



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YS4
Title : Structure of Aspartate-Semialdehyde Dehydrogenase from *Methanococcus jannaschii*
Authors : Faehnle, C.R.; Ohren, J.F.; Viola, R.E.
Deposited on : 2005-02-07
Resolution : 2.29 Å(reported)

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

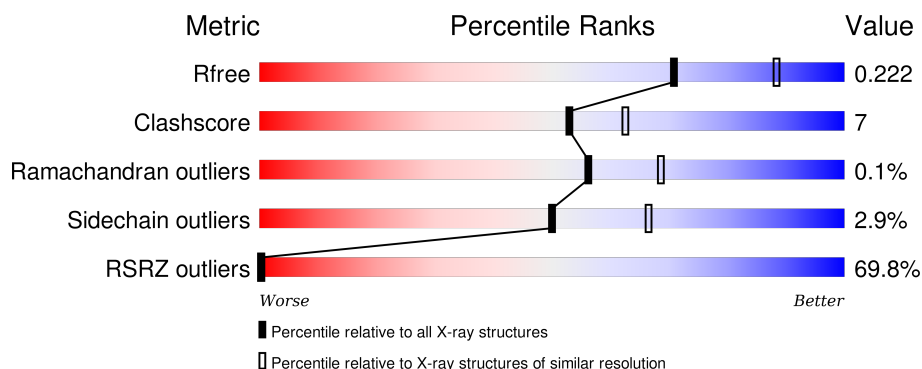
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	
1	B	354	

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	NAP	A	900	X	-	-	-
2	NAP	B	901	X	-	-	X
3	MLA	A	904	-	-	-	X
3	MLA	B	902	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6003 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 Aspartate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2725	1738	454	519	4	10			
1	B	348	Total	C	N	O	S	Se	0	0	0
			2725	1738	454	519	4	10			

There are 20 discrepancies between the modelled and reference sequences:

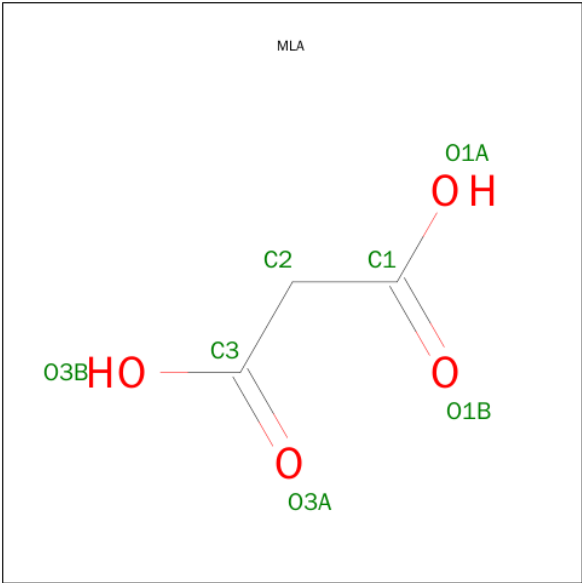
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	33	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	69	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	170	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	183	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	197	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	214	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	271	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	310	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	7	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	33	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	69	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	119	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	170	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	183	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	197	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	214	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	271	MSE	MET	MODIFIED RESIDUE	UNP Q57658
B	310	MSE	MET	MODIFIED RESIDUE	UNP Q57658

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	3	4		
3	A	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		

