Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:44 PM GMT

PDB ID	:	4PT3
Title	:	NADPH complex structure of Aldehyde Dehydrogenase from Bacillus cereus
Authors	:	Ngo, H.P.T.; Hong, S.H.; Oh, D.K.; Kang, L.W.
Deposited on	:	2014-03-10
Resolution	:	2.00 Å(reported)

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

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

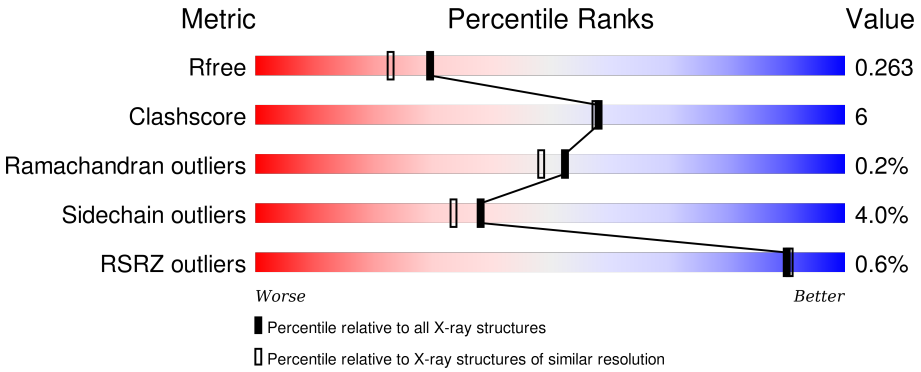
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	87% 11%
1	B	494	85% 13%
1	C	494	% 83% 15%
1	D	494	81% 17%

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	NA	D	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15905 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.

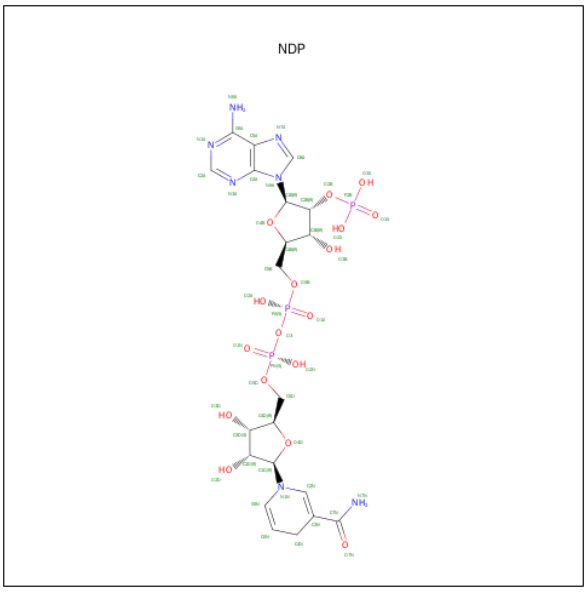
- Molecule 1 is a protein called Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	C	488	Total	C	N	O	S	0	0	0
			3768	2400	626	728	14			
1	D	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		
2	D	1	Total	Na	0	0
			1	1		
2	C	2	Total	Na	0	0
			2	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

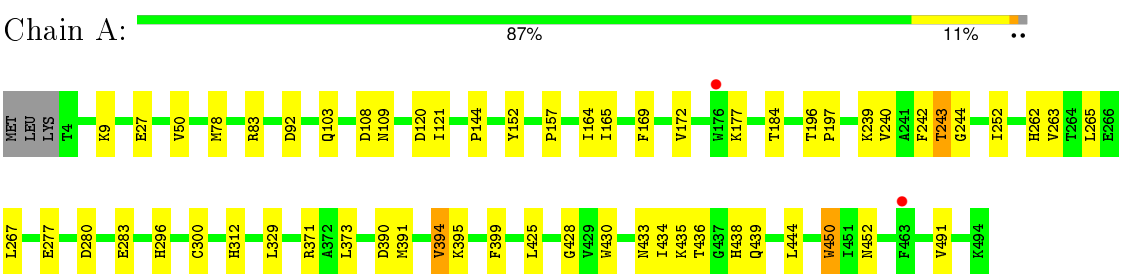
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	167	Total	O	0	0
			167	167		
4	C	110	Total	O	0	0
			110	110		
4	D	136	Total	O	0	0
			136	136		

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.

