



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:47 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

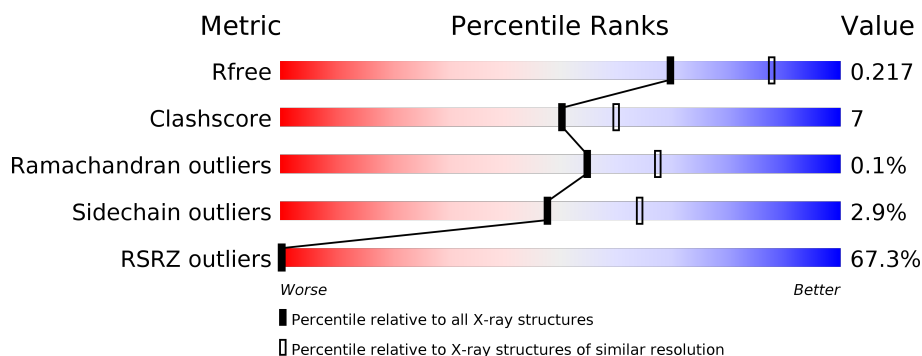
1 Overall quality at a glance

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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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	<div> <div>66%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	354	<div> <div>62%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>

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:

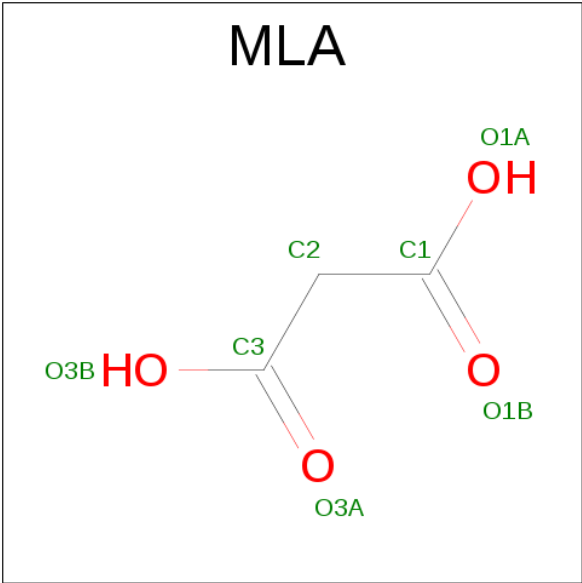
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	33	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	69	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	119	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	170	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	183	MSE	MET	MODIFIED RESIDUE	UNP Q57658
A	197	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: C₂₁H₂₈N₇O₁₇P₃).



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

- 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		

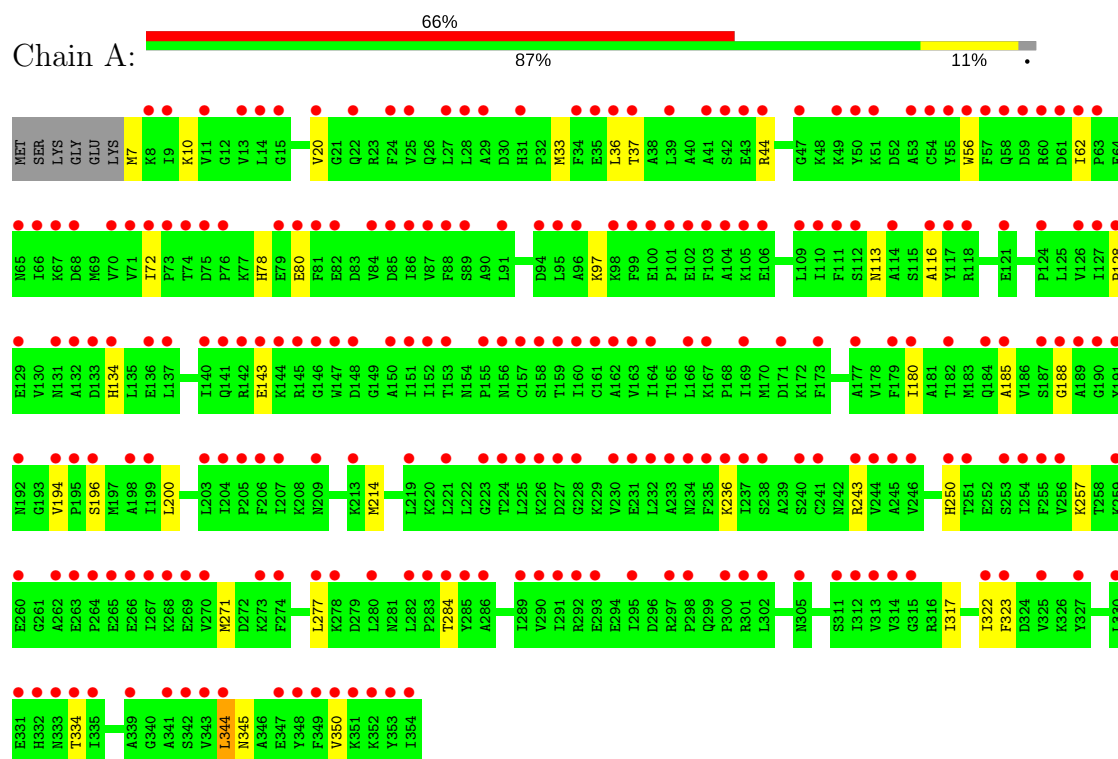
- Molecule 4 is water.