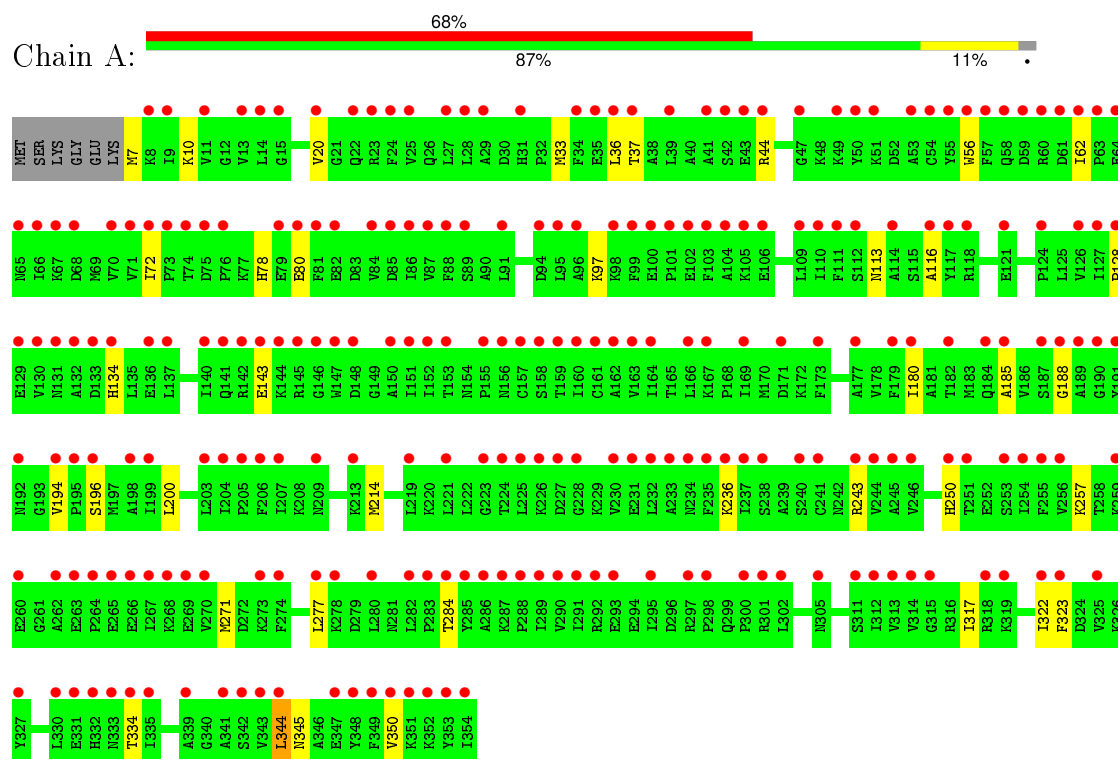
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	223	Total	O	0	0
			223	223		

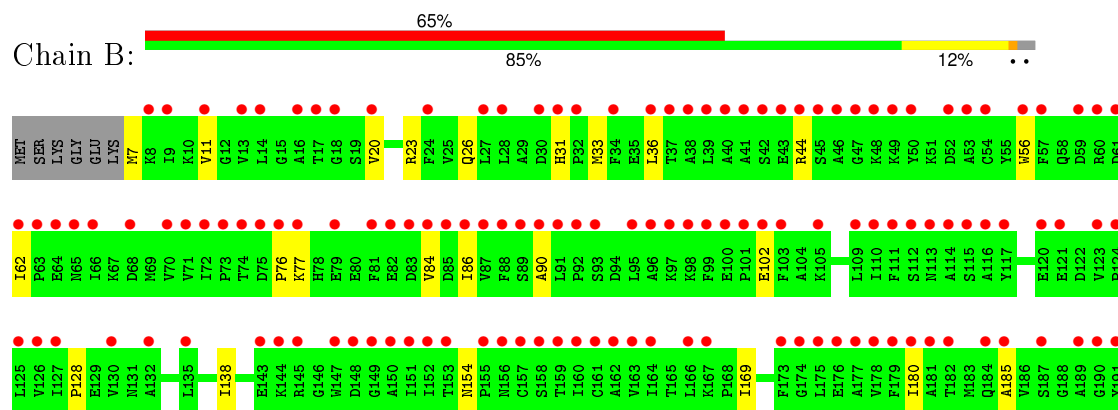
3 Residue-property plots

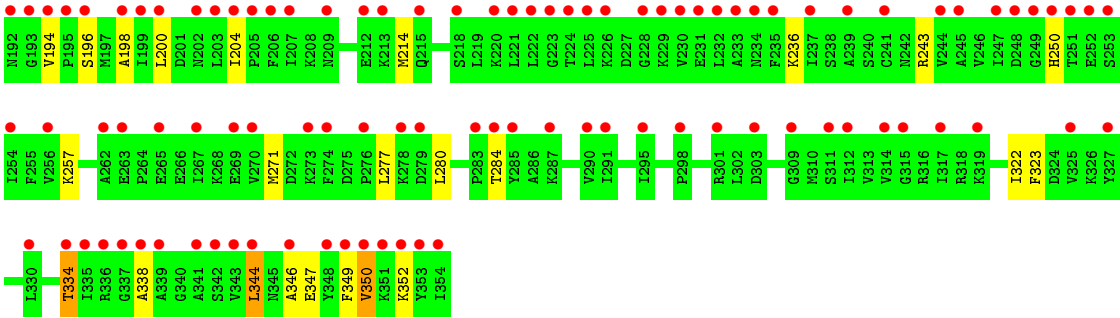
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 1: Aspartate-semialdehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.25Å 95.25Å 297.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 2.29 39.15 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.22-2.29) 99.2 (39.15-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.191 , 0.221 0.196 , 0.222	Depositor DCC
R_{free} test set	3145 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62083 reflections	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	6003	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.35	0/2767	0.51	0/3722
1	B	0.35	0/2767	0.51	0/3722
All	All	0.35	0/5534	0.51	0/7444

