:ALA:HB3	1.87	0.55
1:F:227:TRP:CH2	1:F:231:GLU:HG3	2.41	0.55
1:H:26:GLN:NE2	6:H:1038:HOH:O	2.32	0.55
1:H:341:SER:HB3	1:H:342:ARG:C	2.27	0.55
1:B:148:ALA:HB3	1:B:149:PRO:HD3	1.88	0.55
1:E:173:VAL:HB	1:E:238:VAL:HG22	1.89	0.55
1:H:171:TRP:H	1:H:236:HIS:HD2	1.55	0.54
1:E:17:LEU:HD22	1:E:320:VAL:HG11	1.88	0.54
1:E:239:LEU:HD11	1:E:264:ASN:ND2	2.22	0.54
1:F:180:LEU:HD11	5:F:1250:NAD:C6N	2.38	0.54
1:C:146:GLU:HG3	6:C:1277:HOH:O	2.06	0.54
1:A:189:ARG:HD3	6:A:1114:HOH:O	2.08	0.54
1:G:289:ILE:HD11	3:G:600:FU2:H5	1.90	0.54
1:F:5:MET:HE2	1:F:127:TYR:HD1	1.73	0.54
1:F:329:GLU:HG3	1:F:331:LYS:HD3	1.90	0.54
1:B:324:PHE:O	1:B:328:ARG:HG3	2.07	0.54
1:G:167:ARG:HB2	1:G:168:PRO:HD2	1.90	0.54
1:E:227:TRP:CH2	1:E:231:GLU:HG3	2.43	0.54
6:A:388:HOH:O	1:D:167:ARG:HD2	2.08	0.53
1:E:167:ARG:HB2	1:E:168:PRO:HD2	1.90	0.53
1:A:148:ALA:HB3	1:A:149:PRO:HD3	1.89	0.53
5:G:1250:NAD:O2A	6:G:389:HOH:O	2.18	0.53
1:G:80:ARG:HD2	1:G:132:PRO:O	2.07	0.53
1:F:156:THR:OG1	5:F:1250:NAD:H4N	2.08	0.53
1:E:246:LYS:O	1:E:247:ALA:CB	2.57	0.53
1:F:247:ALA:HA	1:F:250:GLN:HB2	1.89	0.53
1:C:209:ARG:NH1	6:C:624:HOH:O	2.41	0.53
1:F:157:VAL:HG21	1:F:183:VAL:HG13	1.90	0.53
1:F:25:PRO:HB2	1:F:129:VAL:HG23	1.91	0.53
1:F:227:TRP:CZ3	1:F:231:GLU:HG3	2.44	0.53
1:B:319:ASP:O	1:B:323:VAL:HG23	2.08	0.53
1:D:153:ALA:HB2	1:D:335:ARG:NH1	2.24	0.52
1:A:236:HIS:HE1	1:G:100:GLU:OE1	1.90	0.52
1:H:55:VAL:HB	6:H:917:HOH:O	2.09	0.52
1:E:6:LYS:HE2	1:E:19:ILE:CG2	2.40	0.52
1:E:223:ASP:O	6:E:688:HOH:O	2.19	0.52
1:F:289:ILE:HG13	1:F:290:VAL:HG22	1.92	0.51
1:F:44:THR:HG23	1:F:53:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:MET:HB3	1:C:24:VAL:HG22	1.93	0.51
1:C:222:THR:O	1:C:224:PRO:HD3	2.10	0.51
1:G:6:LYS:HD2	1:G:19:ILE:HG22	1.93	0.51
1:E:290:VAL:HG13	5:E:1250:NAD:O7N	2.10	0.51
1:B:100:GLU:OE1	1:H:236:HIS:HE1	1.93	0.51
1:F:173:VAL:HB	1:F:238:VAL:HG22	1.93	0.51
1:F:209:ARG:NH2	6:F:415:HOH:O	2.43	0.51
1:A:246:LYS:O	1:A:250:GLN:HG3	2.10	0.51
1:F:180:LEU:O	1:F:183:VAL:HG12	2.11	0.51
5:G:1250:NAD:H5N	3:G:600:FU2:C1	2.39	0.51
1:H:148:ALA:HB3	1:H:149:PRO:HD3	1.92	0.51
1:H:289:ILE:HG13	1:H:290:VAL:HG22	1.92	0.51
1:F:35:LYS:HE2	1:F:127:TYR:OH	2.11	0.50
1:A:250:GLN:O	1:A:254:MET:HG3	2.11	0.50
1:G:148:ALA:HB3	1:G:149:PRO:HD3	1.91	0.50
1:C:153:ALA:HB2	1:C:335:ARG:NH1	2.26	0.50
1:A:206:ASN:O	1:A:210:ARG:HG2	2.12	0.50
1:G:123:GLY:C	1:G:125:GLY:H	2.14	0.50
1:D:13:PHE:HE1	1:D:57:PRO:HG2	1.77	0.50
1:F:173:VAL:HG22	1:F:196:ALA:HB3	1.93	0.50
1:F:239:LEU:HD11	1:F:264:ASN:ND2	2.26	0.50
1:F:251:ALA:HA	1:F:254:MET:HE2	1.94	0.50
1:G:289:ILE:HG13	1:G:290:VAL:HG22	1.93	0.50
1:G:289:ILE:HD12	3:G:600:FU2:H5	1.92	0.50
1:E:171:TRP:H	1:E:236:HIS:CD2	2.28	0.50
1:C:148:ALA:HB3	1:C:149:PRO:HD3	1.93	0.50
1:H:200:ILE:HB	1:H:220:ARG:HG3	1.94	0.49
1:D:14:GLY:O	6:D:1019:HOH:O	2.19	0.49
1:A:326:ARG:NH1	6:A:1263:HOH:O	2.44	0.49
1:B:276:PHE:O	1:B:280:LEU:HB2	2.12	0.49
1:E:148:ALA:HB3	1:E:149:PRO:HD3	1.94	0.49
1:A:139:PRO:HB2	1:A:141:LYS:HE3	1.95	0.49
1:H:239:LEU:HD11	1:H:264:ASN:ND2	2.28	0.49
1:E:246:LYS:CD	1:E:246:LYS:H	2.17	0.49
1:A:179:GLY:HA3	4:A:701:SO4:O3	2.11	0.49
1:D:185:VAL:O	1:D:189:ARG:HG2	2.13	0.49
1:A:171:TRP:H	1:A:236:HIS:CD2	2.30	0.49
1:C:287:GLY:HA3	1:E:279:VAL:HA	1.94	0.49