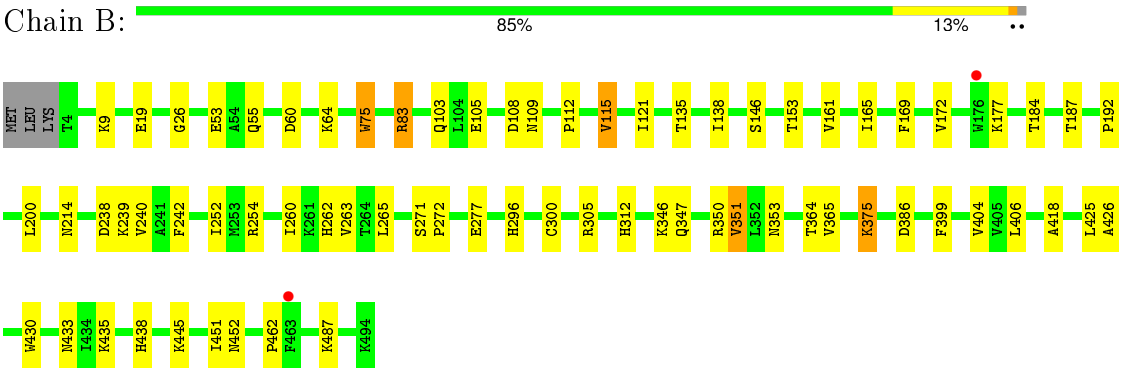
- Molecule 1: Aldehyde dehydrogenase

Chain A:



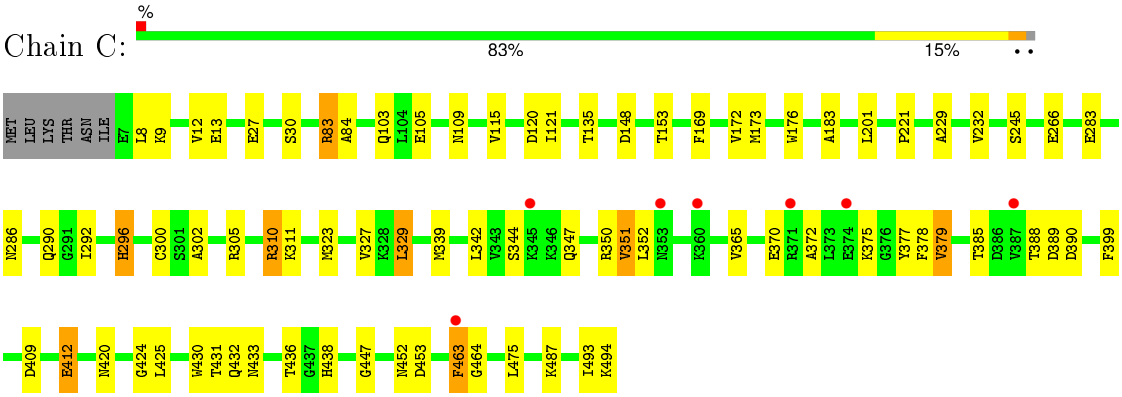
- Molecule 1: Aldehyde dehydrogenase

Chain B:



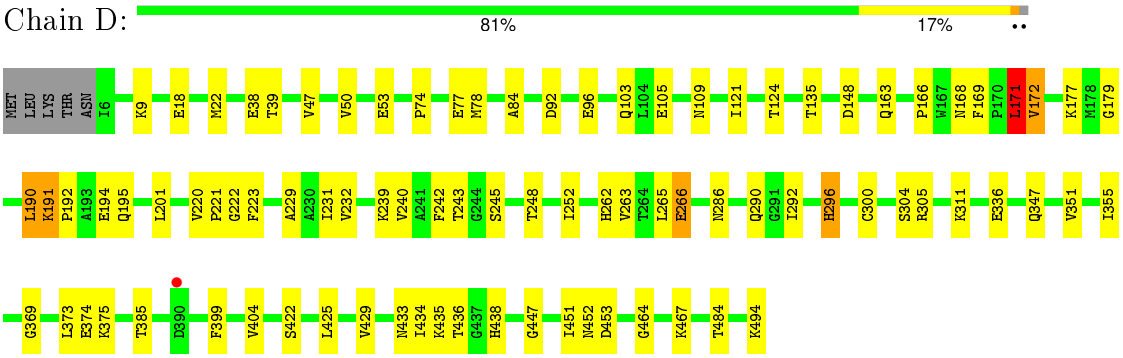
- Molecule 1: Aldehyde dehydrogenase

Chain C:



- Molecule 1: Aldehyde dehydrogenase

Chain D:


81%
17%
MET LEU LYS THR ASN I6 K9 E18 M22 E38 T39 V47 V50 E53 P74 E77 M78 A84 D92 E96 Q103 L104 E105 N109 I121 T124 T135 D148 Q163 P166 W167 N168 F169 P170 L171 V172 K177 M178 G179
L190 K191 P192 A193 E194 Q195 L201 V220 P221 G222 F223 A229 A230 I231 V232 K239 V240 A241 F242 T243 G244 S245 T248 I252 H262 V263 T264 L265 E266 N286 Q290 G291 I292 H296 C300 S304 R305 K311 E336 Q347 V351 I355
G369 L373 E374 K375 T385 D390 F399 V404 S422 L425 V429 N433 I434 K435 T436 G437 H438 G447 I451 N452 D453 G464 K467 T484 K494

