Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:09 PM GMT

PDB ID	:	4H73
Title	:	Thermostable aldehyde dehydrogenase from Pyrobaculum sp. complexed with NADP+
Authors	:	Petrova, T.; Shabalin, I.G.; Bezsudnova, E.Y.; Boyko, K.M.; Mardanov, A.V.; Gumerov, V.M; Ravin, N.V.; Popov , V.O.
Deposited on	:	2012-09-20
Resolution	:	2.40 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:

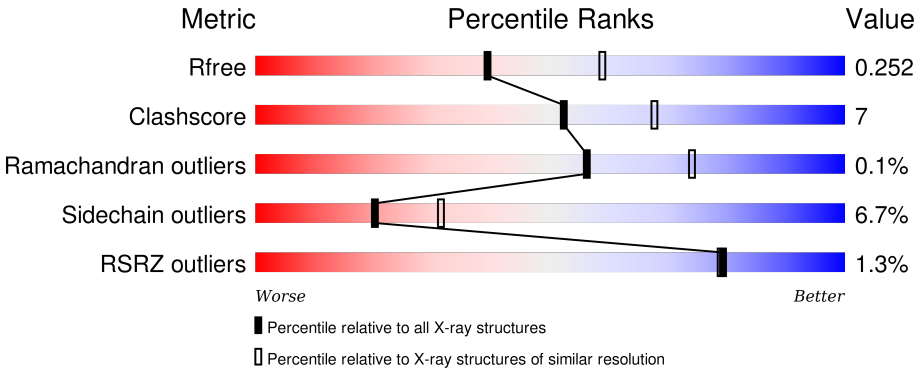
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	491	77% 19%
1	B	491	2% 79% 18%
1	C	491	78% 19%
1	D	491	79% 18%
1	E	491	79% 18%

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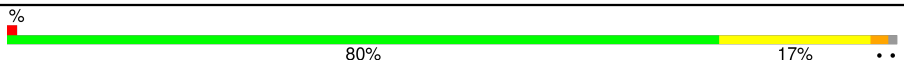
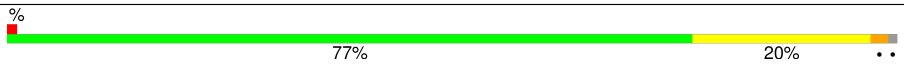
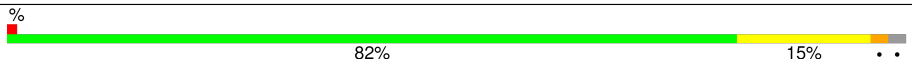
Mol	Chain	Length	Quality of chain
1	F	491	
1	G	491	
1	H	491	

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	NDP	D	500	-	-	-	X
2	NDP	F	500	-	-	-	X

2 Entry composition (i)

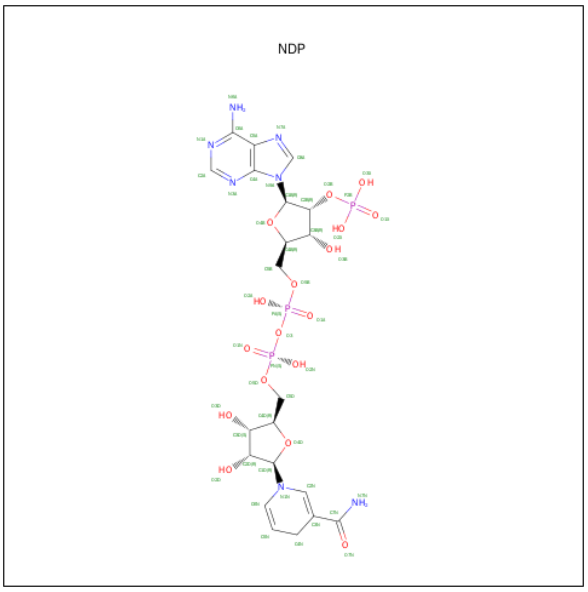
There are 4 unique types of molecules in this entry. The entry contains 31843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3744	2388	651	695	10			
1	B	485	Total	C	N	O	S	0	0	0
			3760	2399	652	698	11			
1	C	485	Total	C	N	O	S	0	0	0
			3762	2400	654	697	11			
1	D	485	Total	C	N	O	S	0	0	0
			3765	2402	656	696	11			
1	E	483	Total	C	N	O	S	0	0	0
			3761	2399	656	696	10			
1	F	485	Total	C	N	O	S	0	0	0
			3771	2405	658	697	11			
1	G	484	Total	C	N	O	S	0	0	0
			3764	2400	657	697	10			
1	H	483	Total	C	N	O	S	0	0	0
			3757	2395	656	696	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

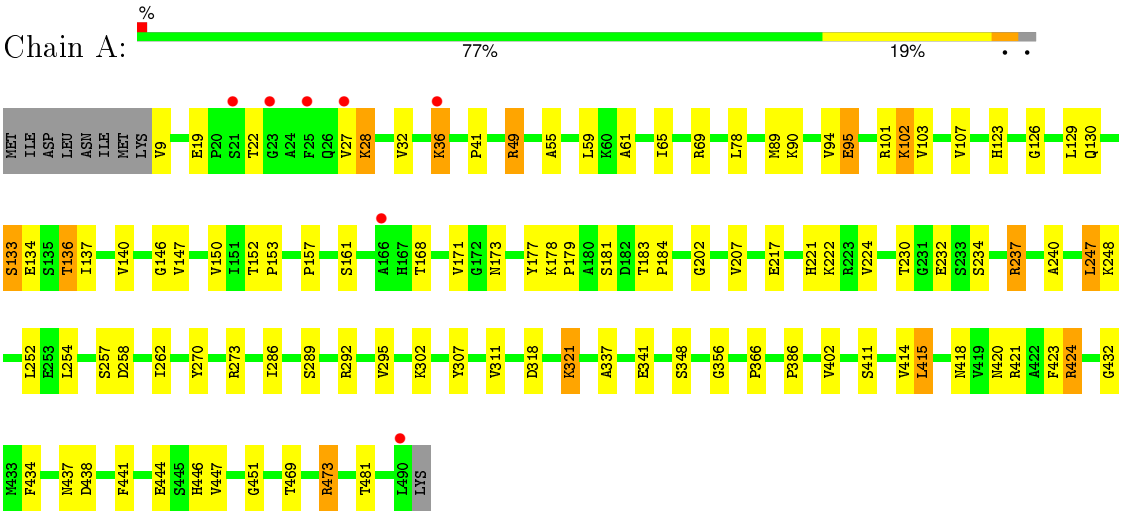
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	175	Total O 175 175	0	0
4	B	179	Total O 179 179	0	0
4	C	192	Total O 192 192	0	0
4	D	184	Total O 184 184	0	0
4	E	201	Total O 201 201	0	0
4	F	179	Total O 179 179	0	0
4	G	226	Total O 226 226	0	0
4	H	171	Total O 171 171	0	0

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.

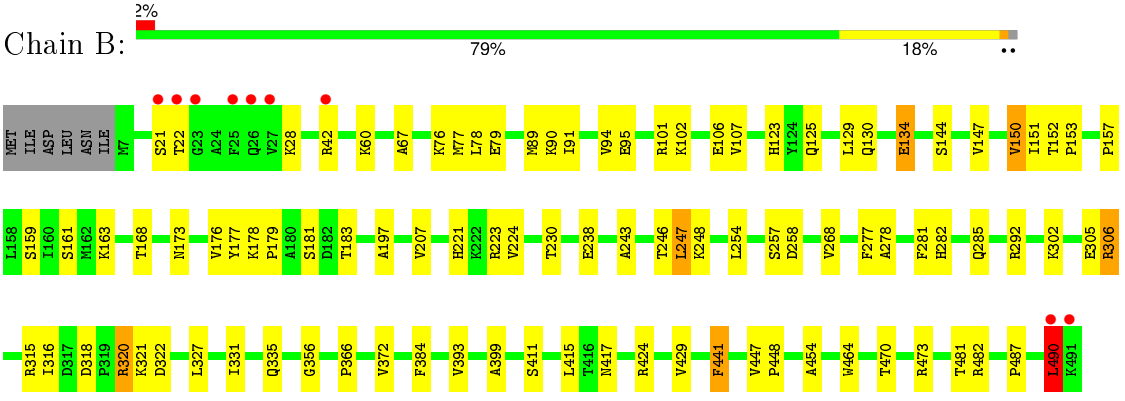
- Molecule 1: Aldehyde dehydrogenase

Chain A:



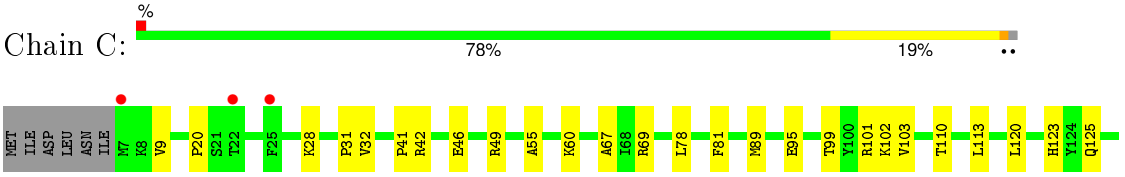
- Molecule 1: Aldehyde dehydrogenase

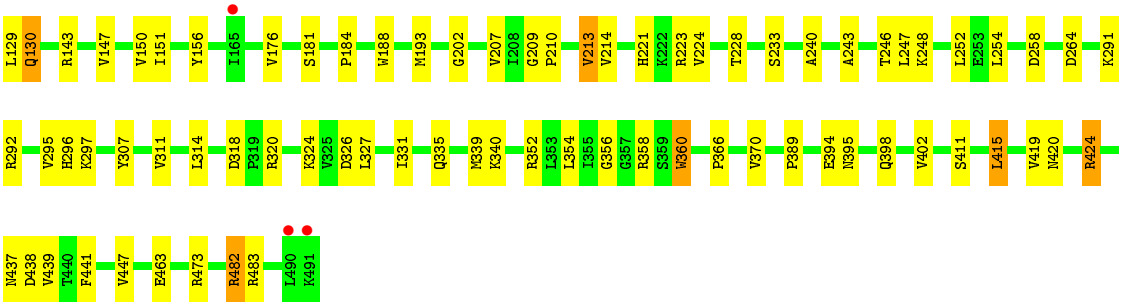
Chain B:



- Molecule 1: Aldehyde dehydrogenase

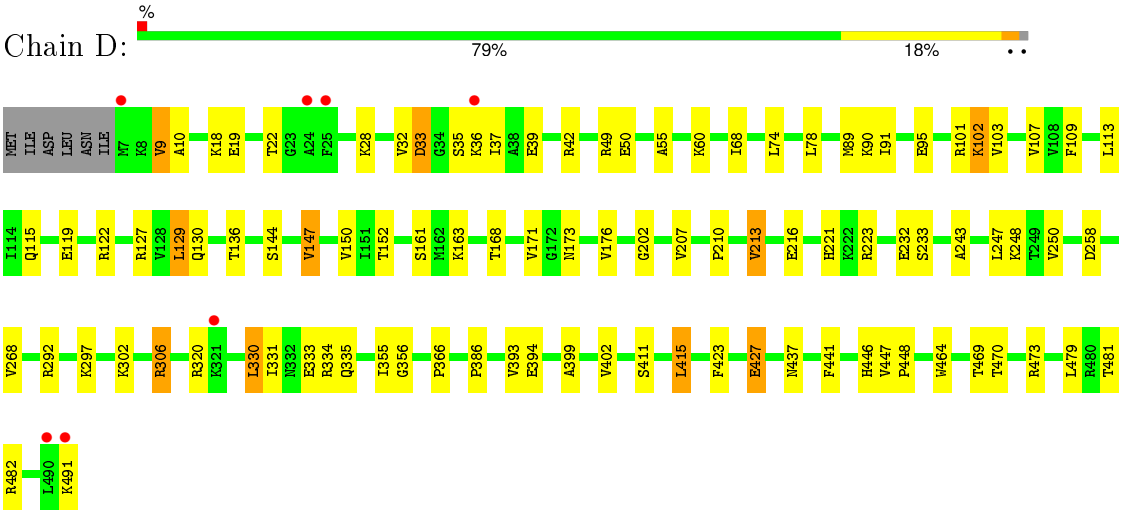
Chain C:





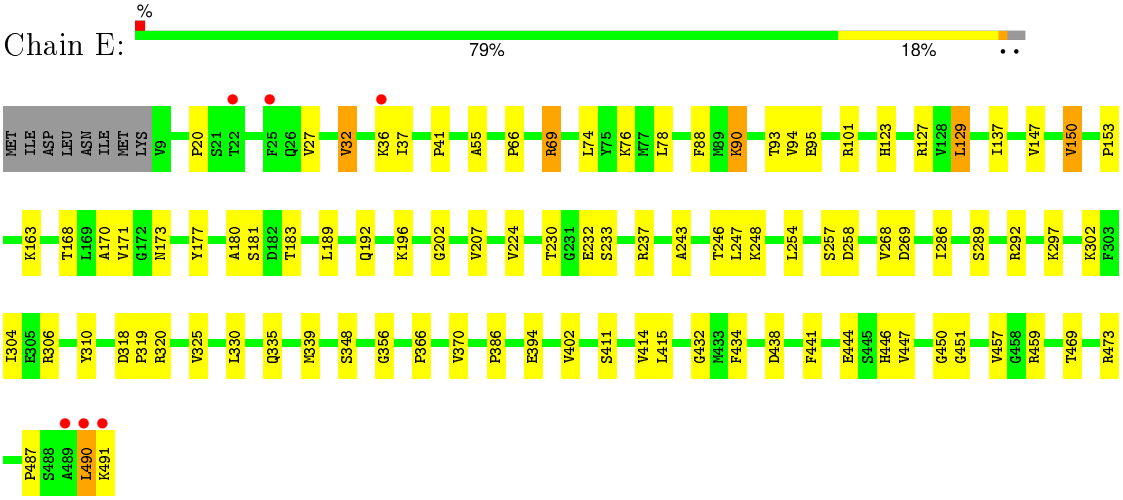
• Molecule 1: Aldehyde dehydrogenase

Chain D:



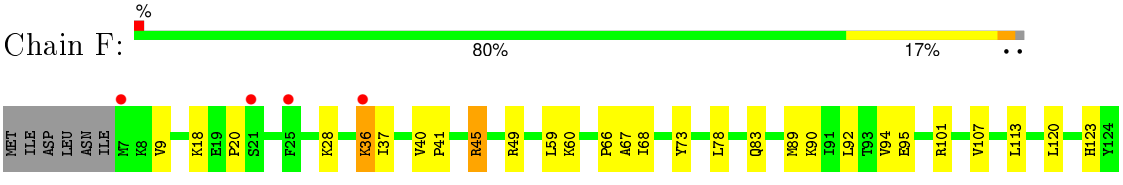
• Molecule 1: Aldehyde dehydrogenase

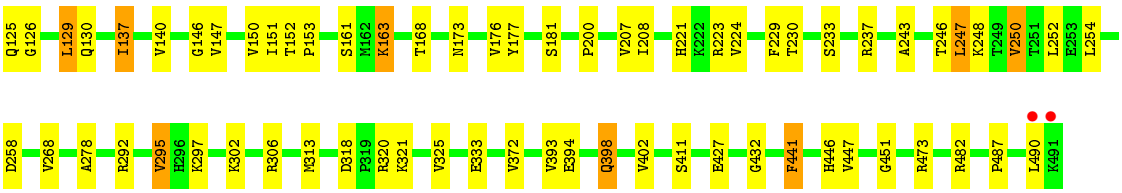
Chain E:



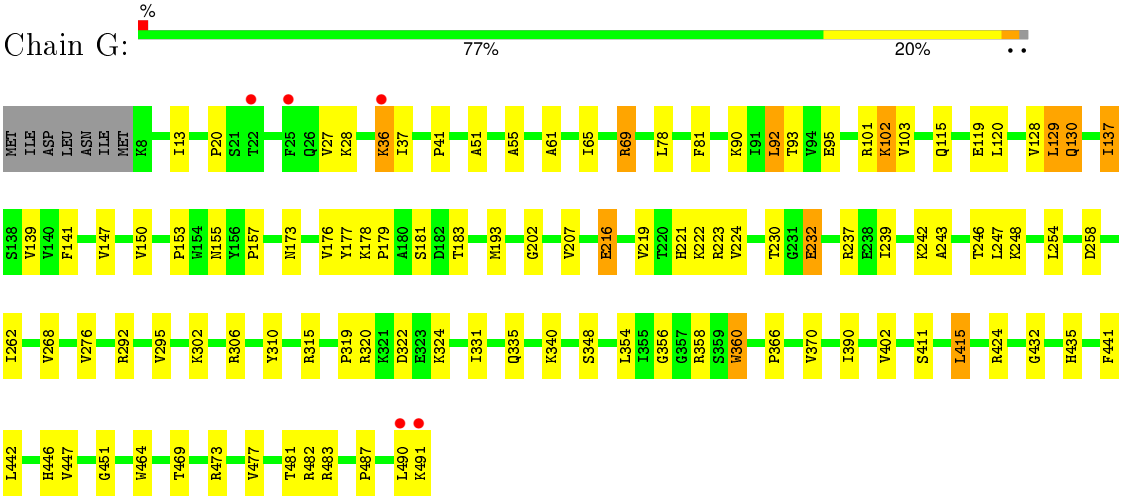
• Molecule 1: Aldehyde dehydrogenase

Chain F:

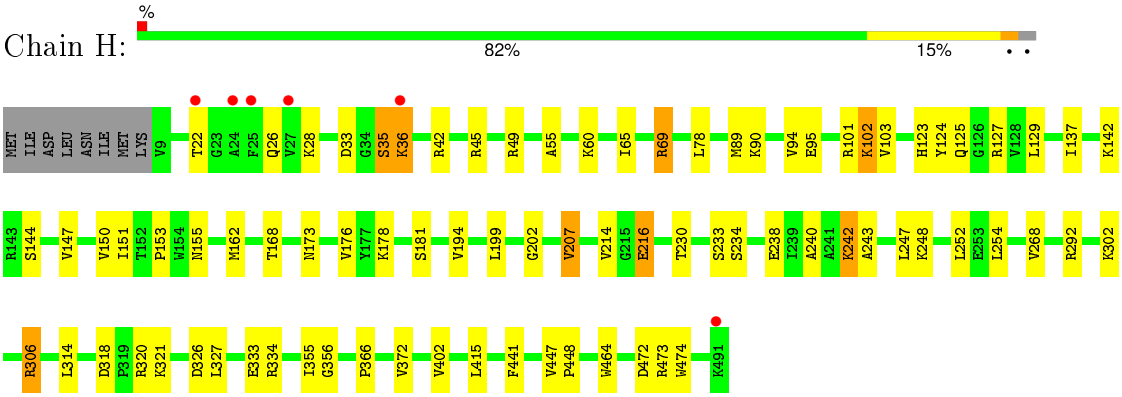




• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	164.21Å 183.77Å 206.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.40 29.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.62-2.40) 94.3 (29.63-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.212 , 0.261 0.201 , 0.252	Depositor DCC
R_{free} test set	11466 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	2 of 228959 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31843	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.22 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3639e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NDP, NI