1:D:53:TRP:HB3	1:D:54:PRO:HD2	1.94	0.49
1:F:5:MET:HE2	1:F:127:TYR:CD1	2.47	0.49
1:G:156:THR:HG21	5:G:1250:NAD:C4N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LYS:HD3	1:C:304:ALA:O	2.13	0.48
1:G:182:HIS:CE1	1:G:183:VAL:HG13	2.48	0.48
1:C:19:ILE:HD12	1:C:19:ILE:N	2.27	0.48
1:A:25:PRO:HB2	1:A:129:VAL:HG23	1.95	0.48
1:E:167:ARG:H	1:E:170:GLN:NE2	2.12	0.48
1:A:171:TRP:H	1:A:236:HIS:HD2	1.61	0.48
1:H:145:VAL:HG12	1:H:312:VAL:HG21	1.95	0.48
1:B:43:HIS:CE1	1:B:327:LEU:HD22	2.49	0.48
1:G:149:PRO:O	1:G:153:ALA:HB3	2.13	0.48
1:F:185:VAL:O	1:F:189:ARG:HG2	2.13	0.48
1:D:90:PRO:HD2	6:D:1142:HOH:O	2.13	0.48
1:E:251:ALA:HA	1:E:254:MET:HE2	1.95	0.48
1:E:225:ALA:HA	1:E:254:MET:HG2	1.95	0.48
1:E:123:GLY:C	1:E:125:GLY:H	2.17	0.48
1:G:171:TRP:H	1:G:236:HIS:HD2	1.61	0.48
1:C:65:HIS:O	1:C:90:PRO:HA	2.14	0.48
1:G:244:SER:HB2	1:G:246:LYS:HE3	1.96	0.47
1:E:86:ARG:HG2	1:E:138:LEU:HB2	1.96	0.47
1:F:246:LYS:O	1:F:247:ALA:CB	2.61	0.47
1:F:217:VAL:HG13	1:F:227:TRP:CD2	2.50	0.47
1:C:171:TRP:H	1:C:236:HIS:HD2	1.62	0.47
1:F:141:LYS:HE3	1:F:304:ALA:HB1	1.96	0.47
1:H:327:LEU:HA	1:H:327:LEU:HD23	1.75	0.47
1:H:133:ASN:ND2	6:H:945:HOH:O	2.47	0.47
1:F:217:VAL:HG22	1:F:227:TRP:CZ3	2.49	0.47
1:E:10:VAL:HG22	1:E:17:LEU:HG	1.96	0.47
1:H:318:ASP:OD2	1:H:318:ASP:N	2.47	0.47
1:D:80:ARG:HD3	1:D:132:PRO:O	2.15	0.47
1:D:33:GLN:HB3	1:D:73:ALA:HB3	1.96	0.47
1:F:290:VAL:HG13	5:F:1250:NAD:O7N	2.15	0.47
1:A:167:ARG:NH1	6:A:1334:HOH:O	2.43	0.47
1:F:325:GLY:O	1:F:329:GLU:HG2	2.15	0.47
1:G:57:PRO:HG3	1:G:118:TYR:CZ	2.50	0.47
1:A:326:ARG:N	1:A:326:ARG:HD2	2.30	0.46
1:F:26:GLN:HA	1:F:27:PRO:HD3	1.80	0.46
1:B:335:ARG:HD2	6:B:359:HOH:O	2.16	0.46
1:B:5:MET:HB3	1:B:24:VAL:HG22	1.96	0.46
1:B:250:GLN:O	1:B:254:MET:HG3	2.16	0.46
1:C:84:GLY:O	6:C:1132:HOH:O	2.21	0.46
1:H:187:TYR:O	1:H:191:MET:HG3	2.16	0.46
1:B:342:ARG:HG3	6:B:900:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:N	1:A:141:LYS:HE2	2.30	0.46
1:A:177:ILE:HB	1:A:204:LYS:HB3	1.97	0.46
1:E:62:ILE:HG22	1:E:124:TYR:HB2	1.97	0.46
1:B:256:ARG:HD3	6:H:1337:HOH:O	2.15	0.46
1:B:265:GLY:O	1:H:279:VAL:HG21	2.15	0.46
1:E:6:LYS:HE2	1:E:19:ILE:HG21	1.98	0.46
1:D:239:LEU:HD11	1:D:264:ASN:ND2	2.31	0.46
1:G:57:PRO:HG3	1:G:118:TYR:CE1	2.50	0.46
1:A:167:ARG:H	1:A:170:GLN:NE2	2.14	0.45
1:G:93:TYR:CE1	1:G:130:ALA:HA	2.51	0.45
1:A:153:ALA:O	1:A:157:VAL:HG22	2.16	0.45
1:B:230:LYS:HA	6:B:1386:HOH:O	2.16	0.45
1:H:80:ARG:HD2	1:H:133:ASN:HA	1.98	0.45
1:A:22:VAL:HB	1:A:23:PRO:HD2	1.98	0.45
1:D:158:TYR:CZ	1:D:162:LYS:HD3	2.51	0.45
1:E:5:MET:HB3	1:E:24:VAL:HG22	1.98	0.45
1:A:322:ASP:O	1:A:326:ARG:HG2	2.16	0.45
1:C:221:ASP:HA	6:C:1361:HOH:O	2.17	0.45
1:F:74:VAL:HG12	1:F:75:GLY:O	2.16	0.45
1:E:155:VAL:HG22	1:E:291:GLY:HA3	1.99	0.45
1:C:33:GLN:HB3	1:C:73:ALA:HB3	1.97	0.45
1:E:218:ASN:N	6:E:1360:HOH:O	2.47	0.45
1:H:91:TRP:O	1:H:115:ASN:HA	2.16	0.45
1:D:42:CYS:SG	1:D:44:THR:HB	2.57	0.45
1:F:225:ALA:HA	1:F:254:MET:HG2	1.98	0.45
1:D:206:ASN:O	1:D:210:ARG:HG2	2.17	0.45
1:A:251:ALA:HA	1:A:254:MET:HE2	1.99	0.45
1:F:290:VAL:H	5:F:1250:NAD:H72N	1.65	0.44
1:H:44:THR:HG23	1:H:53:TRP:CH2	2.53	0.44
1:G:43:HIS:HB3	5:G:1250:NAD:H3D	1.98	0.44
1:E:329:GLU:CB	1:E:331:LYS:HG3	2.47	0.44
1:F:319:ASP:O	1:F:323:VAL:HG23	2.16	0.44