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	2725	0	2756	28	0
1	B	2725	0	2756	41	0
2	A	48	0	25	11	0
2	B	48	0	25	9	0
3	A	14	0	4	3	0
3	B	14	0	4	1	0
4	A	206	0	0	3	0
4	B	223	0	0	2	0
All	All	6003	0	5570	73	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 (73) 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:23:ARG:HG3	1:B:334:THR:HG23	1.37	1.02
1:B:23:ARG:HG3	1:B:334:THR:CG2	1.90	1.00
1:B:20:VAL:HG23	4:B:1051:HOH:O	1.73	0.88
1:A:188:GLY:HA2	2:A:900:NAP:C7N	2.03	0.88
1:A:334:THR:HG22	2:A:900:NAP:O7N	1.77	0.84
1:A:188:GLY:HA2	2:A:900:NAP:N7N	1.97	0.80
1:B:20:VAL:HG22	2:B:901:NAP:N7N	1.98	0.79
1:B:23:ARG:HH21	1:B:26:GLN:HE22	1.37	0.70
1:B:194:VAL:HG21	1:B:243:ARG:HD3	1.73	0.70
1:B:198:ALA:HB1	1:B:204:ILE:HD11	1.75	0.69
1:B:334:THR:HA	2:B:901:NAP:O7N	1.93	0.68
1:B:20:VAL:CG2	2:B:901:NAP:H2N	2.25	0.67
1:B:20:VAL:HG22	2:B:901:NAP:H71N	1.61	0.64
1:B:185:ALA:H	1:B:250:HIS:HD2	1.47	0.63
1:A:185:ALA:H	1:A:250:HIS:HD2	1.48	0.62
2:A:900:NAP:H5N	3:A:904:MLA:O3A	2.00	0.62
1:B:185:ALA:H	1:B:250:HIS:CD2	2.18	0.62
1:B:169:ILE:HD11	1:B:271:MSE:HE3	1.82	0.62
1:B:138:ILE:HD13	1:B:349:PHE:HE2	1.65	0.62
1:B:138:ILE:HD13	1:B:349:PHE:CE2	2.36	0.60
1:B:31:HIS:HD2	1:B:33:MSE:H	1.48	0.60
1:B:20:VAL:CG2	2:B:901:NAP:C2N	2.80	0.59
1:A:128:PRO:HB2	1:A:277:LEU:HD11	1.84	0.59
1:B:76:PRO:HG3	1:B:102:GLU:HB3	1.85	0.58
1:A:271:MSE:HE1	1:A:317:ILE:HD11	1.87	0.56
1:A:194:VAL:HG21	1:A:243:ARG:HD3	1.86	0.55
1:B:20:VAL:HG22	2:B:901:NAP:C2N	2.37	0.55
1:A:236:LYS:HB3	1:B:322:ILE:HG12	1.88	0.54
1:A:185:ALA:H	1:A:250:HIS:CD2	2.26	0.54
1:A:128:PRO:HG2	1:A:344:LEU:HD13	1.91	0.52
1:A:20:VAL:HG23	2:A:900:NAP:C2N	2.39	0.52
1:B:20:VAL:HG22	2:B:901:NAP:C7N	2.40	0.52
1:B:128:PRO:HB2	1:B:277:LEU:HD11	1.92	0.51
1:B:20:VAL:HG22	2:B:901:NAP:H2N	1.92	0.51
1:B:31:HIS:HE1	1:B:347:GLU:OE1	1.92	0.51
1:A:113:ASN:HD21	2:A:900:NAP:C5N	2.23	0.51
2:A:900:NAP:C5N	3:A:904:MLA:C3	2.90	0.50
2:B:901:NAP:H5N	3:B:902:MLA:O1B	2.11	0.50
1:B:128:PRO:HG2	1:B:344:LEU:HD13	1.95	0.49
1:B:346:ALA:O	1:B:350:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:HIS:CD2	1:B:33:MSE:H	2.30	0.48
1:A:78:HIS:HD2	1:A:80:GLU:H	1.62	0.47
1:B:180:ILE:HG21	1:B:214:MSE:HE1	1.96	0.47
1:B:56:TRP:CD2	1:B:62:ILE:HG12	2.48	0.47
1:A:271:MSE:HE1	1:A:317:ILE:CD1	2.45	0.47
2:A:900:NAP:H5N	3:A:904:MLA:C3	2.45	0.46
1:A:284:THR:HG22	1:A:284:THR:O	2.15	0.46
1:B:11:VAL:HG12	1:B:86:ILE:HB	1.97	0.46
1:B:23:ARG:HE	1:B:334:THR:HG21	1.79	0.46
1:B:284:THR:O	1:B:284:THR:HG22	2.16	0.46
1:A:7:MSE:HB3	1:A:33:MSE:HA	1.97	0.46
1:A:128:PRO:HG3	1:A:345:ASN:HD22	1.81	0.45
1:A:194:VAL:CG2	1:A:243:ARG:HD3	2.46	0.44
1:A:243:ARG:HD2	4:A:973:HOH:O	2.16	0.44
1:A:257:LYS:HB2	1:A:323:PHE:CG	2.53	0.44
1:B:20:VAL:HB	1:B:90:ALA:HB1	2.00	0.44
1:B:23:ARG:NH2	1:B:26:GLN:HE22	2.10	0.44
1:B:169:ILE:HD11	1:B:271:MSE:CE	2.47	0.43
1:A:72:ILE:HD13	1:A:80:GLU:HB2	2.00	0.43
1:B:31:HIS:CE1	1:B:347:GLU:OE1	2.70	0.43
1:A:113:ASN:HD21	2:A:900:NAP:C6N	2.31	0.43
1:A:97:LYS:HG3	1:A:116:ALA:HB1	2.01	0.43
1:A:56:TRP:CD2	1:A:62:ILE:HG12	2.54	0.43
2:A:900:NAP:H4N	4:A:986:HOH:O	2.18	0.42
1:B:243:ARG:HD2	4:B:916:HOH:O	2.17	0.42
1:A:180:ILE:HG21	1:A:214:MSE:HE1	2.01	0.42
1:B:198:ALA:HB1	1:B:204:ILE:CD1	2.47	0.42
1:B:257:LYS:HB2	1:B:323:PHE:CG	2.55	0.41
1:A:322:ILE:HG12	1:B:236:LYS:HB3	2.03	0.41
2:A:900:NAP:H2A	4:A:983:HOH:O	2.21	0.41
1:B:196:SER:O	1:B:200:LEU:HB2	2.21	0.41
1:A:196:SER:O	1:A:200:LEU:HB2	2.21	0.41
1:A:10:LYS:HG2	1:A:37:THR:HG21	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	346/354 (98%)	335 (97%)	11 (3%)	0	100	100
1	B	346/354 (98%)	337 (97%)	8 (2%)	1 (0%)	46	57
All	All	692/708 (98%)	672 (97%)	19 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/292 (102%)	291 (98%)	6 (2%)	63	79
1	B	297/292 (102%)	286 (96%)	11 (4%)	41	55
All	All	594/584 (102%)	577 (97%)	17 (3%)	50	66