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	0.42	0/3823	0.60	0/5184
1	B	0.43	0/3839	0.60	0/5204
1	C	0.44	0/3841	0.61	0/5208
1	D	0.45	0/3844	0.62	0/5211
1	E	0.45	0/3840	0.62	0/5205
1	F	0.44	0/3850	0.62	1/5218 (0.0%)
1	G	0.45	0/3842	0.64	0/5207
1	H	0.44	0/3836	0.60	0/5199
All	All	0.44	0/30715	0.61	1/41636 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	295	VAL	CB-CA-C	-5.17	101.57	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	490	LEU	Peptide
1	D	32	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3744	0	3739	61	0
1	B	3760	0	3749	58	0
1	C	3762	0	3751	59	0
1	D	3765	0	3761	47	0
1	E	3761	0	3770	55	0
1	F	3771	0	3771	57	0
1	G	3764	0	3766	62	0
1	H	3757	0	3756	46	0
2	A	31	0	11	2	0
2	B	31	0	11	2	0
2	C	31	0	11	2	0
2	D	31	0	11	0	0
2	E	31	0	11	1	0
2	F	31	0	11	3	0
2	G	31	0	11	1	0
2	H	31	0	11	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	175	0	0	2	0
4	B	179	0	0	2	0
4	C	192	0	0	5	0
4	D	184	0	0	4	0
4	E	201	0	0	3	0
4	F	179	0	0	2	0
4	G	226	0	0	4	0
4	H	171	0	0	2	0
All	All	31843	0	30151	403	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 7.