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.89Å 93.94Å 144.93Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	47.88 – 2.00 47.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.88-2.00) 99.9 (47.88-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.91 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.260 0.213 , 0.263	Depositor DCC
R_{free} test set	7525 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 150310 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15905	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: NDP, NA

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	1.03	1/3870 (0.0%)	0.93	2/5250 (0.0%)
1	B	1.00	2/3870 (0.1%)	0.94	6/5250 (0.1%)
1	C	0.83	0/3847	0.85	2/5218 (0.0%)
1	D	0.89	2/3855 (0.1%)	0.88	5/5229 (0.1%)
All	All	0.94	5/15442 (0.0%)	0.90	15/20947 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	GLY	N-CA	6.56	1.55	1.46
1	A	450	TRP	CB-CG	6.25	1.61	1.50
1	B	75	TRP	CG-CD1	-5.34	1.29	1.36
1	B	462	PRO	CA-C	-5.28	1.42	1.52
1	D	53	GLU	CD-OE2	-5.09	1.20	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	305	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	305	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	108	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	148	ASP	CB-CG-OD1	-5.98	112.91	118.30
1	B	254	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	148	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	83	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	238	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	190	LEU	CA-CB-CG	5.49	127.93	115.30
1	C	305	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	305	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	D	171	LEU	CB-CG-CD2	5.12	119.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	453	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	108	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3791	0	3739	43	0
1	B	3791	0	3739	47	0
1	C	3768	0	3716	50	0
1	D	3776	0	3727	50	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	1	0
3	A	48	0	26	1	0
3	B	48	0	26	1	0
3	C	48	0	26	1	0
3	D	48	0	26	5	0
4	A	167	0	0	3	0
4	B	167	0	0	4	0
4	C	110	0	0	3	0
4	D	136	0	0	5	0
All	All	15905	0	15025	178	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 6.