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	44	ARG
1	A	134	HIS
1	A	143	GLU
1	A	344	LEU

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Mol	Chain	Res	Type
1	A	350	VAL
1	B	7	MSE
1	B	36	LEU
1	B	44	ARG
1	B	77	LYS
1	B	84	VAL
1	B	154	ASN
1	B	280	LEU
1	B	334	THR
1	B	344	LEU
1	B	350	VAL
1	B	352	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	113	ASN
1	A	134	HIS
1	A	250	HIS
1	A	332	HIS
1	A	345	ASN
1	B	26	GLN
1	B	31	HIS
1	B	209	ASN
1	B	250	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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	900	-	42,52,52	1.33	4 (9%)	54,80,80	2.09	8 (14%)
3	MLA	A	903	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLA	A	904	-	0,6,6	0.00	-	0,7,7	0.00	-
2	NAP	B	901	-	42,52,52	1.34	3 (7%)	54,80,80	2.15	9 (16%)
3	MLA	B	902	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLA	B	905	-	0,6,6	0.00	-	0,7,7	0.00	-

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	NAP	A	900	-	1/1/12/12	0/27/67/67	0/5/5/5
3	MLA	A	903	-	-	0/0/4/4	0/0/0/0
3	MLA	A	904	-	-	0/0/4/4	0/0/0/0
2	NAP	B	901	-	2/2/12/12	0/27/67/67	0/5/5/5
3	MLA	B	902	-	-	0/0/4/4	0/0/0/0
3	MLA	B	905	-	-	0/0/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	NAP	O4B-C1B	2.27	1.44	1.41
2	B	901	NAP	C5A-C4A	2.50	1.46	1.40
2	A	900	NAP	C5A-C4A	2.62	1.46	1.40
2	A	900	NAP	O4D-C1D	2.63	1.44	1.41
2	B	901	NAP	O4D-C1D	2.96	1.45	1.41
2	A	900	NAP	C4A-N3A	6.19	1.44	1.35
2	B	901	NAP	C4A-N3A	6.23	1.44	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAP	N3A-C2A-N1A	-7.44	123.20	128.89
2	A	900	NAP	N3A-C2A-N1A	-7.06	123.49	128.89
2	B	901	NAP	PN-O3-PA	-4.59	119.83	132.73
2	A	900	NAP	PN-O3-PA	-4.43	120.28	132.73
2	B	901	NAP	C4A-C5A-N7A	-3.99	105.81	109.48
2	A	900	NAP	C4A-C5A-N7A	-3.81	105.97	109.48
2	B	901	NAP	C3B-C2B-C1B	2.02	106.63	102.73
2	B	901	NAP	C2D-C3D-C4D	2.10	106.93	102.61
2	A	900	NAP	C3N-C7N-N7N	2.13	120.14	117.82
2	B	901	NAP	C4B-O4B-C1B	2.17	112.11	109.72
2	A	900	NAP	C2A-N1A-C6A	2.37	123.00	118.77
2	B	901	NAP	C2A-N1A-C6A	2.38	123.03	118.77
2	A	900	NAP	O4B-C1B-N9A	2.44	113.20	108.10
2	A	900	NAP	C1B-N9A-C4A	3.02	131.50	126.94
2	B	901	NAP	C3N-C7N-N7N	3.24	121.36	117.82
2	A	900	NAP	O4D-C1D-N1N	8.54	117.52	108.13
2	B	901	NAP	O4D-C1D-N1N	9.18	118.21	108.13

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	900	NAP	C1B
2	B	901	NAP	C1B
2	B	901	NAP	C3B

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	NAP	11	0
3	A	904	MLA	3	0
2	B	901	NAP	9	0
3	B	902	MLA	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/354 (95%)	2.98	241 (71%) 0 0	21, 34, 51, 56	0
1	B	338/354 (95%)	2.75	231 (68%) 0 0	22, 33, 48, 55	0
All	All	676/708 (95%)	2.86	472 (69%) 0 0	21, 33, 49, 56	0