All (403) 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:305:GLU:OE1	1:B:306:ARG:NH1	2.15	0.80
1:A:247:LEU:HD21	1:B:254:LEU:HD12	1.63	0.79
1:G:20:PRO:HG3	1:G:41:PRO:HB3	1.65	0.78
1:H:45:ARG:HD2	1:H:49:ARG:HH21	1.51	0.76
1:D:28:LYS:HE2	1:D:95:GLU:HG3	1.69	0.75
1:B:28:LYS:HE2	1:B:95:GLU:HB2	1.67	0.75
1:C:482:ARG:HD3	1:C:483:ARG:H	1.50	0.74
1:D:210:PRO:HG2	1:D:213:VAL:HG13	1.70	0.73
1:C:129:LEU:HD23	1:D:447:VAL:HG12	1.71	0.73
1:C:20:PRO:HG3	1:C:41:PRO:HB3	1.70	0.73
1:D:33:ASP:HB3	1:D:35:SER:H	1.52	0.72
1:E:487:PRO:HG2	1:E:490:LEU:HD22	1.71	0.72
1:E:247:LEU:HD21	1:F:254:LEU:HD12	1.71	0.71
1:B:42:ARG:NH2	4:B:752:HOH:O	2.24	0.69
1:F:28:LYS:HE2	1:F:95:GLU:HG3	1.73	0.69
1:F:41:PRO:HG2	1:F:208:ILE:HB	1.73	0.69
1:E:129:LEU:HD23	1:F:447:VAL:HG12	1.75	0.69
1:G:254:LEU:HD12	1:H:247:LEU:HD21	1.73	0.69
1:E:127:ARG:NH1	4:E:651:HOH:O	2.26	0.67
1:G:221:HIS:HE1	1:G:223:ARG:HG3	1.58	0.67
1:A:147:VAL:HG22	1:A:224:VAL:HA	1.75	0.67
1:G:129:LEU:HD23	1:H:447:VAL:HG12	1.76	0.66
1:C:292:ARG:NH2	1:C:402:VAL:O	2.29	0.66
1:C:210:PRO:HG2	1:C:213:VAL:HG13	1.78	0.66
1:C:246:THR:OG1	1:C:248:LYS:NZ	2.28	0.65
1:F:28:LYS:HE3	1:F:37:ILE:HD12	1.77	0.65
1:C:221:HIS:HE1	1:C:223:ARG:HG3	1.62	0.64
1:G:324:LYS:NZ	4:G:787:HOH:O	2.31	0.64
1:F:292:ARG:NH2	1:F:402:VAL:O	2.32	0.62
1:G:237:ARG:NH2	4:G:805:HOH:O	2.31	0.62
1:A:28:LYS:HE2	1:A:95:GLU:HB2	1.82	0.62
1:A:438:ASP:OD1	1:B:482:ARG:NH2	2.32	0.61
1:A:133:SER:HB2	1:A:136:THR:HG21	1.82	0.61
1:A:254:LEU:HD12	1:B:247:LEU:HD21	1.80	0.61
1:E:318:ASP:OD1	1:E:320:ARG:HD3	1.99	0.61
1:C:424:ARG:NH1	4:C:771:HOH:O	2.34	0.61
1:E:254:LEU:HD12	1:F:247:LEU:HD21	1.83	0.61
1:A:318:ASP:HB3	1:A:321:LYS:HD2	1.83	0.61
1:H:28:LYS:HE2	1:H:95:GLU:HG3	1.82	0.61
1:B:102:LYS:HE3	1:B:282:HIS:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ASP:OD1	1:F:482:ARG:NH2	2.32	0.60
1:D:168:THR:HG22	1:D:173:ASN:HB2	1.83	0.60
1:F:237:ARG:NH1	4:F:737:HOH:O	2.34	0.60
1:E:181:SER:OG	2:E:501:NDP:O3X	2.20	0.60
1:H:33:ASP:OD1	1:H:35:SER:HB3	2.01	0.60
1:G:181:SER:OG	2:G:501:NDP:O3X	2.14	0.60
1:B:181:SER:OG	2:B:500:NDP:O3X	2.16	0.59
1:H:318:ASP:OD1	1:H:320:ARG:HD3	2.02	0.59
1:B:243:ALA:HB1	1:B:248:LYS:HG3	1.84	0.59
1:D:292:ARG:NH2	1:D:402:VAL:O	2.35	0.59
1:G:268:VAL:HG21	1:G:302:LYS:HE3	1.84	0.59
1:E:432:GLY:HA3	1:E:451:GLY:HA2	1.85	0.59
1:G:102:LYS:NZ	1:G:155:ASN:O	2.35	0.59
1:A:420:ASN:O	1:A:424:ARG:HD3	2.02	0.58
1:H:243:ALA:HB1	1:H:248:LYS:HG3	1.85	0.58
1:C:318:ASP:OD1	1:C:320:ARG:HD3	2.02	0.58
1:A:292:ARG:NH2	1:A:402:VAL:O	2.36	0.58
1:F:89:MET:HG3	1:F:107:VAL:HG21	1.86	0.58
1:F:221:HIS:HE1	1:F:223:ARG:HG3	1.69	0.58
1:E:490:LEU:HA	1:E:491:LYS:HB2	1.86	0.57
1:D:297:LYS:HD3	1:D:394:GLU:HG2	1.85	0.57
1:G:447:VAL:HG12	1:H:129:LEU:HD23	1.86	0.57
1:C:314:LEU:HD13	1:C:327:LEU:HD11	1.87	0.57
1:E:257:SER:OG	1:E:292:ARG:HD2	2.04	0.57
1:F:168:THR:HG22	1:F:173:ASN:HB2	1.85	0.57
1:C:147:VAL:HG22	1:C:224:VAL:HA	1.87	0.57
1:C:28:LYS:HE2	1:C:95:GLU:HB2	1.86	0.57
1:E:93:THR:HG23	1:E:319:PRO:HB2	1.85	0.57
1:E:37:ILE:HD11	1:E:94:VAL:HG12	1.87	0.57
1:C:224:VAL:O	1:C:248:LYS:HE3	2.05	0.57
1:A:150:VAL:HG23	1:A:177:TYR:HD1	1.70	0.57
1:H:268:VAL:HG11	1:H:302:LYS:HB3	1.86	0.57
1:G:93:THR:HG23	1:G:319:PRO:HB2	1.87	0.56
1:F:258:ASP:OD2	1:F:411:SER:HB3	2.04	0.56
1:B:318:ASP:HB3	1:B:321:LYS:HG3	1.87	0.56
1:E:246:THR:OG1	1:E:248:LYS:NZ	2.39	0.56
1:B:306:ARG:NE	4:B:712:HOH:O	2.39	0.56
1:C:482:ARG:HD3	1:C:483:ARG:N	2.18	0.56
1:C:254:LEU:HD12	1:D:247:LEU:HD21	1.87	0.56
1:F:20:PRO:HD3	1:F:41:PRO:HB3	1.88	0.56
1:C:297:LYS:HD3	1:C:394:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:HIS:CE1	1:G:223:ARG:HG3	2.38	0.55
1:A:123:HIS:ND1	1:C:120:LEU:HD21	2.21	0.55
1:F:487:PRO:HG2	1:F:490:LEU:HB2	1.88	0.55
1:D:18:LYS:NZ	1:D:50:GLU:OE2	2.37	0.55
1:E:243:ALA:HB1	1:E:248:LYS:HG3	1.88	0.55
1:G:28:LYS:HE2	1:G:95:GLU:HG3	1.89	0.55
1:A:273:ARG:NH2	4:A:688:HOH:O	2.39	0.55
1:F:181:SER:OG	2:F:500:NDP:O3X	2.25	0.55
1:G:487:PRO:HB3	1:H:314:LEU:HD23	1.89	0.55
1:B:153:PRO:HD3	1:B:230:THR:HB	1.88	0.54
1:G:27:VAL:HG11	1:G:36:LYS:HG3	1.89	0.54
1:F:393:VAL:HB	1:F:398:GLN:HB3	1.90	0.54
1:A:168:THR:HG22	1:A:173:ASN:HB2	1.90	0.54
1:G:224:VAL:O	1:G:248:LYS:HE3	2.07	0.54
1:C:258:ASP:OD2	1:C:411:SER:HB3	2.07	0.54
1:E:258:ASP:OD2	1:E:411:SER:HB3	2.08	0.53
1:A:134:GLU:O	1:A:136:THR:HG22	2.07	0.53
1:E:268:VAL:HG21	1:E:302:LYS:HE3	1.89	0.53
1:E:450:GLY:HA3	1:E:459:ARG:HD3	1.90	0.53
1:E:147:VAL:HG22	1:E:224:VAL:HA	1.89	0.53
1:G:153:PRO:HD3	1:G:230:THR:HB	1.90	0.53
1:D:89:MET:HG3	1:D:107:VAL:HG21	1.89	0.53
1:E:366:PRO:HA	1:E:386:PRO:HB2	1.90	0.53
1:A:89:MET:HG2	1:A:103:VAL:HG23	1.89	0.53
1:E:150:VAL:HG13	1:E:177:TYR:HA	1.90	0.53
1:E:168:THR:HG22	1:E:173:ASN:HB2	1.90	0.53
1:D:91:ILE:O	1:D:95:GLU:HB3	2.09	0.52
1:G:137:ILE:HG23	1:G:477:VAL:HB	1.90	0.52
1:C:42:ARG:NH1	4:C:785:HOH:O	2.42	0.52
1:E:55:ALA:HA	1:E:202:GLY:O	2.09	0.52
1:E:74:LEU:HD11	1:E:170:ALA:HB2	1.91	0.52
1:F:94:VAL:HG22	1:F:320:ARG:HD3	1.92	0.52
1:A:153:PRO:HD3	1:A:230:THR:HB	1.92	0.52
1:B:152:THR:HG21	1:B:161:SER:HA	1.90	0.52
1:C:143:ARG:HH12	1:D:427:GLU:HG2	1.74	0.52
1:A:55:ALA:HA	1:A:202:GLY:O	2.10	0.52
1:G:150:VAL:HG22	1:G:177:TYR:HD1	1.75	0.52
1:H:45:ARG:HD2	1:H:49:ARG:NH2	2.23	0.51
1:A:90:LYS:O	1:A:94:VAL:HG23	2.10	0.51
1:E:20:PRO:HD3	1:E:41:PRO:HB3	1.91	0.51
1:D:55:ALA:HA	1:D:202:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:ALA:HA	1:H:202:GLY:O	2.11	0.51
1:A:129:LEU:HD23	1:B:447:VAL:HG12	1.93	0.51
1:D:356:GLY:HA3	1:D:366:PRO:O	2.10	0.51
1:D:115:GLN:O	1:D:119:GLU:HG3	2.11	0.51
1:F:147:VAL:HG22	1:F:224:VAL:HA	1.93	0.51
1:G:258:ASP:OD2	1:G:411:SER:HB3	2.10	0.51
1:F:9:VAL:O	1:F:41:PRO:HD3	2.10	0.51
1:H:240:ALA:HB2	1:H:252:LEU:HD11	1.91	0.51
1:B:134:GLU:OE2	1:C:69:ARG:NH2	2.44	0.51
1:A:414:VAL:HG12	1:A:434:PHE:HE2	1.76	0.51
1:C:243:ALA:HB1	1:C:248:LYS:HG3	1.93	0.51
1:F:83:GLN:NE2	4:F:743:HOH:O	2.43	0.51
1:B:318:ASP:OD2	1:B:320:ARG:NH1	2.44	0.51
1:G:432:GLY:HA3	1:G:451:GLY:HA2	1.93	0.51
1:A:150:VAL:HG23	1:A:177:TYR:CD1	2.45	0.50
1:A:366:PRO:HA	1:A:386:PRO:HB2	1.94	0.50
1:F:250:VAL:HG13	1:F:252:LEU:HG	1.94	0.50
1:F:243:ALA:HB1	1:F:248:LYS:HG3	1.94	0.50
1:A:337:ALA:O	1:A:341:GLU:HG3	2.12	0.50
1:A:157:PRO:HG3	1:A:183:THR:HG21	1.94	0.50
1:C:358:ARG:HB3	1:C:360:TRP:CZ3	2.47	0.50
1:D:415:LEU:HD12	1:D:437:ASN:HA	1.92	0.50
1:C:221:HIS:CE1	1:C:223:ARG:HG3	2.43	0.50
1:B:315:ARG:NH2	1:B:322:ASP:OD2	2.39	0.50
1:G:482:ARG:HG3	1:G:483:ARG:H	1.77	0.50
1:F:67:ALA:HB2	1:G:130:GLN:HG2	1.94	0.50
1:E:123:HIS:CG	1:G:120:LEU:HD21	2.46	0.50
1:B:151:ILE:HG22	2:B:500:NDP:H4B	1.94	0.49
1:B:318:ASP:OD1	1:B:320:ARG:HD3	2.12	0.49
1:B:89:MET:HG3	1:B:107:VAL:HG21	1.94	0.49
1:B:316:ILE:HG12	1:B:327:LEU:HB2	1.93	0.49
1:E:192:GLN:O	1:E:196:LYS:HG3	2.12	0.49
1:B:106:GLU:HG3	1:B:159:SER:HB3	1.92	0.49
1:G:150:VAL:HG22	1:G:177:TYR:CD1	2.47	0.49
1:F:59:LEU:HD21	1:F:146:GLY:HA2	1.95	0.49
1:D:258:ASP:OD2	1:D:411:SER:HB3	2.13	0.49
1:D:268:VAL:HG21	1:D:302:LYS:HE3	1.93	0.49
1:B:258:ASP:OD2	1:B:411:SER:HB3	2.11	0.49
1:C:110:THR:HA	1:C:113:LEU:HD12	1.93	0.49
1:H:326:ASP:O	1:H:327:LEU:HD23	2.12	0.49
1:A:307:TYR:O	1:A:311:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:VAL:HG21	1:D:399:ALA:HB2	1.94	0.49
1:B:178:LYS:NZ	1:B:179:PRO:O	2.43	0.49
1:A:444:GLU:HB2	1:A:447:VAL:HG13	1.95	0.49
1:B:487:PRO:HD2	1:B:490:LEU:HD22	1.95	0.49
1:E:444:GLU:HB2	1:E:447:VAL:HG13	1.95	0.49
1:E:320:ARG:NH2	4:E:713:HOH:O	2.46	0.49
1:E:173:ASN:ND2	1:E:469:THR:HB	2.28	0.49
1:E:224:VAL:O	1:E:248:LYS:HE3	2.13	0.48
1:G:157:PRO:HG3	1:G:183:THR:HG21	1.95	0.48
1:H:356:GLY:HA3	1:H:366:PRO:O	2.12	0.48
1:A:133:SER:HB2	1:A:136:THR:CG2	2.42	0.48
1:C:447:VAL:HG12	1:D:129:LEU:HD23	1.95	0.48
1:E:356:GLY:HA3	1:E:366:PRO:O	2.12	0.48
1:G:173:ASN:ND2	1:G:469:THR:HB	2.28	0.48
1:A:61:ALA:O	1:A:65:ILE:HG23	2.13	0.48
1:G:315:ARG:NH2	1:G:322:ASP:OD2	2.37	0.48
1:A:258:ASP:OD2	1:A:411:SER:HB3	2.14	0.48
1:H:153:PRO:HD3	1:H:230:THR:HB	1.94	0.48
1:B:417:ASN:O	1:C:419:VAL:HG12	2.14	0.48
1:A:49:ARG:HD3	1:A:217:GLU:OE2	2.14	0.48
1:E:153:PRO:HD3	1:E:230:THR:HB	1.96	0.48
1:C:31:PRO:HB3	1:C:331:ILE:O	2.13	0.48
1:F:137:ILE:HD13	1:G:141:PHE:HZ	1.79	0.48
1:E:123:HIS:ND1	1:G:120:LEU:HD21	2.29	0.48
1:G:115:GLN:O	1:G:119:GLU:HG3	2.13	0.48
1:C:55:ALA:HA	1:C:202:GLY:O	2.14	0.48
1:C:438:ASP:OD1	1:D:482:ARG:NH2	2.47	0.47
1:G:237:ARG:HG2	1:H:247:LEU:HD13	1.96	0.47
1:C:420:ASN:O	1:C:424:ARG:HD3	2.14	0.47
1:C:463:GLU:OE2	1:D:127:ARG:NH2	2.47	0.47
1:F:66:PRO:HB2	1:F:68:ILE:HG22	1.96	0.47
1:A:237:ARG:HG3	1:B:247:LEU:HD13	1.95	0.47
1:E:32:VAL:HG11	1:E:320:ARG:HH11	1.78	0.47
1:A:318:ASP:O	1:A:321:LYS:HB2	2.15	0.47
1:H:306:ARG:HA	1:H:306:ARG:HD3	1.64	0.47
1:E:292:ARG:NH2	1:E:402:VAL:O	2.47	0.47
1:C:209:GLY:HA3	1:C:214:VAL:HG21	1.96	0.47
1:F:432:GLY:HA3	1:F:451:GLY:HA2	1.96	0.47
1:H:355:ILE:HG12	1:H:356:GLY:N	2.30	0.47
1:C:99:THR:HG21	1:C:326:ASP:O	2.15	0.47
1:G:55:ALA:HA	1:G:202:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:HIS:HE1	1:B:223:ARG:HG3	1.80	0.47
1:E:414:VAL:HG12	1:E:434:PHE:HE2	1.79	0.47
1:A:181:SER:O	1:A:184:PRO:HD3	2.15	0.47