1:D:43:HIS:CE1	1:D:327:LEU:HD22	2.53	0.44
1:G:239:LEU:HD11	1:G:264:ASN:ND2	2.33	0.44
1:F:319:ASP:O	1:F:322:ASP:HB2	2.18	0.44
1:E:160:GLY:O	1:E:164:THR:HG23	2.18	0.44
1:H:46:LEU:HD23	1:H:324:PHE:CD2	2.53	0.44
1:F:244:SER:O	1:F:248:PHE:CD2	2.71	0.44
1:G:171:TRP:H	1:G:236:HIS:CD2	2.36	0.44
1:E:217:VAL:HG22	1:E:227:TRP:CZ3	2.52	0.43
1:B:279:VAL:HB	1:H:266:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:GLY:O	1:G:329:GLU:HG2	2.18	0.43
1:A:265:GLY:O	1:G:279:VAL:HG21	2.18	0.43
1:F:6:LYS:HD2	1:F:317:LEU:HD13	2.01	0.43
1:G:200:ILE:HG22	1:G:220:ARG:HG2	2.00	0.43
1:D:5:MET:HB3	1:D:24:VAL:HG22	2.00	0.43
1:F:246:LYS:HB3	1:F:246:LYS:HE2	1.72	0.43
1:C:41:VAL:HG22	1:C:124:TYR:OH	2.19	0.43
1:E:5:MET:O	1:E:21:GLU:HA	2.19	0.43
1:G:252:ILE:O	6:G:870:HOH:O	2.20	0.43
1:G:160:GLY:O	1:G:164:THR:HG23	2.18	0.43
1:A:153:ALA:HB2	1:A:335:ARG:NH1	2.33	0.43
1:A:9:VAL:HG22	1:A:62:ILE:HG12	1.99	0.43
1:H:139:PRO:HB2	1:H:141:LYS:HD3	2.01	0.43
1:E:255:VAL:HG22	1:E:259:GLY:HA3	1.99	0.43
1:D:151:LEU:HD13	1:D:296:LEU:HD11	2.01	0.43
1:D:324:PHE:O	1:D:328:ARG:HG3	2.18	0.43
1:C:35:LYS:O	1:C:69:GLY:HA3	2.18	0.43
1:G:215:VAL:HG21	1:G:231:GLU:HG2	1.99	0.43
1:C:185:VAL:O	1:C:189:ARG:HG2	2.18	0.43
1:H:123:GLY:C	1:H:125:GLY:H	2.21	0.43
1:D:174:ILE:HG12	1:D:195:VAL:HG13	2.00	0.43
1:E:8:ALA:HB2	1:E:317:LEU:HD21	2.00	0.43
1:B:281:LYS:HE2	1:B:283:ILE:HD11	2.00	0.43
1:G:173:VAL:HG22	1:G:196:ALA:HB3	1.99	0.42
1:F:53:TRP:CZ3	3:F:600:FU2:H4	2.54	0.42
1:F:176:GLY:O	1:F:181:GLY:HA3	2.19	0.42
1:E:44:THR:HG23	1:E:53:TRP:CH2	2.53	0.42
1:F:155:VAL:HG22	1:F:291:GLY:HA3	2.01	0.42
1:F:280:LEU:HD22	1:F:280:LEU:HA	1.92	0.42
1:F:91:TRP:O	1:F:115:ASN:HA	2.19	0.42
1:F:13:PHE:CZ	1:F:57:PRO:HD2	2.55	0.42
1:E:177:ILE:HA	1:E:181:GLY:HA3	2.01	0.42
1:B:88:GLY:HA3	1:B:151:LEU:HD11	2.00	0.42
1:G:289:ILE:HD11	3:G:600:FU2:C5	2.48	0.42
1:C:25:PRO:HB2	1:C:129:VAL:CG2	2.49	0.42
1:H:276:PHE:CE2	1:H:280:LEU:HD12	2.54	0.42
1:E:46:LEU:HD22	1:E:328:ARG:CZ	2.49	0.42
1:E:255:VAL:HG21	1:E:259:GLY:HA3	2.01	0.42
1:C:219:ALA:HA	1:C:222:THR:O	2.18	0.42
1:D:13:PHE:CE1	1:D:57:PRO:HG2	2.53	0.42
1:B:239:LEU:HD11	1:B:264:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ALA:HB2	1:C:317:LEU:HD21	2.01	0.42
1:G:289:ILE:O	1:G:289:ILE:HG23	2.20	0.42
1:D:335:ARG:HD3	6:D:373:HOH:O	2.18	0.42
1:C:319:ASP:O	1:C:323:VAL:HG23	2.20	0.42
1:H:160:GLY:O	1:H:164:THR:HG23	2.19	0.42
1:C:175:SER:HB3	1:C:240:VAL:HA	2.00	0.42
1:C:160:GLY:O	1:C:164:THR:HG23	2.19	0.42
1:B:80:ARG:HD3	1:B:132:PRO:O	2.18	0.42
1:F:266:LEU:N	1:F:267:PRO:CD	2.82	0.42
1:F:6:LYS:HD2	1:F:317:LEU:CD1	2.49	0.42
1:C:167:ARG:HB2	1:C:168:PRO:HD2	2.02	0.42
1:A:218:ASN:OD1	1:A:220:ARG:HB3	2.19	0.42
1:G:273:THR:HG22	1:G:275:ILE:HD13	2.01	0.42
1:H:74:VAL:HG13	1:H:78:VAL:HB	2.02	0.42
1:C:236:HIS:HE1	1:E:100:GLU:OE2	2.03	0.42
1:C:42:CYS:SG	1:C:44:THR:HB	2.60	0.42
1:D:171:TRP:H	1:D:236:HIS:HD2	1.68	0.42
1:C:279:VAL:HB	1:E:266:LEU:HD21	2.02	0.42
1:B:206:ASN:O	1:B:210:ARG:HG2	2.19	0.42
1:H:289:ILE:HA	5:H:1250:NAD:O7N	2.20	0.41
1:G:262:ALA:HA	1:G:286:ARG:O	2.20	0.41
1:B:163:VAL:HB	1:B:286:ARG:HD3	2.01	0.41
1:G:134:TYR:CD2	1:G:293:ARG:HD3	2.55	0.41
1:D:211:LEU:HD12	1:D:211:LEU:HA	1.82	0.41
1:C:314:THR:HA	1:C:337:VAL:O	2.19	0.41
1:E:59:LEU:HA	1:E:60:PRO:HA	1.79	0.41