All (472) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	12.2
1	B	63	PRO	11.1
1	B	53	ALA	9.3
1	A	84	VAL	8.9
1	A	230	VAL	8.4
1	A	81	PHE	8.2
1	B	76	PRO	7.9
1	A	226	LYS	7.8
1	B	72	ILE	7.8
1	B	73	PRO	7.6
1	A	44	ARG	7.5
1	A	280	LEU	7.3
1	A	104	ALA	7.2
1	A	53	ALA	7.1
1	A	147	TRP	6.8
1	B	70	VAL	6.8
1	A	70	VAL	6.6
1	B	207	ILE	6.5
1	B	95	LEU	6.3
1	A	263	GLU	6.2
1	A	99	PHE	6.1
1	B	99	PHE	6.1
1	B	47	GLY	6.1
1	B	71	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	267	ILE	6.1
1	B	77	LYS	5.9
1	B	9	ILE	5.9
1	B	152	ILE	5.8
1	A	286	ALA	5.8
1	B	20	VAL	5.8
1	A	289	ILE	5.7
1	A	56	TRP	5.6
1	A	354	ILE	5.6
1	A	98	LYS	5.5
1	B	226	LYS	5.5
1	A	237	ILE	5.5
1	A	162	ALA	5.4
1	B	225	LEU	5.4
1	B	45	SER	5.4
1	B	274	PHE	5.4
1	A	274	PHE	5.3
1	A	89	SER	5.2
1	B	314	VAL	5.2
1	A	31	HIS	5.1
1	B	49	LYS	5.1
1	A	43	GLU	5.1
1	B	91	LEU	5.1
1	A	353	TYR	5.0
1	B	59	ASP	5.0
1	A	169	ILE	5.0
1	A	227	ASP	5.0
1	A	253	SER	4.9
1	A	28	LEU	4.9
1	A	50	TYR	4.9
1	A	277	LEU	4.9
1	B	335	ILE	4.9
1	B	68	ASP	4.8
1	A	189	ALA	4.8
1	A	225	LEU	4.8
1	A	87	VAL	4.8
1	B	163	VAL	4.8
1	A	68	ASP	4.7
1	A	143	GLU	4.7
1	A	91	LEU	4.7
1	B	74	THR	4.7
1	B	235	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	93	SER	4.7
1	B	130	VAL	4.7
1	A	9	ILE	4.7
1	B	189	ALA	4.6
1	A	101	PRO	4.6
1	B	40	ALA	4.6
1	B	162	ALA	4.6
1	A	349	PHE	4.6
1	A	341	ALA	4.5
1	A	8	LYS	4.5
1	B	123	VAL	4.5
1	B	312	ILE	4.4
1	A	194	VAL	4.4
1	B	285	TYR	4.4
1	A	75	ASP	4.4
1	A	109	LEU	4.4
1	B	153	THR	4.4
1	B	265	GLU	4.4
1	A	25	VAL	4.4
1	A	59	ASP	4.3
1	B	54	CYS	4.3
1	A	80	GLU	4.3
1	B	103	PHE	4.3
1	A	62	ILE	4.3
1	A	63	PRO	4.3
1	A	148	ASP	4.3
1	A	350	VAL	4.3
1	B	120	GLU	4.3
1	A	42	SER	4.3
1	B	334	THR	4.3
1	B	192	ASN	4.2
1	A	140	ILE	4.2
1	A	151	ILE	4.2
1	B	178	VAL	4.2
1	B	161	CYS	4.2
1	B	187	SER	4.2
1	A	177	ALA	4.2
1	B	17	THR	4.2
1	B	221	LEU	4.2
1	B	150	ALA	4.2
1	A	142	ARG	4.2
1	A	330	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	101	PRO	4.2
1	A	76	PRO	4.1
1	A	96	ALA	4.1
1	A	36	LEU	4.1
1	A	232	LEU	4.1
1	A	278	LYS	4.1
1	A	34	PHE	4.1
1	B	34	PHE	4.0
1	B	174	GLY	4.0
1	B	232	LEU	4.0
1	B	270	VAL	4.0
1	A	74	THR	4.0
1	A	246	VAL	4.0
1	A	37	THR	4.0