All (178) 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:83:ARG:HD3	4:B:722:HOH:O	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:THR:OG1	4:D:605:HOH:O	1.88	0.91
1:C:388:THR:OG1	1:C:390:ASP:OD1	1.95	0.82
1:B:9:LYS:H	1:B:103:GLN:HE22	1.24	0.82
2:D:501:NA:NA	4:D:605:HOH:O	1.52	0.81
1:C:300:CYS:SG	1:C:425:LEU:HD21	2.23	0.78
1:B:438:HIS:HE1	1:C:438:HIS:HE1	1.34	0.76
1:A:9:LYS:H	1:A:103:GLN:HE22	1.33	0.75
1:A:239:LYS:HZ3	1:A:262:HIS:HD2	1.32	0.74
1:D:467:LYS:O	4:D:622:HOH:O	2.05	0.74
1:A:243:THR:HG21	4:A:729:HOH:O	1.88	0.73
1:A:300:CYS:SG	1:A:425:LEU:HD21	2.29	0.72
1:A:391:MET:HB2	1:A:394:VAL:HG13	1.73	0.70
1:D:9:LYS:H	1:D:103:GLN:HE22	1.39	0.69
1:B:19:GLU:OE2	4:B:717:HOH:O	2.09	0.69
1:A:433:ASN:HD22	1:A:436:THR:H	1.44	0.66
1:B:239:LYS:HZ3	1:B:262:HIS:HD2	1.43	0.66
1:D:300:CYS:HB3	3:D:502:NDP:H72N	1.60	0.65
1:C:286:ASN:O	1:C:290:GLN:HG2	1.98	0.64
1:C:169:PHE:HB3	1:C:172:VAL:HG22	1.80	0.64
1:B:75:TRP:CH2	1:B:83:ARG:HD2	2.33	0.64
1:C:9:LYS:H	1:C:103:GLN:HE22	1.46	0.62
1:B:438:HIS:HE1	1:C:438:HIS:CE1	2.18	0.62
1:D:229:ALA:HA	1:D:232:VAL:HG12	1.82	0.61
1:C:173:MET:HG2	1:C:176:TRP:CZ3	2.35	0.61
1:C:310:ARG:HD2	1:C:409:ASP:OD2	2.00	0.61
1:A:438:HIS:HE1	1:D:438:HIS:HE1	1.48	0.61
1:A:438:HIS:CE1	1:D:438:HIS:HE1	2.18	0.61
1:D:172:VAL:HG13	4:D:662:HOH:O	2.01	0.61
1:D:201:LEU:HD11	1:D:221:PRO:HG3	1.84	0.60
1:B:300:CYS:SG	1:B:425:LEU:HD21	2.41	0.60
1:C:84:ALA:HB2	1:C:135:THR:OG1	2.02	0.59
1:D:292:ILE:HD13	1:D:304:SER:HA	1.84	0.59
1:B:165:ILE:HD11	4:B:623:HOH:O	2.02	0.59
1:A:239:LYS:NZ	1:A:262:HIS:HD2	2.01	0.58
1:C:388:THR:O	1:C:390:ASP:N	2.37	0.58
1:D:245:SER:HB3	3:D:502:NDP:O4D	2.04	0.57
1:D:347:GLN:O	1:D:351:VAL:HG13	2.05	0.57
1:B:438:HIS:CE1	1:C:438:HIS:HE1	2.20	0.57
1:C:83:ARG:HH11	1:C:83:ARG:HG3	1.69	0.57
1:C:201:LEU:HD11	1:C:221:PRO:HG3	1.87	0.57
1:C:412:GLU:CD	1:C:412:GLU:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ALA:HB2	1:D:135:THR:OG1	2.06	0.56
1:D:300:CYS:SG	1:D:425:LEU:HD21	2.46	0.55
1:D:195:GLN:OE1	3:D:502:NDP:O1X	2.25	0.55
1:D:433:ASN:HD22	1:D:436:THR:H	1.54	0.55
1:D:191:LYS:NZ	3:D:502:NDP:O2X	2.41	0.54
1:A:300:CYS:HG	1:A:425:LEU:HD21	1.73	0.53
1:A:312:HIS:HD2	4:A:739:HOH:O	1.92	0.53
1:D:286:ASN:O	1:D:290:GLN:HG2	2.09	0.53
1:B:272:PRO:HG3	1:B:418:ALA:HB1	1.89	0.53
1:C:120:ASP:O	1:C:172:VAL:HG12	2.09	0.52
1:D:262:HIS:HE1	4:D:716:HOH:O	1.92	0.51
1:C:352:LEU:HD21	1:C:370:GLU:O	2.11	0.51
1:A:277:GLU:O	1:A:312:HIS:HE1	1.92	0.51
1:D:38:GLU:OE1	1:D:47:VAL:HG21	2.10	0.51
1:B:404:VAL:HG23	1:B:406:LEU:HD11	1.92	0.51
1:B:364:THR:OG1	1:B:386:ASP:OD2	2.20	0.50
1:A:280:ASP:OD1	1:A:283:GLU:HG2	2.11	0.50
1:A:435:LYS:HG2	1:C:493:ILE:HA	1.93	0.50
1:C:433:ASN:HD22	1:C:436:THR:H	1.59	0.50