1:A:224:VAL:O	1:A:248:LYS:HE3	2.15	0.46
1:G:358:ARG:HB3	1:G:360:TRP:CZ3	2.50	0.46
1:A:102:LYS:HG3	1:A:103:VAL:N	2.29	0.46
1:E:304:ILE:HD13	1:E:370:VAL:HG11	1.97	0.46
1:C:415:LEU:HD12	1:C:437:ASN:HA	1.97	0.46
1:F:73:TYR:CE1	1:F:200:PRO:HD3	2.51	0.46
1:D:168:THR:HG23	1:D:469:THR:HG21	1.98	0.46
1:E:36:LYS:HD2	4:E:691:HOH:O	2.16	0.46
1:F:152:THR:HG21	1:F:161:SER:HA	1.96	0.46
1:F:229:PHE:HE1	2:F:500:NDP:O4B	1.98	0.46
1:F:67:ALA:CB	1:G:130:GLN:HG2	2.46	0.46
1:A:9:VAL:N	1:A:41:PRO:HD3	2.30	0.46
1:F:36:LYS:N	1:F:36:LYS:HD2	2.31	0.46
1:B:90:LYS:O	1:B:94:VAL:HG23	2.16	0.46
1:D:221:HIS:HE1	1:D:223:ARG:HG3	1.81	0.46
1:A:415:LEU:HD12	1:A:437:ASN:HA	1.98	0.46
1:E:168:THR:HG23	1:E:469:THR:HG21	1.98	0.46
1:D:479:LEU:O	4:D:728:HOH:O	2.21	0.46
1:D:355:ILE:HG12	1:D:356:GLY:N	2.31	0.46
1:A:240:ALA:HB2	1:A:252:LEU:HD11	1.98	0.46
1:C:307:TYR:O	1:C:311:VAL:HG23	2.15	0.46
1:D:448:PRO:HD3	1:D:464:TRP:CH2	2.51	0.46
1:B:448:PRO:HD3	1:B:464:TRP:CZ3	2.50	0.45
1:C:356:GLY:HA3	1:C:366:PRO:O	2.16	0.45
1:D:144:SER:HA	1:D:470:THR:HG22	1.97	0.45
1:G:356:GLY:HA3	1:G:366:PRO:O	2.16	0.45
1:B:424:ARG:HD2	4:D:728:HOH:O	2.16	0.45
1:C:438:ASP:OD1	1:C:439:VAL:N	2.45	0.45
1:G:331:ILE:HG22	1:G:335:GLN:HG3	1.98	0.45
1:B:331:ILE:HG22	1:B:335:GLN:HG3	1.99	0.45
1:B:277:PHE:O	1:B:281:PHE:HB2	2.16	0.45
1:D:28:LYS:HE3	1:D:37:ILE:HD12	1.99	0.45
1:D:109:PHE:CE2	1:D:113:LEU:HD11	2.51	0.45
1:F:318:ASP:O	1:F:321:LYS:HB2	2.17	0.45
1:E:297:LYS:NZ	1:E:394:GLU:OE1	2.46	0.45
1:C:324:LYS:NZ	4:C:780:HOH:O	2.49	0.45
1:A:217:GLU:O	1:A:221:HIS:HB2	2.16	0.45
1:F:278:ALA:HA	1:F:441:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:SER:O	1:B:292:ARG:NH1	2.50	0.45
1:C:395:ASN:OD1	1:C:398:GLN:HB2	2.16	0.45
1:B:246:THR:OG1	1:B:248:LYS:NZ	2.47	0.45
1:A:152:THR:HG21	1:A:161:SER:HA	1.98	0.45
1:H:233:SER:HA	1:H:254:LEU:HB3	1.97	0.45
1:A:89:MET:HG3	1:A:107:VAL:HG21	1.97	0.45
1:G:128:VAL:HG22	1:G:139:VAL:HG12	1.99	0.45
1:F:45:ARG:HD2	1:F:49:ARG:NH2	2.31	0.45
1:B:168:THR:HG23	1:B:173:ASN:HB2	1.99	0.45
1:H:102:LYS:NZ	1:H:155:ASN:O	2.46	0.45
1:H:89:MET:HE3	1:H:103:VAL:HG23	1.98	0.45
1:A:270:TYR:CE1	1:B:481:THR:HG23	2.51	0.44
1:H:49:ARG:NH2	4:H:697:HOH:O	2.49	0.44
1:G:178:LYS:NZ	1:G:179:PRO:O	2.48	0.44
1:D:68:ILE:HG13	1:D:122:ARG:HD2	1.98	0.44
1:B:144:SER:HA	1:B:470:THR:HG22	1.99	0.44
1:F:36:LYS:H	1:F:36:LYS:HD2	1.82	0.44
1:B:356:GLY:HA3	1:B:366:PRO:O	2.16	0.44
1:H:448:PRO:HB3	1:H:464:TRP:CG	2.53	0.44
1:G:262:ILE:HG12	1:G:415:LEU:HD22	1.98	0.44
1:A:173:ASN:ND2	1:A:469:THR:HB	2.32	0.44
1:H:448:PRO:HB3	1:H:464:TRP:CD1	2.52	0.44
1:B:91:ILE:HD13	1:B:91:ILE:HA	1.83	0.44
1:G:92:LEU:HB3	1:G:103:VAL:CG1	2.48	0.44
1:F:150:VAL:HG22	1:F:177:TYR:HD1	1.83	0.44
1:G:232:GLU:HG2	4:G:749:HOH:O	2.18	0.44
1:A:168:THR:HG23	1:A:469:THR:HG21	2.00	0.44
1:D:448:PRO:HB3	1:D:464:TRP:CE2	2.53	0.44
1:D:330:LEU:HD11	1:D:386:PRO:HD3	2.00	0.43
1:F:153:PRO:HD3	1:F:230:THR:HB	2.00	0.43
1:B:268:VAL:HG21	1:B:302:LYS:HE3	2.00	0.43
1:F:306:ARG:HA	1:F:306:ARG:HD3	1.78	0.43
1:C:291:LYS:O	1:C:389:PRO:HD2	2.18	0.43
1:D:33:ASP:OD2	1:D:320:ARG:NH2	2.49	0.43
1:H:207:VAL:HG22	1:H:214:VAL:HG11	2.00	0.43
1:B:76:LYS:HD3	1:B:197:ALA:O	2.18	0.43
1:D:331:ILE:HG22	1:D:335:GLN:HG3	1.99	0.43
1:C:9:VAL:HB	1:C:188:TRP:CG	2.53	0.43
1:G:306:ARG:HG3	1:G:310:TYR:CE2	2.54	0.43
1:E:27:VAL:HG11	1:E:36:LYS:HG3	1.99	0.43
1:H:168:THR:HG22	1:H:173:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG11	1:A:318:ASP:OD1	2.18	0.43
1:D:355:ILE:HG12	1:D:356:GLY:H	1.84	0.43
1:H:151:ILE:HG22	2:H:500:NDP:H4B	2.01	0.43
1:C:102:LYS:HE2	1:C:156:TYR:CZ	2.54	0.43
1:B:157:PRO:HG3	1:B:183:THR:HG21	2.01	0.43
1:D:152:THR:HG21	1:D:161:SER:HA	2.01	0.43
1:H:60:LYS:HE3	1:H:60:LYS:HB2	1.79	0.43
1:D:306:ARG:HD3	1:D:306:ARG:HA	1.81	0.43
1:F:113:LEU:HD22	1:F:163:LYS:HB2	2.00	0.43
1:F:40:VAL:CG1	1:F:208:ILE:HG21	2.49	0.43
1:C:49:ARG:NH2	4:C:635:HOH:O	2.51	0.43
1:D:9:VAL:HG13	1:D:39:GLU:O	2.18	0.43
1:F:224:VAL:O	1:F:248:LYS:HE3	2.19	0.43
1:A:27:VAL:HG11	1:A:36:LYS:NZ	2.34	0.43
1:C:354:LEU:HD11	1:C:370:VAL:HG13	2.00	0.43
1:H:65:ILE:HD12	1:H:69:ARG:HB3	1.99	0.43
1:G:464:TRP:NE1	1:H:472:ASP:OD1	2.38	0.43
1:E:180:ALA:HB3	1:E:183:THR:OG1	2.18	0.43
1:D:243:ALA:HB1	1:D:248:LYS:HG3	2.01	0.42
1:G:354:LEU:HD11	1:G:370:VAL:HG13	2.01	0.42
1:G:102:LYS:HG3	1:G:103:VAL:N	2.33	0.42
1:E:447:VAL:HG12	1:F:129:LEU:HD23	2.00	0.42
1:E:286:ILE:HB	1:E:289:SER:HB2	2.02	0.42
1:B:130:GLN:HG2	1:C:67:ALA:CB	2.50	0.42
1:C:46:GLU:HG2	4:C:782:HOH:O	2.18	0.42
1:E:66:PRO:HG2	1:E:69:ARG:HG3	2.00	0.42
1:C:264:ASP:HB3	1:C:296:HIS:ND1	2.34	0.42
1:F:150:VAL:HG22	1:F:177:TYR:CD1	2.55	0.42
1:E:269:ASP:OD1	1:E:310:TYR:OH	2.24	0.42
1:F:151:ILE:HG22	2:F:500:NDP:H4B	2.01	0.42
1:D:102:LYS:HG3	1:D:103:VAL:N	2.35	0.42
1:C:181:SER:OG	2:C:501:NDP:O3X	2.29	0.42
1:C:240:ALA:HB2	1:C:252:LEU:HD11	2.01	0.42
1:B:77:MET:HE3	1:B:77:MET:HB3	1.83	0.42
1:G:13:ILE:HG23	1:G:51:ALA:HA	2.02	0.42
1:B:150:VAL:HG13	1:B:177:TYR:HA	2.01	0.42
1:G:216:GLU:OE2	1:G:242:LYS:NZ	2.52	0.42
1:B:306:ARG:HD3	1:B:306:ARG:HA	1.71	0.42
1:G:81:PHE:HB2	1:G:193:MET:SD	2.59	0.42
1:H:194:VAL:HG13	1:H:199:LEU:HD22	2.01	0.42
1:G:292:ARG:NH2	1:G:402:VAL:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HE2	2:A:501:NDP:H1B	2.02	0.42
1:A:418:ASN:OD1	1:A:421:ARG:HG3	2.20	0.42
1:C:151:ILE:HG22	2:C:501:NDP:H4B	2.02	0.42
1:A:423:PHE:HZ	1:D:423:PHE:HZ	1.68	0.42
1:C:335:GLN:O	1:C:339:MET:HG2	2.19	0.42
1:A:286:ILE:HB	1:A:289:SER:HB2	2.00	0.42
1:H:124:TYR:CZ	1:H:142:LYS:HE3	2.55	0.42
1:B:448:PRO:HD3	1:B:464:TRP:CH2	2.55	0.42
1:B:76:LYS:O	1:B:79:GLU:HG2	2.20	0.42
1:F:126:GLY:HA3	1:F:140:VAL:O	2.19	0.42
1:H:36:LYS:HD3	1:H:36:LYS:HA	1.89	0.42
1:C:89:MET:HE3	1:C:103:VAL:HG23	2.02	0.42
1:A:126:GLY:HA3	1:A:140:VAL:O	2.20	0.42
1:B:224:VAL:O	1:B:248:LYS:HE3	2.19	0.41
1:F:120:LEU:HD21	1:H:123:HIS:CG	2.55	0.41
1:H:292:ARG:NH2	1:H:402:VAL:O	2.53	0.41
1:C:81:PHE:HB2	1:C:193:MET:SD	2.60	0.41
1:H:26:GLN:HG3	1:H:42:ARG:HB2	2.03	0.41
1:F:246:THR:OG1	1:F:248:LYS:NZ	2.41	0.41
1:A:49:ARG:HD2	4:A:702:HOH:O	2.20	0.41
1:E:237:ARG:HG2	1:F:247:LEU:HD13	2.02	0.41
1:E:123:HIS:CE1	1:G:120:LEU:HD11	2.55	0.41
1:D:147:VAL:HG13	1:D:223:ARG:O	2.19	0.41
1:G:65:ILE:HD12	1:G:69:ARG:HB2	2.01	0.41
1:G:435:HIS:CE1	1:G:442:LEU:HB2	2.55	0.41
1:C:181:SER:O	1:C:184:PRO:HD3	2.20	0.41
1:H:123:HIS:O	1:H:125:GLN:HG3	2.20	0.41
1:B:393:VAL:HG21	1:B:399:ALA:HB2	2.02	0.41
1:B:67:ALA:HB2	1:C:130:GLN:HG2	2.02	0.41
1:H:162:MET:HB3	1:H:162:MET:HE3	1.97	0.41
1:E:90:LYS:O	1:E:94:VAL:HG23	2.20	0.41
1:D:10:ALA:HB1	1:D:18:LYS:O	2.21	0.41
1:E:444:GLU:O	1:E:447:VAL:HG22	2.21	0.41
1:A:232:GLU:H	2:A:501:NDP:PA	2.43	0.41
1:F:268:VAL:HG21	1:F:302:LYS:HE3	2.03	0.41
1:B:278:ALA:HA	1:B:441:PHE:CE2	2.56	0.41
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.83	0.41
1:G:219:VAL:HG21	1:G:239:ILE:HG12	2.02	0.41
1:H:318:ASP:HB3	1:H:321:LYS:HG2	2.03	0.41
1:H:178:LYS:HE2	2:H:500:NDP:H1B	2.02	0.41
1:H:181:SER:OG	2:H:500:NDP:O3X	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:LYS:HD2	1:F:394:GLU:HG2	2.02	0.41
1:E:88:PHE:CE2	1:E:189:LEU:HB3	2.56	0.41
1:E:490:LEU:HD13	1:F:313:MET:HE1	2.03	0.41
1:G:243:ALA:HB1	1:G:248:LYS:HG3	2.01	0.41
1:F:224:VAL:HB	1:F:248:LYS:HE2	2.02	0.41
1:H:355:ILE:HG12	1:H:356:GLY:H	1.86	0.41
1:E:306:ARG:HA	1:E:306:ARG:HD3	1.68	0.41
1:F:123:HIS:O	1:F:125:GLN:HG3	2.21	0.41
1:B:285:GLN:HB3	1:B:384:PHE:CE1	2.55	0.41
1:E:335:GLN:O	1:E:339:MET:HG2	2.21	0.41
1:A:247:LEU:HD23	1:B:454:ALA:HA	2.03	0.41
1:G:276:VAL:HG21	1:G:310:TYR:HB2	2.03	0.41
1:A:178:LYS:HA	1:A:179:PRO:HD2	1.93	0.41
1:D:334:ARG:NH1	4:D:749:HOH:O	2.31	0.41
1:A:123:HIS:CG	1:C:120:LEU:HD21	2.56	0.40
1:A:356:GLY:HA3	1:A:366:PRO:O	2.22	0.40
1:F:45:ARG:HH11	1:F:49:ARG:NH2	2.19	0.40
1:G:435:HIS:HE1	1:H:474:TRP:CZ3	2.39	0.40
1:A:262:ILE:HG13	1:A:415:LEU:HD22	2.02	0.40
1:G:370:VAL:HG12	1:G:390:ILE:HB	2.03	0.40
1:B:67:ALA:CB	1:C:130:GLN:HG2	2.52	0.40
1:G:424:ARG:HD2	4:G:746:HOH:O	2.21	0.40
1:A:432:GLY:HA3	1:A:451:GLY:HA2	2.02	0.40
1:D:130:GLN:HG3	4:D:623:HOH:O	2.21	0.40
1:B:123:HIS:O	1:B:125:GLN:HG3	2.21	0.40
1:F:45:ARG:HH11	1:F:49:ARG:HH22	1.70	0.40
1:G:61:ALA:O	1:G:65:ILE:HG23	2.21	0.40
1:C:123:HIS:O	1:C:125:GLN:HG3	2.21	0.40
2:H:500:NDP:N6A	4:H:717:HOH:O	2.36	0.40
1:H:216:GLU:OE1	1:H:242:LYS:NZ	2.39	0.40
1:G:28:LYS:HE3	1:G:37:ILE:HD12	2.04	0.40
1:G:246:THR:OG1	1:G:248:LYS:NZ	2.41	0.40
1:H:448:PRO:HB3	1:H:464:TRP:CD2	2.56	0.40
1:A:473:ARG:NH2	1:B:429:VAL:O	2.55	0.40
1:A:59:LEU:HD21	1:A:146:GLY:HA2	2.03	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	480/491 (98%)	464 (97%)	16 (3%)	0	100 100
1	B	483/491 (98%)	471 (98%)	12 (2%)	0	100 100
1	C	483/491 (98%)	469 (97%)	13 (3%)	1 (0%)	52 69
1	D	483/491 (98%)	470 (97%)	13 (3%)	0	100 100
1	E	481/491 (98%)	468 (97%)	12 (2%)	1 (0%)	52 69
1	F	483/491 (98%)	471 (98%)	12 (2%)	0	100 100
1	G	482/491 (98%)	468 (97%)	14 (3%)	0	100 100
1	H	481/491 (98%)	474 (98%)	7 (2%)	0	100 100
All	All	3856/3928 (98%)	3755 (97%)	99 (3%)	2 (0%)	56 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	32	VAL
1	C	32	VAL