1	B	338	ALA	4.0
1	B	117	TYR	4.0
1	B	251	THR	4.0
1	A	223	GLY	4.0
1	A	82	GLU	4.0
1	A	240	SER	4.0
1	B	343	VAL	3.9
1	A	54	CYS	3.9
1	A	285	TYR	3.9
1	A	327	TYR	3.9
1	A	348	TYR	3.9
1	B	56	TRP	3.9
1	A	11	VAL	3.9
1	A	72	ILE	3.9
1	A	204	ILE	3.9
1	A	27	LEU	3.9
1	B	14	LEU	3.9
1	A	158	SER	3.8
1	A	199	ILE	3.8
1	A	270	VAL	3.8
1	A	314	VAL	3.8
1	A	94	ASP	3.8
1	B	102	GLU	3.8
1	B	151	ILE	3.8
1	A	88	PHE	3.8
1	B	336	ARG	3.8
1	A	251	THR	3.7
1	B	180	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	73	PRO	3.7
1	B	198	ALA	3.7
1	B	195	PRO	3.7
1	A	118	ARG	3.7
1	A	136	GLU	3.7
1	A	339	ALA	3.7
1	A	313	VAL	3.7
1	B	96	ALA	3.7
1	B	341	ALA	3.7
1	A	161	CYS	3.7
1	A	191	TYR	3.7
1	B	191	TYR	3.7
1	A	282	LEU	3.6
1	B	114	ALA	3.6
1	B	245	ALA	3.6
1	B	158	SER	3.6
1	A	129	GLU	3.6
1	B	110	ILE	3.6
1	B	204	ILE	3.6
1	A	198	ALA	3.6
1	A	264	PRO	3.6
1	B	143	GLU	3.6
1	A	160	ILE	3.6
1	A	207	ILE	3.6
1	A	112	SER	3.6
1	A	105	LYS	3.6
1	B	254	ILE	3.6
1	B	181	ALA	3.6
1	A	145	ARG	3.5
1	A	273	LYS	3.5
1	A	322	ILE	3.5
1	B	86	ILE	3.5
1	A	188	GLY	3.5
1	B	209	ASN	3.5
1	B	212	GLU	3.5
1	B	36	LEU	3.5
1	B	349	PHE	3.5
1	B	348	TYR	3.5
1	A	110	ILE	3.5
1	A	312	ILE	3.5
1	B	237	ILE	3.5
1	B	46	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	250	HIS	3.5
1	B	353	TYR	3.5
1	A	332	HIS	3.5
1	B	16	ALA	3.5
1	B	13	VAL	3.5
1	A	243	ARG	3.4
1	A	141	GLN	3.4
1	B	57	PHE	3.4
1	A	260	GLU	3.4
1	B	61	ASP	3.4
1	A	66	ILE	3.4
1	A	228	GLY	3.4
1	B	125	LEU	3.4
1	A	236	LYS	3.4
1	A	344	LEU	3.4
1	A	111	PHE	3.4
1	A	164	ILE	3.4
1	A	71	VAL	3.4
1	B	109	LEU	3.4
1	A	180	ILE	3.4
1	B	317	ILE	3.4
1	A	29	ALA	3.4
1	A	163	VAL	3.3
1	A	334	THR	3.3
1	B	85	ASP	3.3
1	B	132	ALA	3.3
1	A	283	PRO	3.3
1	A	244	VAL	3.3
1	A	39	LEU	3.3
1	A	58	GLN	3.3
1	B	84	VAL	3.3
1	A	24	PHE	3.3
1	B	176	GLU	3.3
1	B	350	VAL	3.3
1	B	164	ILE	3.3
1	A	51	LYS	3.3
1	B	194	VAL	3.3
1	B	206	PHE	3.3
1	B	228	GLY	3.3
1	B	337	GLY	3.3
1	A	187	SER	3.3
1	A	342	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	244	VAL	3.3
1	A	269	GLU	3.2
1	B	319	LYS	3.2
1	A	291	ILE	3.2
1	A	126	VAL	3.2
1	B	155	PRO	3.2
1	A	173	PHE	3.2
1	B	179	PHE	3.2
1	A	284	THR	3.2
1	A	297	ARG	3.2
1	A	132	ALA	3.2
1	B	135	LEU	3.2