1:F:148:ALA:N	1:F:149:PRO:HD2	2.36	0.41
1:D:314:THR:HA	1:D:337:VAL:O	2.20	0.41
1:E:289:ILE:HG23	1:E:289:ILE:O	2.20	0.41
1:H:56:LYS:N	1:H:56:LYS:HD2	2.34	0.41
1:F:93:TYR:CE1	1:F:130:ALA:HA	2.55	0.41
1:D:189:ARG:CG	1:D:189:ARG:NH1	2.76	0.41
1:G:264:ASN:O	5:G:1250:NAD:C2N	2.69	0.41
1:F:250:GLN:O	1:F:254:MET:HG3	2.21	0.41
1:C:51:GLY:HA2	6:C:354:HOH:O	2.20	0.41
1:F:13:PHE:CD1	1:F:51:GLY:HA3	2.55	0.41
1:A:290:VAL:HG13	3:A:600:FU2:H6	2.02	0.41
1:E:19:ILE:N	1:E:19:ILE:HD12	2.35	0.41
1:A:227:TRP:O	1:A:231:GLU:HB2	2.20	0.41
1:C:62:ILE:HA	1:C:63:PRO:HD3	1.90	0.41
1:D:189:ARG:HG3	1:D:189:ARG:NH1	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:LEU:HD23	1:E:317:LEU:O	2.20	0.41
1:A:215:VAL:HG11	1:A:227:TRP:HZ3	1.85	0.41
1:C:177:ILE:HB	1:C:204:LYS:HB3	2.03	0.41
1:E:243:VAL:O	1:E:243:VAL:CG1	2.68	0.41
1:E:250:GLN:O	1:E:254:MET:HG3	2.20	0.41
1:D:236:HIS:HE1	1:F:100:GLU:OE2	2.04	0.41
1:A:239:LEU:HD11	1:A:264:ASN:ND2	2.36	0.41
1:F:183:VAL:HG22	1:F:187:TYR:CE1	2.56	0.41
1:E:91:TRP:O	1:E:115:ASN:HA	2.21	0.41
1:B:316:LYS:HE2	1:B:316:LYS:HA	2.03	0.41
1:D:25:PRO:HB2	1:D:129:VAL:HG23	2.03	0.41
1:B:57:PRO:HB3	1:B:118:TYR:O	2.21	0.41
1:E:173:VAL:HG22	1:E:196:ALA:HB3	2.01	0.41
1:E:320:VAL:HG12	1:E:321:ASN:N	2.35	0.41
1:E:74:VAL:CG1	1:E:78:VAL:HB	2.51	0.41
1:H:245:PRO:O	1:H:248:PHE:HB2	2.21	0.40
1:A:275:ILE:HG12	1:G:271:PHE:HD2	1.86	0.40
1:F:244:SER:O	1:F:246:LYS:O	2.39	0.40
1:E:317:LEU:O	1:E:320:VAL:HG23	2.21	0.40
1:B:189:ARG:NH2	6:B:1359:HOH:O	2.46	0.40
1:D:176:GLY:O	1:D:181:GLY:HA3	2.21	0.40
1:B:143:GLY:O	1:B:146:GLU:HG2	2.20	0.40
1:E:329:GLU:HB2	1:E:331:LYS:HG3	2.04	0.40
1:A:243:VAL:HG11	1:G:275:ILE:HG21	2.03	0.40
1:C:324:PHE:O	1:C:328:ARG:HG3	2.21	0.40
1:G:316:LYS:HD2	1:G:316:LYS:H	1.87	0.40
1:F:342:ARG:CD	1:F:342:ARG:N	2.84	0.40
1:A:319:ASP:O	1:A:323:VAL:HG23	2.20	0.40
1:F:17:LEU:N	1:F:321:ASN:OD1	2.55	0.40
1:E:141:LYS:HE2	1:E:141:LYS:H	1.80	0.40
1:A:5:MET:HB2	1:A:126:GLU:HB2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLU:OE2	6:C:692:HOH:O[1_455]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	328 (97%)	9 (3%)	1 (0%)	46	57
1	B	338/340 (99%)	328 (97%)	8 (2%)	2 (1%)	30	36
1	C	338/340 (99%)	326 (96%)	11 (3%)	1 (0%)	46	57
1	D	338/340 (99%)	328 (97%)	9 (3%)	1 (0%)	46	57
1	E	338/340 (99%)	320 (95%)	14 (4%)	4 (1%)	16	16
1	F	338/340 (99%)	323 (96%)	14 (4%)	1 (0%)	46	57
1	G	338/340 (99%)	330 (98%)	7 (2%)	1 (0%)	46	57
1	H	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	46	57
All	All	2704/2720 (99%)	2608 (96%)	84 (3%)	12 (0%)	39	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	221	ASP
1	A	290	VAL
1	B	290	VAL
1	C	290	VAL
1	D	290	VAL
1	E	290	VAL
1	E	341	SER
1	F	290	VAL
1	G	290	VAL
1	H	290	VAL
1	E	247	ALA
1	B	231	GLU

5.3.2 Protein sidechains

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	261/261 (100%)	254 (97%)	7 (3%)	52 70
1	B	261/261 (100%)	254 (97%)	7 (3%)	52 70
1	C	261/261 (100%)	255 (98%)	6 (2%)	58 75
1	D	261/261 (100%)	255 (98%)	6 (2%)	58 75
1	E	261/261 (100%)	253 (97%)	8 (3%)	47 64
1	F	261/261 (100%)	256 (98%)	5 (2%)	65 81
1	G	261/261 (100%)	253 (97%)	8 (3%)	47 64
1	H	261/261 (100%)	252 (97%)	9 (3%)	44 59
All	All	2088/2088 (100%)	2032 (97%)	56 (3%)	52 70