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	395/408 (97%)	364 (92%)	31 (8%)	16 24
1	B	395/408 (97%)	374 (95%)	21 (5%)	28 44
1	C	395/408 (97%)	375 (95%)	20 (5%)	29 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	396/408 (97%)	361 (91%)	35 (9%)	12 18
1	E	398/408 (98%)	375 (94%)	23 (6%)	25 39
1	F	397/408 (97%)	371 (94%)	26 (6%)	21 33
1	G	397/408 (97%)	368 (93%)	29 (7%)	17 27
1	H	396/408 (97%)	369 (93%)	27 (7%)	20 31
All	All	3169/3264 (97%)	2957 (93%)	212 (7%)	20 31

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	22	THR
1	A	28	LYS
1	A	36	LYS
1	A	49	ARG
1	A	69	ARG
1	A	78	LEU
1	A	95	GLU
1	A	101	ARG
1	A	102	LYS
1	A	130	GLN
1	A	133	SER
1	A	136	THR
1	A	137	ILE
1	A	171	VAL
1	A	207	VAL
1	A	222	LYS
1	A	234	SER
1	A	237	ARG
1	A	247	LEU
1	A	257	SER
1	A	295	VAL
1	A	302	LYS
1	A	321	LYS
1	A	348	SER
1	A	415	LEU
1	A	424	ARG
1	A	441	PHE
1	A	446	HIS
1	A	473	ARG