1	A	315	GLY	3.2
1	A	290	VAL	3.2
1	A	300	PRO	3.2
1	B	327	TYR	3.2
1	A	238	SER	3.2
1	B	82	GLU	3.2
1	B	196	SER	3.2
1	A	49	LYS	3.2
1	A	157	CYS	3.1
1	B	223	GLY	3.1
1	A	57	PHE	3.1
1	A	103	PHE	3.1
1	B	11	VAL	3.1
1	B	44	ARG	3.1
1	A	13	VAL	3.1
1	B	279	ASP	3.1
1	B	156	ASN	3.1
1	B	83	ASP	3.1
1	B	200	LEU	3.1
1	B	233	ALA	3.1
1	A	235	PHE	3.1
1	A	153	THR	3.0
1	B	342	SER	3.0
1	A	100	GLU	3.0
1	B	24	PHE	3.0
1	B	231	GLU	3.0
1	A	203	LEU	3.0
1	B	88	PHE	3.0
1	B	66	ILE	3.0
1	A	182	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	218	SER	3.0
1	A	156	ASN	3.0
1	A	206	PHE	3.0
1	A	255	PHE	3.0
1	B	354	ILE	3.0
1	B	229	LYS	3.0
1	A	116	ALA	3.0
1	A	185	ALA	3.0
1	B	38	ALA	3.0
1	B	62	ILE	3.0
1	B	27	LEU	3.0
1	B	147	TRP	2.9
1	B	126	VAL	2.9
1	B	121	GLU	2.9
1	B	115	SER	2.9
1	B	276	PRO	2.9
1	B	256	VAL	2.9
1	B	89	SER	2.9
1	A	265	GLU	2.9
1	A	166	LEU	2.9
1	A	121	GLU	2.9
1	B	65	ASN	2.9
1	B	230	VAL	2.9
1	A	65	ASN	2.9
1	B	30	ASP	2.9
1	A	117	TYR	2.9
1	A	295	ILE	2.9
1	B	252	GLU	2.8
1	A	352	LYS	2.8
1	B	39	LEU	2.8
1	B	157	CYS	2.8
1	B	8	LYS	2.8
1	A	15	GLY	2.8
1	B	177	ALA	2.8
1	B	290	VAL	2.8
1	B	149	GLY	2.8
1	B	32	PRO	2.8
1	B	248	ASP	2.8
1	B	263	GLU	2.8
1	B	291	ILE	2.8
1	A	192	ASN	2.8
1	B	41	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	159	THR	2.8
1	B	87	VAL	2.8
1	B	173	PHE	2.8
1	B	309	GLY	2.8
1	A	146	GLY	2.7
1	B	127	ILE	2.7
1	B	199	ILE	2.7
1	A	256	VAL	2.7
1	A	60	ARG	2.7
1	B	344	LEU	2.7
1	A	128	PRO	2.7
1	A	335	ILE	2.7
1	A	41	ALA	2.7
1	A	134	HIS	2.7
1	A	331	GLU	2.7
1	B	352	LYS	2.7
1	A	250	HIS	2.7
1	A	221	LEU	2.7
1	A	131	ASN	2.7
1	A	241	CYS	2.7
1	B	224	THR	2.7
1	A	133	ASP	2.7
1	A	245	ALA	2.6
1	A	231	GLU	2.6
1	A	61	ASP	2.6
1	B	278	LYS	2.6
1	B	298	PRO	2.6
1	B	325	VAL	2.6
1	A	254	ILE	2.6
1	B	234	ASN	2.6
1	A	14	LEU	2.6
1	A	85	ASP	2.6
1	A	323	PHE	2.6
1	A	124	PRO	2.6
1	A	233	ALA	2.6
1	A	22	GLN	2.6
1	A	205	PRO	2.6
1	B	284	THR	2.6
1	A	102	GLU	2.5
1	A	333	ASN	2.5
1	B	166	LEU	2.5
1	B	203	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	303	ASP	2.5
1	B	42	SER	2.5
1	A	351	LYS	2.5
1	A	224	THR	2.5
1	A	127	ILE	2.5
1	A	55	TYR	2.5
1	B	167	LYS	2.5
1	B	185	ALA	2.5
1	A	298	PRO	2.5
1	B	31	HIS	2.5