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	CYS
1	A	100	GLU
1	A	141	LYS
1	A	207	LEU
1	A	217	VAL
1	A	222	THR
1	A	317	LEU
1	B	42	CYS
1	B	96	CYS
1	B	207	LEU
1	B	222	THR
1	B	231	GLU
1	B	317	LEU
1	B	318	ASP
1	C	42	CYS
1	C	140	ASP
1	C	189	ARG
1	C	211	LEU
1	C	250	GLN
1	C	317	LEU
1	D	42	CYS
1	D	96	CYS
1	D	207	LEU

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Mol	Chain	Res	Type
1	D	211	LEU
1	D	222	THR
1	D	333	GLU
1	E	4	MET
1	E	140	ASP
1	E	141	LYS
1	E	198	VAL
1	E	217	VAL
1	E	246	LYS
1	E	312	VAL
1	E	327	LEU
1	F	217	VAL
1	F	280	LEU
1	F	316	LYS
1	F	327	LEU
1	F	342	ARG
1	G	80	ARG
1	G	83	GLU
1	G	96	CYS
1	G	215	VAL
1	G	246	LYS
1	G	280	LEU
1	G	316	LYS
1	G	317	LEU
1	H	21	GLU
1	H	76	SER
1	H	96	CYS
1	H	204	LYS
1	H	217	VAL
1	H	317	LEU
1	H	318	ASP
1	H	327	LEU
1	H	342	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	43	HIS
1	A	170	GLN
1	A	236	HIS
1	A	264	ASN

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	170	GLN
1	B	236	HIS
1	C	26	GLN
1	C	170	GLN
1	C	236	HIS
1	C	264	ASN
1	D	65	HIS
1	D	236	HIS
1	E	114	GLN
1	E	170	GLN
1	E	236	HIS
1	E	305	HIS
1	F	43	HIS
1	F	170	GLN
1	F	236	HIS
1	G	104	GLN
1	G	114	GLN
1	G	170	GLN
1	G	206	ASN
1	G	236	HIS
1	H	170	GLN
1	H	229	GLN
1	H	236	HIS

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 41 ligands modelled in this entry, 16 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
3	FU2	A	600	-	4,7,7	2.76	1 (25%)	2,8,8	1.02	0
4	SO4	A	701	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.11	0
3	FU2	B	600	-	4,7,7	2.74	1 (25%)	2,8,8	1.03	0
4	SO4	B	701	-	4,4,4	0.21	0	6,6,6	0.09	0
4	SO4	B	702	-	4,4,4	0.21	0	6,6,6	0.11	0
3	FU2	C	600	-	4,7,7	2.65	1 (25%)	2,8,8	0.99	0
4	SO4	C	701	-	4,4,4	0.21	0	6,6,6	0.09	0
4	SO4	C	702	-	4,4,4	0.22	0	6,6,6	0.15	0
3	FU2	D	600	-	4,7,7	2.70	1 (25%)	2,8,8	1.03	0
4	SO4	D	701	-	4,4,4	0.21	0	6,6,6	0.10	0
4	SO4	D	702	-	4,4,4	0.20	0	6,6,6	0.13	0
5	NAD	E	1250	-	38,48,48	2.55	16 (42%)	47,73,73	2.75	19 (40%)
3	FU2	E	600	2	4,7,7	2.64	1 (25%)	2,8,8	1.00	0
4	SO4	E	702	-	4,4,4	0.22	0	6,6,6	0.08	0
5	NAD	F	1250	-	38,48,48	2.54	16 (42%)	47,73,73	2.67	17 (36%)
3	FU2	F	600	2	4,7,7	2.65	1 (25%)	2,8,8	1.03	0
4	SO4	F	702	-	4,4,4	0.23	0	6,6,6	0.14	0
5	NAD	G	1250	-	38,48,48	2.52	15 (39%)	47,73,73	2.89	19 (40%)
3	FU2	G	600	2	4,7,7	2.64	1 (25%)	2,8,8	0.98	0
4	SO4	G	702	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	G	703	-	4,4,4	0.23	0	6,6,6	0.10	0
5	NAD	H	1250	-	38,48,48	2.54	16 (42%)	47,73,73	2.71	19 (40%)
4	SO4	H	702	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	H	703	-	4,4,4	0.25	0	6,6,6	0.14	0

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
3	FU2	A	600	-	-	0/0/2/2	0/0/1/1
4	SO4	A	701	-	-	0/0/0/0	0/0/0/0
4	SO4	A	702	-	-	0/0/0/0	0/0/0/0
3	FU2	B	600	-	-	0/0/2/2	0/0/1/1
4	SO4	B	701	-	-	0/0/0/0	0/0/0/0
4	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	FU2	C	600	-	-	0/0/2/2	0/0/1/1
4	SO4	C	701	-	-	0/0/0/0	0/0/0/0
4	SO4	C	702	-	-	0/0/0/0	0/0/0/0
3	FU2	D	600	-	-	0/0/2/2	0/0/1/1
4	SO4	D	701	-	-	0/0/0/0	0/0/0/0
4	SO4	D	702	-	-	0/0/0/0	0/0/0/0
5	NAD	E	1250	-	-	0/22/62/62	0/5/5/5
3	FU2	E	600	2	-	0/0/2/2	0/0/1/1
4	SO4	E	702	-	-	0/0/0/0	0/0/0/0
5	NAD	F	1250	-	-	0/22/62/62	0/5/5/5
3	FU2	F	600	2	-	0/0/2/2	0/0/1/1
4	SO4	F	702	-	-	0/0/0/0	0/0/0/0