1:D:194:GLU:OE2	1:D:223:PHE:CE1	2.64	0.50
1:C:266:GLU:HB3	4:C:685:HOH:O	2.12	0.49
1:D:239:LYS:HD3	1:D:240:VAL:N	2.27	0.49
1:C:12:VAL:HG21	1:C:103:GLN:HE21	1.76	0.49
1:D:355:ILE:HD13	1:D:369:GLY:HA2	1.93	0.49
1:D:447:GLY:HA3	1:D:464:GLY:O	2.13	0.49
1:B:445:LYS:CE	4:B:618:HOH:O	2.61	0.49
1:A:263:VAL:HG12	1:A:265:LEU:HG	1.95	0.49
1:D:263:VAL:HG12	1:D:265:LEU:HG	1.95	0.49
1:D:242:PHE:CG	1:D:252:ILE:HD13	2.48	0.49
1:A:239:LYS:HZ3	1:A:262:HIS:CD2	2.22	0.48
1:A:165:ILE:HD11	1:A:177:LYS:HG3	1.95	0.48
1:A:263:VAL:CG1	1:A:265:LEU:HG	2.43	0.48
1:C:296:HIS:CD2	1:C:339:MET:HG3	2.48	0.48
1:B:375:LYS:HD2	1:B:375:LYS:N	2.28	0.48
1:B:239:LYS:NZ	1:B:262:HIS:HD2	2.11	0.48
1:D:194:GLU:HB3	1:D:222:GLY:O	2.14	0.48
1:A:92:ASP:OD2	4:A:725:HOH:O	2.20	0.48
1:A:169:PHE:HB3	1:A:172:VAL:CG1	2.44	0.47
1:C:229:ALA:HA	1:C:232:VAL:HG12	1.95	0.47
1:C:172:VAL:HG13	4:C:652:HOH:O	2.13	0.47
1:B:242:PHE:CD1	1:B:252:ILE:CD1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:HG22	1:B:187:THR:O	2.14	0.47
1:B:165:ILE:HG22	1:B:177:LYS:HE2	1.97	0.47
1:D:191:LYS:HB2	1:D:231:ILE:CD1	2.45	0.47
1:A:165:ILE:CD1	1:A:177:LYS:HG3	2.45	0.47
1:B:271:SER:HB3	1:B:426:ALA:O	2.15	0.47
1:B:83:ARG:HG2	1:B:135:THR:HG21	1.97	0.46
1:B:75:TRP:CZ2	1:B:83:ARG:HD2	2.50	0.46
1:D:239:LYS:HZ3	1:D:262:HIS:HD2	1.63	0.46
1:B:60:ASP:OD2	1:B:64:LYS:NZ	2.49	0.46
1:B:438:HIS:CE1	1:C:438:HIS:CE1	3.00	0.45
1:D:300:CYS:HB3	3:D:502:NDP:N7N	2.30	0.45
1:A:164:ILE:HD13	3:A:503:NDP:H2A	1.99	0.45
1:C:352:LEU:CD2	1:C:370:GLU:O	2.64	0.45
1:D:163:GLN:NE2	1:D:177:LYS:HB3	2.32	0.45
1:D:92:ASP:O	1:D:96:GLU:HG3	2.16	0.45
1:D:242:PHE:CD1	1:D:252:ILE:HD13	2.51	0.45
1:B:263:VAL:HG12	1:B:265:LEU:HG	1.97	0.45
1:A:428:GLY:HA2	1:A:450:TRP:O	2.17	0.45
1:B:300:CYS:HB3	3:B:503:NDP:O7N	2.17	0.45
1:B:112:PRO:HB2	1:B:115:VAL:HG13	1.97	0.45
1:D:74:PRO:O	1:D:78:MET:HB2	2.17	0.45
1:B:169:PHE:HB3	1:B:172:VAL:CG1	2.47	0.45
1:C:148:ASP:HB3	1:C:494:LYS:HG3	1.99	0.44
1:D:191:LYS:HG2	1:D:220:VAL:O	2.17	0.44
1:D:296:HIS:N	1:D:296:HIS:CD2	2.83	0.44
1:C:430:TRP:CE3	1:C:452:ASN:HA	2.53	0.44
1:D:169:PHE:HB3	1:D:172:VAL:HG22	1.99	0.44
1:A:240:VAL:CG1	1:A:263:VAL:HG22	2.47	0.44
1:A:244:GLY:O	1:A:267:LEU:HA	2.17	0.44
1:A:491:VAL:HG22	1:B:451:ILE:HD12	2.00	0.44
1:C:365:VAL:O	1:C:365:VAL:CG2	2.66	0.44
1:B:153:THR:HA	1:B:487:LYS:O	2.17	0.44
1:A:395:LYS:HB2	1:A:395:LYS:HE3	1.86	0.44
1:A:239:LYS:NZ	1:A:262:HIS:CD2	2.83	0.44
1:D:194:GLU:OE2	1:D:223:PHE:HE1	2.01	0.44
1:D:168:ASN:N	1:D:168:ASN:OD1	2.49	0.43
1:C:372:ALA:HB3	1:C:378:PHE:HB3	2.00	0.43
1:C:327:VAL:HG11	1:C:339:MET:HE3	1.99	0.43
1:C:169:PHE:HB3	1:C:172:VAL:CG2	2.46	0.43
1:C:176:TRP:CD1	1:C:475:LEU:HD21	2.54	0.43