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Mol	Chain	Res	Type
1	A	481	THR
1	B	21	SER
1	B	22	THR
1	B	60	LYS
1	B	78	LEU
1	B	101	ARG
1	B	129	LEU
1	B	134	GLU
1	B	147	VAL
1	B	150	VAL
1	B	163	LYS
1	B	176	VAL
1	B	207	VAL
1	B	238	GLU
1	B	247	LEU
1	B	306	ARG
1	B	320	ARG
1	B	372	VAL
1	B	415	LEU
1	B	441	PHE
1	B	473	ARG
1	B	490	LEU
1	C	60	LYS
1	C	78	LEU
1	C	101	ARG
1	C	130	GLN
1	C	150	VAL
1	C	176	VAL
1	C	207	VAL
1	C	213	VAL
1	C	228	THR
1	C	233	SER
1	C	247	LEU
1	C	295	VAL
1	C	340	LYS
1	C	352	ARG
1	C	360	TRP
1	C	415	LEU
1	C	424	ARG
1	C	441	PHE
1	C	473	ARG
1	C	482	ARG

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Mol	Chain	Res	Type
1	D	9	VAL
1	D	19	GLU
1	D	22	THR
1	D	33	ASP
1	D	36	LYS
1	D	42	ARG
1	D	49	ARG
1	D	60	LYS
1	D	78	LEU
1	D	90	LYS
1	D	101	ARG
1	D	102	LYS
1	D	129	LEU
1	D	136	THR
1	D	147	VAL
1	D	150	VAL
1	D	163	LYS
1	D	171	VAL
1	D	176	VAL
1	D	207	VAL
1	D	213	VAL
1	D	216	GLU
1	D	232	GLU
1	D	233	SER
1	D	250	VAL
1	D	306	ARG
1	D	330	LEU
1	D	333	GLU
1	D	415	LEU
1	D	427	GLU
1	D	441	PHE
1	D	446	HIS
1	D	473	ARG
1	D	481	THR
1	D	491	LYS
1	E	69	ARG
1	E	76	LYS
1	E	78	LEU
1	E	90	LYS
1	E	95	GLU
1	E	101	ARG
1	E	129	LEU

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Mol	Chain	Res	Type
1	E	137	ILE
1	E	150	VAL
1	E	163	LYS
1	E	171	VAL
1	E	207	VAL
1	E	232	GLU
1	E	233	SER
1	E	325	VAL
1	E	330	LEU
1	E	348	SER
1	E	415	LEU
1	E	441	PHE
1	E	446	HIS
1	E	457	VAL
1	E	473	ARG
1	E	490	LEU
1	F	18	LYS
1	F	36	LYS
1	F	45	ARG
1	F	60	LYS
1	F	78	LEU
1	F	90	LYS
1	F	92	LEU
1	F	101	ARG
1	F	129	LEU
1	F	130	GLN
1	F	137	ILE
1	F	163	LYS
1	F	176	VAL
1	F	207	VAL
1	F	233	SER
1	F	247	LEU
1	F	250	VAL
1	F	295	VAL
1	F	325	VAL
1	F	333	GLU
1	F	372	VAL
1	F	398	GLN
1	F	427	GLU
1	F	441	PHE
1	F	446	HIS
1	F	473	ARG

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Mol	Chain	Res	Type
1	G	36	LYS
1	G	69	ARG
1	G	78	LEU
1	G	90	LYS
1	G	92	LEU
1	G	101	ARG
1	G	102	LYS
1	G	129	LEU
1	G	130	GLN
1	G	137	ILE
1	G	147	VAL
1	G	176	VAL
1	G	207	VAL
1	G	216	GLU
1	G	222	LYS
1	G	232	GLU
1	G	247	LEU
1	G	295	VAL
1	G	320	ARG
1	G	340	LYS
1	G	348	SER
1	G	360	TRP
1	G	415	LEU
1	G	441	PHE
1	G	446	HIS
1	G	473	ARG
1	G	481	THR
1	G	490	LEU
1	G	491	LYS
1	H	22	THR
1	H	35	SER
1	H	36	LYS
1	H	69	ARG
1	H	78	LEU
1	H	90	LYS
1	H	94	VAL
1	H	101	ARG
1	H	102	LYS
1	H	127	ARG
1	H	137	ILE
1	H	144	SER
1	H	147	VAL

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Mol	Chain	Res	Type
1	H	150	VAL
1	H	176	VAL
1	H	207	VAL
1	H	216	GLU
1	H	234	SER
1	H	238	GLU
1	H	242	LYS
1	H	306	ARG
1	H	333	GLU
1	H	334	ARG
1	H	372	VAL
1	H	415	LEU
1	H	441	PHE
1	H	473	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	192	GLN
1	G	398	GLN
1	H	115	GLN

5.3.3 RNA (i)

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)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	A	501	-	26,33,52	1.66	4 (15%)	34,52,80	2.15	5 (14%)
2	NDP	B	500	-	26,33,52	1.74	6 (23%)	34,52,80	2.58	7 (20%)
2	NDP	C	501	-	26,33,52	1.68	4 (15%)	34,52,80	2.21	6 (17%)
2	NDP	D	500	-	26,33,52	1.69	5 (19%)	34,52,80	2.28	8 (23%)
2	NDP	E	501	-	26,33,52	1.64	4 (15%)	34,52,80	2.15	5 (14%)
2	NDP	F	500	-	26,33,52	1.68	4 (15%)	34,52,80	2.29	7 (20%)
2	NDP	G	501	-	26,33,52	1.67	3 (11%)	34,52,80	2.16	5 (14%)
2	NDP	H	500	-	26,33,52	1.68	5 (19%)	34,52,80	2.24	8 (23%)