5	NAD	G	1250	-	-	0/22/62/62	0/5/5/5
3	FU2	G	600	2	-	0/0/2/2	0/0/1/1
4	SO4	G	702	-	-	0/0/0/0	0/0/0/0
4	SO4	G	703	-	-	0/0/0/0	0/0/0/0
5	NAD	H	1250	-	-	0/22/62/62	0/5/5/5
4	SO4	H	702	-	-	0/0/0/0	0/0/0/0
4	SO4	H	703	-	-	0/0/0/0	0/0/0/0

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1250	NAD	C2B-C3B	-5.04	1.39	1.53
5	E	1250	NAD	C2B-C3B	-5.02	1.39	1.53
5	F	1250	NAD	C2B-C3B	-5.02	1.39	1.53
5	G	1250	NAD	C2B-C3B	-5.00	1.39	1.53
5	G	1250	NAD	O3D-C3D	-3.01	1.35	1.43
5	H	1250	NAD	O3D-C3D	-2.92	1.36	1.43
5	F	1250	NAD	O3D-C3D	-2.83	1.36	1.43
5	E	1250	NAD	O3D-C3D	-2.80	1.36	1.43
5	G	1250	NAD	C2D-C3D	-2.47	1.46	1.53
5	H	1250	NAD	C2D-C3D	-2.40	1.46	1.53
5	F	1250	NAD	C2D-C3D	-2.36	1.47	1.53
5	H	1250	NAD	O2D-C2D	-2.36	1.37	1.43
5	E	1250	NAD	O4B-C4B	-2.36	1.39	1.45
5	H	1250	NAD	O4B-C1B	-2.33	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1250	NAD	C2D-C3D	-2.33	1.47	1.53
5	E	1250	NAD	O5B-C5B	-2.33	1.35	1.44
5	G	1250	NAD	O5B-C5B	-2.30	1.35	1.44
5	E	1250	NAD	O4B-C1B	-2.27	1.38	1.41
5	H	1250	NAD	O4B-C4B	-2.26	1.39	1.45
5	F	1250	NAD	O4B-C4B	-2.24	1.39	1.45
5	H	1250	NAD	O5B-C5B	-2.24	1.35	1.44
5	F	1250	NAD	O2D-C2D	-2.23	1.37	1.43
5	G	1250	NAD	O2D-C2D	-2.22	1.37	1.43
5	F	1250	NAD	O5B-C5B	-2.21	1.35	1.44
5	G	1250	NAD	O4B-C4B	-2.19	1.40	1.45
5	E	1250	NAD	O2D-C2D	-2.16	1.37	1.43
5	G	1250	NAD	O4B-C1B	-2.16	1.38	1.41
5	F	1250	NAD	O4B-C1B	-2.14	1.38	1.41
5	H	1250	NAD	C5D-C4D	-2.12	1.44	1.51
5	F	1250	NAD	C5D-C4D	-2.12	1.44	1.51
5	E	1250	NAD	C5D-C4D	-2.05	1.45	1.51
5	G	1250	NAD	C5D-C4D	-2.00	1.45	1.51
5	F	1250	NAD	O7N-C7N	2.10	1.28	1.24
5	E	1250	NAD	O7N-C7N	2.14	1.28	1.24
5	H	1250	NAD	O7N-C7N	2.28	1.29	1.24
5	G	1250	NAD	C4N-C3N	2.42	1.43	1.39
5	H	1250	NAD	C4N-C3N	2.44	1.43	1.39
5	E	1250	NAD	C4N-C3N	2.59	1.43	1.39
5	F	1250	NAD	C4N-C3N	2.64	1.43	1.39
5	F	1250	NAD	C6N-N1N	2.91	1.43	1.35
5	H	1250	NAD	C6N-N1N	2.91	1.43	1.35
5	G	1250	NAD	C6N-N1N	2.93	1.43	1.35
5	E	1250	NAD	C6N-N1N	2.96	1.43	1.35
5	G	1250	NAD	C5N-C4N	3.73	1.46	1.38
5	H	1250	NAD	C3N-C7N	3.82	1.56	1.50
5	E	1250	NAD	C5N-C4N	3.84	1.46	1.38
5	G	1250	NAD	C3N-C7N	3.86	1.56	1.50
5	F	1250	NAD	C5N-C4N	3.89	1.46	1.38
5	F	1250	NAD	C3N-C7N	3.93	1.56	1.50
5	E	1250	NAD	C3N-C7N	3.97	1.56	1.50
5	H	1250	NAD	C5N-C4N	4.00	1.47	1.38
5	F	1250	NAD	C6N-C5N	4.75	1.49	1.38
5	E	1250	NAD	C6N-C5N	4.76	1.49	1.38
5	G	1250	NAD	C6N-C5N	4.78	1.49	1.38
5	H	1250	NAD	C6N-C5N	4.93	1.49	1.38
5	G	1250	NAD	C7N-N7N	5.00	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1250	NAD	C7N-N7N	5.02	1.43	1.33
5	F	1250	NAD	C7N-N7N	5.05	1.43	1.33
5	E	1250	NAD	C7N-N7N	5.12	1.43	1.33
3	G	600	FU2	OXT-C1	5.22	1.38	1.21
3	E	600	FU2	OXT-C1	5.24	1.38	1.21
3	F	600	FU2	OXT-C1	5.26	1.38	1.21
3	C	600	FU2	OXT-C1	5.27	1.38	1.21
3	D	600	FU2	OXT-C1	5.32	1.38	1.21
3	B	600	FU2	OXT-C1	5.41	1.38	1.21
3	A	600	FU2	OXT-C1	5.42	1.38	1.21
5	H	1250	NAD	C2N-C3N	7.69	1.50	1.39
5	E	1250	NAD	C2N-C3N	7.83	1.50	1.39
5	G	1250	NAD	C2N-C3N	7.85	1.50	1.39
5	F	1250	NAD	C2N-C3N	7.91	1.51	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1250	NAD	N3A-C2A-N1A	-8.07	122.72	128.89
5	E	1250	NAD	N3A-C2A-N1A	-8.05	122.73	128.89
5	H	1250	NAD	N3A-C2A-N1A	-7.89	122.85	128.89
5	G	1250	NAD	N3A-C2A-N1A	-7.86	122.87	128.89