1:C:84:ALA:HB2	1:C:135:THR:HG1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:THR:HA	1:D:266:GLU:O	2.18	0.43
1:D:374:GLU:OE1	1:D:374:GLU:HA	2.19	0.43
1:B:425:LEU:HD12	1:B:425:LEU:HA	1.89	0.43
1:B:53:GLU:CD	1:B:55:GLN:HE22	2.22	0.43
1:D:245:SER:HG	1:D:248:THR:HG1	1.63	0.43
1:A:435:LYS:O	1:A:439:GLN:HG3	2.19	0.43
1:A:157:PRO:HB3	1:A:184:THR:O	2.18	0.43
1:B:239:LYS:HD3	1:B:240:VAL:N	2.34	0.43
1:C:135:THR:HG22	1:C:183:ALA:HA	2.01	0.43
1:C:300:CYS:SG	1:C:463:PHE:HZ	2.41	0.42
1:C:245:SER:HB3	3:C:503:NDP:O4D	2.18	0.42
1:C:365:VAL:O	1:C:365:VAL:HG23	2.19	0.42
1:B:430:TRP:HA	1:B:452:ASN:OD1	2.19	0.42
1:C:323:MET:O	1:C:327:VAL:HG23	2.19	0.42
1:B:277:GLU:O	1:B:312:HIS:HE1	2.01	0.42
1:A:430:TRP:HA	1:A:452:ASN:OD1	2.19	0.42
1:D:22:MET:CG	1:D:221:PRO:HD2	2.50	0.42
1:A:444:LEU:O	1:B:487:LYS:NZ	2.51	0.42
1:D:451:ILE:O	1:D:452:ASN:HB2	2.18	0.42
1:B:433:ASN:HA	1:C:432:GLN:O	2.20	0.42
1:A:196:THR:N	1:A:197:PRO:CD	2.83	0.42
1:C:153:THR:HA	1:C:487:LYS:O	2.20	0.42
1:A:242:PHE:CD1	1:A:252:ILE:CD1	3.03	0.42
1:A:78:MET:SD	1:A:83:ARG:HG2	2.60	0.42
1:D:191:LYS:HD3	1:D:192:PRO:O	2.18	0.41
1:A:390:ASP:O	1:A:395:LYS:HE2	2.19	0.41
1:D:124:THR:HG21	1:D:171:LEU:HD13	2.01	0.41
1:B:346:LYS:O	1:B:350:ARG:HG3	2.20	0.41
1:B:26:GLY:HA3	1:B:214:ASN:HD22	1.86	0.41
1:C:342:LEU:HD22	1:C:379:VAL:CG1	2.50	0.41
1:C:329:LEU:HD12	1:C:378:PHE:HD2	1.85	0.41
1:C:420:ASN:HB3	4:C:695:HOH:O	2.20	0.41
1:A:434:ILE:HA	1:D:434:ILE:HB	2.02	0.41
1:A:9:LYS:H	1:A:103:GLN:NE2	2.10	0.41
1:D:163:GLN:HB2	1:D:190:LEU:HD23	2.01	0.41
1:B:192:PRO:HG3	1:B:200:LEU:HD23	2.02	0.41
1:C:292:ILE:HD12	1:C:302:ALA:HB1	2.02	0.41
1:A:27:GLU:HA	1:A:27:GLU:OE2	2.19	0.41
1:B:260:ILE:O	1:B:260:ILE:HG22	2.20	0.41
1:C:347:GLN:O	1:C:351:VAL:HG13	2.21	0.41
1:A:83:ARG:HB3	1:A:83:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLY:HA3	1:C:464:GLY:O	2.20	0.41
1:C:412:GLU:N	1:C:412:GLU:CD	2.72	0.41
1:D:433:ASN:HD21	1:D:435:LYS:HB2	1.85	0.41
1:C:8:LEU:HB3	1:C:13:GLU:HG3	2.02	0.41
1:A:144:PRO:HG2	1:A:144:PRO:O	2.21	0.41
1:B:347:GLN:O	1:B:351:VAL:HG13	2.21	0.40
1:C:344:SER:HA	1:C:377:TYR:CD2	2.56	0.40
1:B:435:LYS:HE2	1:D:494:LYS:O	2.21	0.40
1:B:26:GLY:HA3	1:B:214:ASN:ND2	2.37	0.40
1:B:138:ILE:HD13	1:B:184:THR:HG22	2.01	0.40
1:A:152:TYR:OH	1:B:438:HIS:HD2	2.04	0.40
1:A:177:LYS:HZ1	1:A:243:THR:CG2	2.34	0.40
1:B:375:LYS:CD	1:B:375:LYS:N	2.85	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	489/494 (99%)	475 (97%)	14 (3%)	0	100	100
1	B	489/494 (99%)	468 (96%)	21 (4%)	0	100	100
1	C	486/494 (98%)	457 (94%)	26 (5%)	3 (1%)	30	22
1	D	487/494 (99%)	462 (95%)	24 (5%)	1 (0%)	52	48
All	All	1951/1976 (99%)	1862 (95%)	85 (4%)	4 (0%)	52	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	389	ASP
1	C	310	ARG