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	NDP	A	501	-	-	0/17/37/77	0/3/3/5
2	NDP	B	500	-	-	0/17/37/77	0/3/3/5
2	NDP	C	501	-	-	0/17/37/77	0/3/3/5
2	NDP	D	500	-	-	0/17/37/77	0/3/3/5
2	NDP	E	501	-	-	0/17/37/77	0/3/3/5
2	NDP	F	500	-	-	0/17/37/77	0/3/3/5
2	NDP	G	501	-	-	0/17/37/77	0/3/3/5
2	NDP	H	500	-	-	0/17/37/77	0/3/3/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NDP	C3B-C2B	-5.14	1.41	1.53
2	D	500	NDP	C3B-C2B	-4.89	1.42	1.53
2	H	500	NDP	C3B-C2B	-4.88	1.42	1.53
2	F	500	NDP	C3B-C2B	-4.84	1.42	1.53
2	A	501	NDP	C3B-C2B	-4.80	1.42	1.53
2	G	501	NDP	C3B-C2B	-4.79	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	NDP	C3B-C2B	-4.75	1.42	1.53
2	C	501	NDP	C3B-C2B	-4.67	1.42	1.53
2	B	500	NDP	O4B-C4B	-2.29	1.39	1.45
2	D	500	NDP	O4B-C4B	-2.19	1.40	1.45
2	A	501	NDP	P2B-O2X	-2.15	1.47	1.54
2	F	500	NDP	O4B-C4B	-2.15	1.40	1.45
2	D	500	NDP	P2B-O2X	-2.13	1.47	1.54
2	F	500	NDP	C3B-C4B	-2.13	1.47	1.53
2	C	501	NDP	O4B-C4B	-2.12	1.40	1.45
2	D	500	NDP	C3B-C4B	-2.12	1.47	1.53
2	C	501	NDP	C3B-C4B	-2.09	1.47	1.53
2	H	500	NDP	O4B-C4B	-2.08	1.40	1.45
2	E	501	NDP	P2B-O2X	-2.06	1.47	1.54
2	B	500	NDP	P2B-O2X	-2.06	1.47	1.54
2	H	500	NDP	C3B-C4B	-2.06	1.47	1.53
2	G	501	NDP	P2B-O3X	-2.05	1.47	1.54
2	A	501	NDP	O4B-C4B	-2.04	1.40	1.45
2	B	500	NDP	C3B-C4B	-2.03	1.47	1.53
2	B	500	NDP	P2B-O3X	-2.01	1.47	1.54
2	E	501	NDP	C3B-C4B	-2.01	1.47	1.53
2	H	500	NDP	P2B-O2X	-2.00	1.47	1.54
2	H	500	NDP	C6A-N6A	4.65	1.49	1.34
2	F	500	NDP	C6A-N6A	4.71	1.49	1.34
2	E	501	NDP	C6A-N6A	4.75	1.49	1.34
2	D	500	NDP	C6A-N6A	4.76	1.49	1.34
2	A	501	NDP	C6A-N6A	4.79	1.49	1.34
2	B	500	NDP	C6A-N6A	4.92	1.50	1.34
2	G	501	NDP	C6A-N6A	4.92	1.50	1.34
2	C	501	NDP	C6A-N6A	4.93	1.50	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	NDP	C1B-N9A-C4A	-9.55	112.54	126.94
2	B	500	NDP	N3A-C2A-N1A	-8.50	122.39	128.89
2	F	500	NDP	C1B-N9A-C4A	-8.29	114.44	126.94
2	C	501	NDP	C1B-N9A-C4A	-8.07	114.76	126.94
2	A	501	NDP	C1B-N9A-C4A	-7.83	115.12	126.94
2	H	500	NDP	N3A-C2A-N1A	-7.77	122.95	128.89
2	G	501	NDP	N3A-C2A-N1A	-7.68	123.01	128.89
2	C	501	NDP	N3A-C2A-N1A	-7.66	123.03	128.89
2	D	500	NDP	C1B-N9A-C4A	-7.65	115.40	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	NDP	C1B-N9A-C4A	-7.52	115.60	126.94
2	F	500	NDP	N3A-C2A-N1A	-7.28	123.32	128.89
2	G	501	NDP	C1B-N9A-C4A	-7.28	115.96	126.94
2	H	500	NDP	C1B-N9A-C4A	-7.26	115.99	126.94
2	D	500	NDP	N3A-C2A-N1A	-7.25	123.34	128.89
2	A	501	NDP	N3A-C2A-N1A	-7.23	123.36	128.89
2	E	501	NDP	N3A-C2A-N1A	-7.21	123.37	128.89
2	B	500	NDP	PA-O3-PN	-3.99	119.29	132.67
2	B	500	NDP	C4A-C5A-N7A	-3.38	106.37	109.48
2	D	500	NDP	O4B-C1B-C2B	-3.13	100.94	106.60
2	F	500	NDP	C4A-C5A-N7A	-3.05	106.67	109.48
2	G	501	NDP	C4A-C5A-N7A	-2.97	106.75	109.48
2	H	500	NDP	O4B-C1B-C2B	-2.96	101.25	106.60
2	D	500	NDP	P2B-O2B-C2B	-2.84	114.75	121.56
2	E	501	NDP	C4A-C5A-N7A	-2.80	106.90	109.48
2	F	500	NDP	O4B-C1B-C2B	-2.79	101.55	106.60
2	A	501	NDP	C4A-C5A-N7A	-2.79	106.91	109.48
2	A	501	NDP	PA-O3-PN	-2.76	123.43	132.67
2	D	500	NDP	C4A-C5A-N7A	-2.71	106.99	109.48
2	H	500	NDP	PA-O3-PN	-2.62	123.90	132.67
2	F	500	NDP	PA-O3-PN	-2.54	124.14	132.67
2	B	500	NDP	C4B-O4B-C1B	-2.39	107.09	109.72
2	C	501	NDP	C4A-C5A-N7A	-2.27	107.39	109.48
2	C	501	NDP	O4B-C1B-C2B	-2.27	102.50	106.60
2	C	501	NDP	PA-O3-PN	-2.26	125.09	132.67
2	H	500	NDP	P2B-O2B-C2B	-2.23	116.21	121.56
2	H	500	NDP	C4A-C5A-N7A	-2.21	107.45	109.48
2	E	501	NDP	O4B-C1B-C2B	-2.14	102.73	106.60
2	D	500	NDP	PA-O3-PN	-2.03	125.85	132.67
2	G	501	NDP	O4B-C1B-C2B	-2.01	102.97	106.60
2	H	500	NDP	O5B-C5B-C4B	2.00	116.50	109.12
2	B	500	NDP	O5B-C5B-C4B	2.24	117.36	109.12
2	C	501	NDP	O3-PA-O5B	2.42	109.35	102.94
2	A	501	NDP	O3-PA-O5B	2.54	109.68	102.94
2	D	500	NDP	O5B-C5B-C4B	2.54	118.50	109.12
2	B	500	NDP	O3-PA-O5B	2.60	109.84	102.94
2	F	500	NDP	O5B-C5B-C4B	2.62	118.76	109.12
2	F	500	NDP	O3-PA-O5B	2.68	110.05	102.94
2	H	500	NDP	O3-PA-O5B	2.78	110.32	102.94
2	D	500	NDP	O3-PA-O5B	3.39	111.93	102.94
2	E	501	NDP	O3-PA-O5B	3.56	112.37	102.94
2	G	501	NDP	O3-PA-O5B	3.95	113.41	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	2	0
2	B	500	NDP	2	0
2	C	501	NDP	2	0
2	E	501	NDP	1	0
2	F	500	NDP	3	0
2	G	501	NDP	1	0
2	H	500	NDP	4	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	482/491 (98%)	-0.17	7 (1%)	76 75	27, 38, 58, 77	0
1	B	485/491 (98%)	-0.27	9 (1%)	70 69	25, 37, 54, 73	0
1	C	485/491 (98%)	-0.27	6 (1%)	81 81	25, 37, 52, 87	0
1	D	485/491 (98%)	-0.24	7 (1%)	78 77	25, 35, 54, 79	0
1	E	483/491 (98%)	-0.28	6 (1%)	81 81	25, 34, 51, 77	0
1	F	485/491 (98%)	-0.23	6 (1%)	81 81	24, 35, 55, 78	0
1	G	484/491 (98%)	-0.30	5 (1%)	84 83	25, 34, 50, 80	0
1	H	483/491 (98%)	-0.26	6 (1%)	81 81	25, 37, 56, 74	0
All	All	3872/3928 (98%)	-0.25	52 (1%)	79 79	24, 36, 54, 87	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	491	LYS	7.7
1	D	491	LYS	6.6
1	C	491	LYS	5.9
1	E	491	LYS	5.5
1	B	491	LYS	5.5
1	A	25	PHE	5.2
1	G	491	LYS	4.9
1	B	25	PHE	4.7
1	H	491	LYS	4.7
1	C	490	LEU	4.6
1	G	490	LEU	4.5
1	A	36	LYS	4.0
1	D	321	LYS	4.0
1	E	25	PHE	3.9
1	G	25	PHE	3.9
1	C	7	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	490	LEU	3.6
1	H	22	THR	3.6
1	B	21	SER	3.4
1	F	25	PHE	3.3
1	H	25	PHE	3.2
1	F	36	LYS	3.2
1	D	25	PHE	3.1
1	E	36	LYS	3.0
1	H	36	LYS	3.0
1	G	36	LYS	2.9
1	A	490	LEU	2.9
1	D	490	LEU	2.9
1	F	7	MET	2.8
1	E	22	THR	2.7
1	H	27	VAL	2.7
1	B	490	LEU	2.6
1	E	490	LEU	2.6
1	B	22	THR	2.6
1	C	25	PHE	2.6
1	A	27	VAL	2.6
1	B	27	VAL	2.5
1	C	165	ILE	2.4
1	B	23	GLY	2.3
1	D	24	ALA	2.3
1	A	23	GLY	2.3
1	A	166	ALA	2.3
1	E	489	ALA	2.3
1	D	36	LYS	2.2
1	D	7	MET	2.2
1	A	21	SER	2.2
1	C	22	THR	2.2
1	F	21	SER	2.2
1	H	24	ALA	2.1
1	G	22	THR	2.1
1	B	26	GLN	2.1
1	B	42	ARG	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
2	NDP	F	500	31/48	0.83	0.23	2.10	39,47,56,56	31
2	NDP	D	500	31/48	0.88	0.22	2.00	34,45,53,59	31
2	NDP	E	501	31/48	0.86	0.20	1.96	38,46,55,56	31
2	NDP	H	500	31/48	0.87	0.21	1.79	41,48,57,61	31
2	NDP	G	501	31/48	0.87	0.19	1.76	34,44,55,59	31
2	NDP	B	500	31/48	0.91	0.17	1.02	38,46,53,54	19
2	NDP	A	501	31/48	0.84	0.20	0.88	40,51,61,65	31
2	NDP	C	501	31/48	0.89	0.17	0.76	34,45,56,62	31
3	NI	C	502	1/1	0.98	0.12	-	43,43,43,43	0
3	NI	A	502	1/1	0.98	0.14	-	44,44,44,44	0
3	NI	G	502	1/1	0.98	0.14	-	44,44,44,44	0
3	NI	E	502	1/1	0.98	0.15	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.