5	G	1250	NAD	C5N-C6N-N1N	-6.43	109.34	120.47
5	H	1250	NAD	C5N-C6N-N1N	-6.30	109.58	120.47
5	E	1250	NAD	C5N-C6N-N1N	-6.29	109.59	120.47
5	F	1250	NAD	C5N-C6N-N1N	-6.27	109.62	120.47
5	G	1250	NAD	C6N-C5N-C4N	-6.23	110.03	119.44
5	E	1250	NAD	C6N-C5N-C4N	-5.91	110.52	119.44
5	F	1250	NAD	C6N-C5N-C4N	-5.90	110.53	119.44
5	G	1250	NAD	C5N-C4N-C3N	-5.68	113.19	120.33
5	H	1250	NAD	C4B-O4B-C1B	-5.03	104.19	109.72
5	H	1250	NAD	C6N-C5N-C4N	-4.91	112.03	119.44
5	E	1250	NAD	PN-O3-PA	-4.80	119.24	132.73
5	H	1250	NAD	C5N-C4N-C3N	-4.80	114.30	120.33
5	E	1250	NAD	C5N-C4N-C3N	-4.70	114.43	120.33
5	G	1250	NAD	C3N-C2N-N1N	-4.69	114.96	120.36
5	F	1250	NAD	PN-O3-PA	-4.60	119.80	132.73
5	G	1250	NAD	PN-O3-PA	-4.56	119.91	132.73
5	F	1250	NAD	C5N-C4N-C3N	-4.54	114.63	120.33
5	H	1250	NAD	PN-O3-PA	-4.53	120.00	132.73
5	G	1250	NAD	C4B-O4B-C1B	-4.44	104.84	109.72
5	E	1250	NAD	C4B-O4B-C1B	-4.36	104.93	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1250	NAD	C4N-C3N-C7N	-4.35	109.59	121.09
5	H	1250	NAD	C2N-C3N-C7N	-4.34	106.69	119.31
5	E	1250	NAD	C4N-C3N-C7N	-4.30	109.72	121.09
5	G	1250	NAD	C4N-C3N-C7N	-4.14	110.15	121.09
5	H	1250	NAD	C4N-C3N-C7N	-3.97	110.59	121.09
5	G	1250	NAD	C4D-O4D-C1D	-3.94	105.39	109.72
5	E	1250	NAD	C3N-C2N-N1N	-3.69	116.11	120.36
5	F	1250	NAD	C2N-C3N-C7N	-3.68	108.62	119.31
5	H	1250	NAD	C4D-O4D-C1D	-3.67	105.69	109.72
5	E	1250	NAD	C2N-C3N-C7N	-3.65	108.71	119.31
5	G	1250	NAD	C2N-C3N-C7N	-3.61	108.83	119.31
5	F	1250	NAD	C4B-O4B-C1B	-3.53	105.84	109.72
5	E	1250	NAD	C4A-C5A-N7A	-3.52	106.24	109.48
5	G	1250	NAD	C2N-C3N-C4N	-3.48	114.42	118.29
5	G	1250	NAD	C4A-C5A-N7A	-3.44	106.31	109.48
5	F	1250	NAD	C4A-C5A-N7A	-3.44	106.32	109.48
5	E	1250	NAD	C4D-O4D-C1D	-3.38	106.00	109.72
5	F	1250	NAD	C3N-C2N-N1N	-3.38	116.47	120.36
5	H	1250	NAD	C4A-C5A-N7A	-3.36	106.39	109.48
5	H	1250	NAD	C3N-C2N-N1N	-3.03	116.88	120.36
5	F	1250	NAD	C4D-O4D-C1D	-2.81	106.63	109.72
5	H	1250	NAD	C2N-C3N-C4N	-2.53	115.48	118.29
5	G	1250	NAD	O7N-C7N-N7N	-2.37	119.26	122.59
5	E	1250	NAD	C1B-N9A-C4A	-2.22	123.59	126.94
5	E	1250	NAD	C2N-C3N-C4N	-2.13	115.92	118.29
5	H	1250	NAD	O7N-C7N-N7N	-2.10	119.64	122.59
5	H	1250	NAD	O3-PN-O5D	2.07	108.44	102.94
5	F	1250	NAD	O5B-C5B-C4B	2.08	116.78	109.12
5	E	1250	NAD	O5D-C5D-C4D	2.15	117.06	109.12
5	G	1250	NAD	O3-PA-O5B	2.23	108.85	102.94
5	G	1250	NAD	O5D-C5D-C4D	2.37	117.87	109.12
5	G	1250	NAD	O3-PN-O5D	2.39	109.27	102.94
5	F	1250	NAD	O3-PN-O5D	2.40	109.29	102.94
5	H	1250	NAD	O5D-C5D-C4D	2.43	118.07	109.12
5	E	1250	NAD	O4B-C1B-N9A	2.45	113.23	108.10
5	H	1250	NAD	O4B-C1B-N9A	2.51	113.36	108.10
5	H	1250	NAD	O3-PA-O5B	2.64	109.94	102.94
5	F	1250	NAD	C2B-C1B-N9A	2.65	118.34	114.29
5	E	1250	NAD	O3-PA-O5B	2.66	109.99	102.94
5	G	1250	NAD	C2B-C1B-N9A	2.67	118.37	114.29
5	F	1250	NAD	O4B-C1B-N9A	2.71	113.76	108.10
5	E	1250	NAD	O3-PN-O5D	2.75	110.22	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1250	NAD	O3-PA-O5B	2.82	110.42	102.94
5	G	1250	NAD	O4B-C1B-N9A	2.90	114.16	108.10
5	E	1250	NAD	C2B-C1B-N9A	3.06	118.96	114.29
5	H	1250	NAD	C2B-C1B-N9A	3.29	119.31	114.29
5	F	1250	NAD	O4D-C1D-N1N	3.33	111.80	108.13
5	E	1250	NAD	O4D-C1D-N1N	3.55	112.04	108.13
5	H	1250	NAD	O4D-C1D-N1N	3.74	112.25	108.13