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Mol	Chain	Res	Type
1	D	166	PRO
1	C	424	GLY

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	398/401 (99%)	388 (98%)	10 (2%)	55	55
1	B	398/401 (99%)	387 (97%)	11 (3%)	51	50
1	C	395/401 (98%)	375 (95%)	20 (5%)	29	23
1	D	396/401 (99%)	374 (94%)	22 (6%)	26	20
All	All	1587/1604 (99%)	1524 (96%)	63 (4%)	38	33

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	109	ASN
1	A	121	ILE
1	A	243	THR
1	A	296	HIS
1	A	329	LEU
1	A	371	ARG
1	A	373	LEU
1	A	394	VAL
1	A	399	PHE
1	B	105	GLU
1	B	109	ASN
1	B	115	VAL
1	B	121	ILE
1	B	146	SER
1	B	296	HIS
1	B	351	VAL
1	B	353	ASN
1	B	365	VAL

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Mol	Chain	Res	Type
1	B	375	LYS
1	B	399	PHE
1	C	27	GLU
1	C	30	SER
1	C	83	ARG
1	C	105	GLU
1	C	109	ASN
1	C	115	VAL
1	C	121	ILE
1	C	283	GLU
1	C	296	HIS
1	C	311	LYS
1	C	329	LEU
1	C	350	ARG
1	C	351	VAL
1	C	375	LYS
1	C	379	VAL
1	C	385	THR
1	C	399	PHE
1	C	412	GLU
1	C	431	THR
1	C	463	PHE
1	D	18	GLU
1	D	50	VAL
1	D	77	GLU
1	D	105	GLU
1	D	109	ASN
1	D	121	ILE
1	D	171	LEU
1	D	172	VAL
1	D	191	LYS
1	D	266	GLU
1	D	296	HIS
1	D	311	LYS
1	D	336	GLU
1	D	373	LEU
1	D	375	LYS
1	D	385	THR
1	D	399	PHE
1	D	404	VAL
1	D	422	SER
1	D	429	VAL

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Mol	Chain	Res	Type
1	D	453	ASP
1	D	484	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	103	GLN
1	A	114	GLN
1	A	214	ASN
1	A	262	HIS
1	A	312	HIS
1	A	325	ASN
1	A	326	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	482	ASN
1	B	55	GLN
1	B	103	GLN
1	B	114	GLN
1	B	214	ASN
1	B	262	HIS
1	B	312	HIS
1	B	325	ASN
1	B	326	ASN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	482	ASN
1	C	103	GLN
1	C	114	GLN
1	C	214	ASN
1	C	262	HIS
1	C	325	ASN
1	C	326	ASN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	442	ASN
1	C	482	ASN
1	D	103	GLN

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Mol	Chain	Res	Type
1	D	114	GLN
1	D	214	ASN
1	D	262	HIS
1	D	312	HIS
1	D	325	ASN
1	D	326	ASN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	442	ASN
1	D	482	ASN

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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	NDP	A	503	-	42,52,52	1.03	4 (9%)	55,80,80	1.69	9 (16%)
3	NDP	B	503	-	42,52,52	1.00	2 (4%)	55,80,80	1.64	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NDP	C	503	-	42,52,52	1.50	9 (21%)	55,80,80	1.57	8 (14%)
3	NDP	D	502	-	42,52,52	1.19	5 (11%)	55,80,80	1.68	9 (16%)