1	A	20	VAL	2.5
1	B	148	ASP	2.5
1	A	347	GLU	2.5
1	B	220	LYS	2.4
1	A	343	VAL	2.4
1	B	81	PHE	2.4
1	A	293	GLU	2.4
1	B	112	SER	2.4
1	A	184	GLN	2.4
1	B	52	ASP	2.4
1	B	283	PRO	2.4
1	A	137	LEU	2.4
1	A	259	LYS	2.4
1	B	295	ILE	2.4
1	A	190	GLY	2.4
1	B	111	PHE	2.4
1	A	150	ALA	2.4
1	B	247	ILE	2.4
1	B	105	LYS	2.4
1	A	179	PHE	2.4
1	A	262	ALA	2.4
1	B	37	THR	2.4
1	B	124	PRO	2.4
1	A	268	LYS	2.4
1	A	302	LEU	2.4
1	B	351	LYS	2.4
1	B	90	ALA	2.4
1	A	106	GLU	2.3
1	A	171	ASP	2.3
1	A	234	ASN	2.3
1	B	144	LYS	2.3
1	B	145	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	205	PRO	2.3
1	B	159	THR	2.3
1	B	43	GLU	2.3
1	B	311	SER	2.3
1	A	219	LEU	2.3
1	B	113	ASN	2.3
1	B	160	ILE	2.3
1	A	114	ALA	2.3
1	B	64	GLU	2.3
1	A	305	ASN	2.3
1	A	195	PRO	2.3
1	B	269	GLU	2.3
1	A	152	ILE	2.3
1	B	339	ALA	2.3
1	A	167	LYS	2.3
1	A	213	LYS	2.3
1	B	330	LEU	2.3
1	B	267	ILE	2.2
1	B	48	LYS	2.2
1	A	196	SER	2.2
1	B	50	TYR	2.2
1	A	266	GLU	2.2
1	A	301	ARG	2.2
1	B	92	PRO	2.2
1	A	311	SER	2.2
1	B	184	GLN	2.2
1	A	144	LYS	2.2
1	B	273	LYS	2.2
1	A	325	VAL	2.2
1	B	213	LYS	2.2
1	B	239	ALA	2.2
1	B	79	GLU	2.2
1	B	315	GLY	2.2
1	A	209	ASN	2.2
1	B	202	ASN	2.2
1	B	262	ALA	2.2
1	A	86	ILE	2.2
1	B	75	ASP	2.1
1	B	190	GLY	2.1
1	A	155	PRO	2.1
1	A	95	LEU	2.1
1	B	175	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	253	SER	2.1
1	A	292	ARG	2.1
1	B	100	GLU	2.1
1	A	130	VAL	2.1
1	A	67	LYS	2.1
1	B	98	LYS	2.1
1	B	346	ALA	2.1
1	B	249	GLY	2.1
1	B	287	LYS	2.1
1	A	35	GLU	2.1
1	A	79	GLU	2.1
1	B	222	LEU	2.1
1	B	18	GLY	2.1
1	B	60	ARG	2.1
1	A	64	GLU	2.1
1	B	28	LEU	2.1
1	A	23	ARG	2.1
1	A	319	LYS	2.1
1	B	193	GLY	2.0
1	A	318	ARG	2.0
1	B	301	ARG	2.0
1	B	241	CYS	2.0
1	A	287	LYS	2.0
1	B	97	LYS	2.0
1	B	215	GLN	2.0
1	B	182	THR	2.0
1	B	116	ALA	2.0
1	A	288	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MLA	B	902	7/7	0.46	0.62	7.26	101,101,102,102	0
3	MLA	A	904	7/7	0.72	0.40	2.05	64,65,66,66	0
2	NAP	B	901	48/48	0.60	0.44	1.42	74,89,99,99	0
2	NAP	A	900	48/48	0.72	0.32	0.50	72,86,96,96	0
3	MLA	B	905	7/7	0.47	0.31	-0.26	35,35,35,35	0
3	MLA	A	903	7/7	0.74	0.23	-0.92	30,31,32,32	0

6.5 Other polymers

There are no such residues in this entry.