5	G	1250	NAD	O4D-C1D-N1N	4.77	113.37	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FU2	1	0
4	A	701	SO4	2	0
5	E	1250	NAD	3	0
3	E	600	FU2	2	0
5	F	1250	NAD	6	0
3	F	600	FU2	1	0
5	G	1250	NAD	5	0
3	G	600	FU2	6	0
5	H	1250	NAD	4	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	340/340 (100%)	-0.49	1 (0%) 94 96	19, 28, 41, 73	0
1	B	340/340 (100%)	-0.39	3 (0%) 85 89	19, 28, 41, 69	0
1	C	340/340 (100%)	-0.36	1 (0%) 94 96	18, 30, 45, 54	0
1	D	340/340 (100%)	-0.42	1 (0%) 94 96	18, 30, 45, 53	0
1	E	340/340 (100%)	-0.16	3 (0%) 85 89	22, 35, 54, 73	0
1	F	340/340 (100%)	-0.13	10 (2%) 55 64	22, 35, 55, 66	0
1	G	340/340 (100%)	-0.48	0 100 100	20, 28, 42, 55	0
1	H	340/340 (100%)	-0.46	0 100 100	19, 28, 43, 57	0
All	All	2720/2720 (100%)	-0.36	19 (0%) 89 92	18, 30, 48, 73	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	14	GLY	4.6
1	E	245	PRO	4.1
1	B	333	GLU	3.5
1	F	217	VAL	3.5
1	A	98	TYR	3.5
1	E	342	ARG	3.3
1	F	125	GLY	3.1
1	F	17	LEU	3.0
1	F	222	THR	2.8
1	B	98	TYR	2.8
1	E	227	TRP	2.7
1	F	203	ALA	2.4
1	B	342	ARG	2.3
1	F	313	SER	2.3
1	C	333	GLU	2.3
1	F	324	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	125	GLY	2.1
1	F	52	ASP	2.1
1	F	243	VAL	2.1

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	FU2	G	600	7/7	0.74	0.39	24.91	30,34,37,40	0
2	ZN	H	500	1/1	0.99	0.12	6.16	26,26,26,26	0
4	SO4	B	701	5/5	0.94	0.31	5.75	33,45,48,52	0
3	FU2	C	600	7/7	0.92	0.23	4.88	30,30,34,35	0
2	ZN	H	501	1/1	0.99	0.16	4.88	28,28,28,28	0
3	FU2	B	600	7/7	0.84	0.22	4.76	22,26,31,31	0
4	SO4	C	701	5/5	0.98	0.16	3.63	33,35,38,40	0
5	NAD	E	1250	44/44	0.82	0.21	2.44	33,42,47,48	0
4	SO4	C	702	5/5	0.98	0.14	1.94	41,41,48,49	0
2	ZN	E	501	1/1	0.99	0.13	1.70	27,27,27,27	0
2	ZN	C	501	1/1	0.99	0.15	1.64	31,31,31,31	0
5	NAD	G	1250	44/44	0.91	0.15	1.62	24,30,35,37	0
2	ZN	D	501	1/1	0.99	0.14	1.50	30,30,30,30	0
5	NAD	F	1250	44/44	0.88	0.19	1.25	29,42,46,48	0
2	ZN	G	501	1/1	0.99	0.15	1.22	27,27,27,27	0
5	NAD	H	1250	44/44	0.92	0.14	1.16	23,30,37,41	0
3	FU2	E	600	7/7	0.90	0.15	1.14	30,36,38,39	0
4	SO4	A	701	5/5	0.97	0.15	1.11	37,49,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FU2	F	600	7/7	0.90	0.18	1.02	32,36,40,40	0
4	SO4	F	702	5/5	0.92	0.19	0.84	41,41,46,48	0
3	FU2	A	600	7/7	0.92	0.12	0.65	21,25,31,31	0
2	ZN	F	501	1/1	0.99	0.12	0.56	25,25,25,25	0
2	ZN	C	500	1/1	0.98	0.11	0.44	31,31,31,31	0
4	SO4	G	703	5/5	0.95	0.11	0.21	28,30,35,36	0
4	SO4	B	702	5/5	0.96	0.11	0.07	41,42,53,55	0
2	ZN	B	501	1/1	0.99	0.14	0.02	29,29,29,29	0
3	FU2	D	600	7/7	0.94	0.10	-0.22	28,31,32,35	0
4	SO4	G	702	5/5	0.94	0.11	-0.24	37,42,47,54	0
2	ZN	A	501	1/1	0.99	0.11	-0.28	30,30,30,30	0
4	SO4	E	702	5/5	0.96	0.10	-0.42	35,39,44,46	0
2	ZN	G	500	1/1	0.96	0.08	-1.07	27,27,27,27	0
2	ZN	A	500	1/1	0.99	0.09	-1.21	33,33,33,33	0
2	ZN	E	500	1/1	0.98	0.09	-1.28	37,37,37,37	0
4	SO4	D	701	5/5	0.97	0.10	-1.31	36,37,47,48	0
4	SO4	D	702	5/5	0.97	0.09	-1.39	37,38,46,49	0
4	SO4	A	702	5/5	0.97	0.07	-1.72	41,42,51,52	0
2	ZN	D	500	1/1	0.99	0.06	-1.96	32,32,32,32	0
4	SO4	H	703	5/5	0.98	0.07	-2.56	27,29,33,35	0
4	SO4	H	702	5/5	0.98	0.05	-2.93	40,40,49,55	0
2	ZN	B	500	1/1	0.99	0.07	-3.47	34,34,34,34	0
2	ZN	F	500	1/1	0.97	0.06	-	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.