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	NDP	A	503	-	-	0/30/77/77	0/5/5/5
3	NDP	B	503	-	-	0/30/77/77	0/5/5/5
3	NDP	C	503	-	-	0/30/77/77	0/5/5/5
3	NDP	D	502	-	-	0/30/77/77	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	NDP	P2B-O2X	-2.86	1.44	1.54
3	C	503	NDP	P2B-O3X	-2.74	1.44	1.54
3	C	503	NDP	PA-O2A	-2.56	1.44	1.54
3	C	503	NDP	C4A-N3A	-2.53	1.31	1.35
3	C	503	NDP	C5A-N7A	-2.33	1.31	1.39
3	C	503	NDP	O4D-C4D	-2.15	1.40	1.45
3	C	503	NDP	C2N-C3N	2.05	1.39	1.34
3	A	503	NDP	O4B-C1B	2.34	1.44	1.41
3	D	502	NDP	O4B-C1B	2.35	1.44	1.41
3	A	503	NDP	C2N-C3N	2.51	1.40	1.34
3	A	503	NDP	C5A-C4A	2.66	1.46	1.40
3	C	503	NDP	C5A-C4A	2.75	1.46	1.40
3	C	503	NDP	C6N-C5N	2.80	1.38	1.33
3	D	502	NDP	C2A-N3A	2.93	1.37	1.32
3	A	503	NDP	C6N-C5N	2.98	1.39	1.33
3	D	502	NDP	C2N-C3N	2.99	1.42	1.34
3	B	503	NDP	C6N-C5N	3.01	1.39	1.33
3	D	502	NDP	C6N-C5N	3.24	1.39	1.33
3	D	502	NDP	C5A-C4A	3.28	1.47	1.40
3	B	503	NDP	C5A-C4A	3.59	1.48	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	NDP	N3A-C2A-N1A	-7.00	123.54	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	NDP	N3A-C2A-N1A	-6.85	123.65	128.89
3	A	503	NDP	N3A-C2A-N1A	-6.85	123.65	128.89
3	C	503	NDP	N3A-C2A-N1A	-5.89	124.38	128.89
3	C	503	NDP	C2D-C1D-N1N	-3.76	103.19	113.34
3	A	503	NDP	C1B-N9A-C4A	-3.56	121.57	126.94
3	B	503	NDP	C1B-N9A-C4A	-3.50	121.66	126.94
3	B	503	NDP	C2D-C1D-N1N	-3.34	104.33	113.34
3	D	502	NDP	C4A-C5A-N7A	-3.31	106.44	109.48
3	A	503	NDP	C4A-C5A-N7A	-3.26	106.48	109.48
3	D	502	NDP	C2D-C1D-N1N	-3.17	104.77	113.34
3	A	503	NDP	C2D-C1D-N1N	-3.14	104.85	113.34
3	B	503	NDP	C4A-C5A-N7A	-3.09	106.64	109.48
3	D	502	NDP	C1B-N9A-C4A	-2.52	123.14	126.94
3	D	502	NDP	PN-O3-PA	-2.28	126.32	132.73
3	B	503	NDP	C1D-N1N-C2N	-2.25	116.99	120.91
3	C	503	NDP	C4A-C5A-N7A	-2.17	107.48	109.48
3	C	503	NDP	PN-O3-PA	-2.04	127.01	132.73
3	C	503	NDP	P2B-O2B-C2B	2.00	126.36	121.56
3	A	503	NDP	C6N-N1N-C2N	2.02	123.71	118.52
3	A	503	NDP	O2N-PN-O1N	2.02	123.47	112.53
3	D	502	NDP	O4D-C4D-C5D	2.23	117.28	109.32
3	B	503	NDP	O4D-C1D-N1N	2.34	113.00	108.07
3	B	503	NDP	C2A-N1A-C6A	2.42	123.09	118.77
3	D	502	NDP	O2X-P2B-O1X	2.57	118.86	110.58
3	C	503	NDP	O2X-P2B-O1X	2.98	120.18	110.58
3	B	503	NDP	O4B-C1B-N9A	3.08	114.54	108.10
3	A	503	NDP	O3X-P2B-O2X	3.20	119.57	107.38
3	A	503	NDP	O4D-C1D-N1N	3.24	114.92	108.07
3	D	502	NDP	C4B-O4B-C1B	3.30	113.34	109.72
3	C	503	NDP	C4B-O4B-C1B	3.59	113.67	109.72
3	A	503	NDP	O4B-C1B-N9A	3.65	115.74	108.10
3	D	502	NDP	O4D-C1D-N1N	4.05	116.62	108.07
3	C	503	NDP	O4D-C1D-N1N	4.24	117.02	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NDP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	NDP	1	0
3	C	503	NDP	1	0
3	D	502	NDP	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	491/494 (99%)	-0.30	2 (0%)	93	93	14, 26, 40, 55	0
1	B	491/494 (99%)	-0.14	2 (0%)	93	93	15, 27, 43, 58	0
1	C	488/494 (98%)	0.05	7 (1%)	78	78	19, 34, 56, 72	0
1	D	489/494 (98%)	-0.06	1 (0%)	95	95	18, 33, 50, 63	0
All	All	1959/1976 (99%)	-0.12	12 (0%)	90	90	14, 30, 49, 72	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	LYS	3.7
1	B	176	TRP	3.3
1	C	387	VAL	3.3
1	B	463	PHE	3.0
1	C	345	LYS	2.5
1	C	374	GLU	2.5
1	C	463	PHE	2.4
1	C	353	ASN	2.3
1	C	371	ARG	2.3
1	A	176	TRP	2.2
1	D	390	ASP	2.1
1	A	463	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	NA	D	501	1/1	0.92	0.15	2.84	39,39,39,39	0
3	NDP	A	503	48/48	0.90	0.14	1.17	37,45,50,51	0
3	NDP	D	502	48/48	0.91	0.13	0.73	41,55,64,66	0
3	NDP	B	503	48/48	0.93	0.12	0.16	30,39,42,49	0
3	NDP	C	503	48/48	0.92	0.13	-0.07	41,49,54,60	0
2	NA	A	501	1/1	0.97	0.08	-0.42	22,22,22,22	0
2	NA	B	501	1/1	0.95	0.10	-0.45	26,26,26,26	0
2	NA	C	502	1/1	0.90	0.07	-1.80	38,38,38,38	0
2	NA	C	501	1/1	0.97	0.07	-2.73	37,37,37,37	0
2	NA	A	502	1/1	0.95	0.05	-3.38	30,30,30,30	0
2	NA	B	502	1/1	0.94	0.06	-3.39	31,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.