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

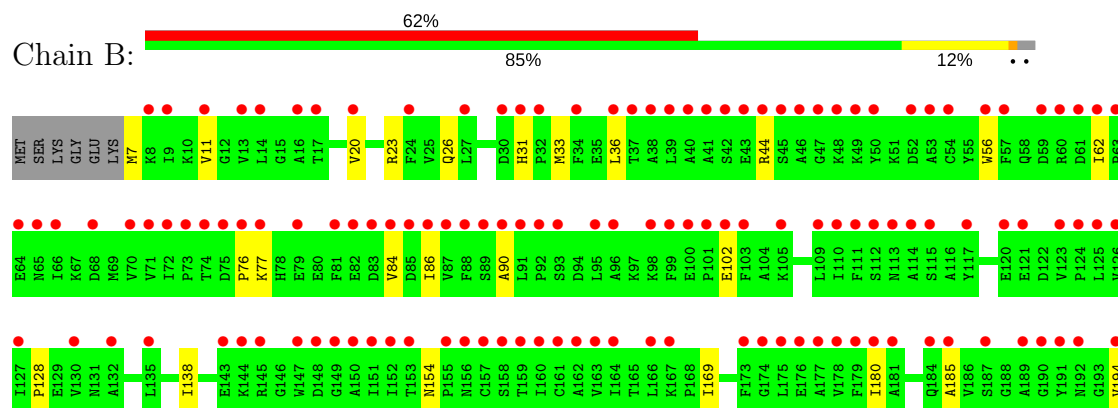
3 Residue-property plots

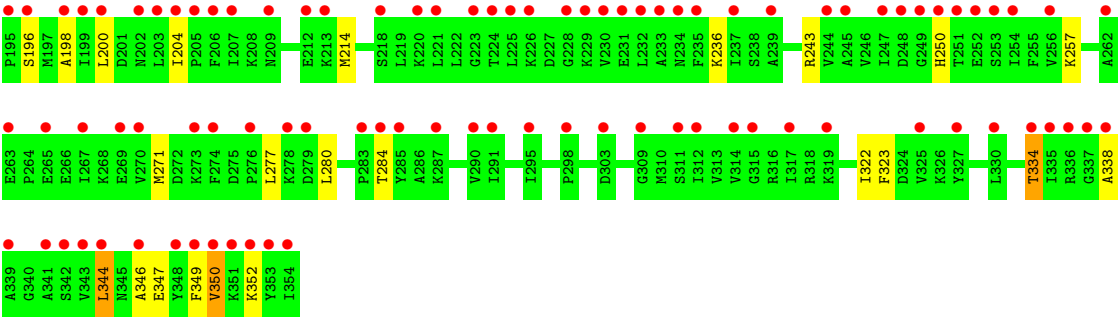
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 0.190 , 0.217	Depositor DCC
R_{free} test set	3147 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)	0.39 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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:A:188:GLY:HA2	2:A:900:NAP:C7N	2.03	0.88
1:B:20:VAL:HG23	4:B:1051:HOH:O	1.73	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:169:ILE:HD11	1:B:271:MSE:HE3	1.82	0.62
1:B:185:ALA:H	1:B:250:HIS:CD2	2.18	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:31:HIS:HE1	1:B:347:GLU:OE1	1.92	0.51
1:B:20:VAL:HG22	2:B:901:NAP:H2N	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:A:72:ILE:HD13	1:A:80:GLU:HB2	2.00	0.43
1:B:169:ILE:HD11	1:B:271:MSE:CE	2.47	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/354 (98%)	335 (97%)	11 (3%)	0	100	100
1	B	346/354 (98%)	337 (97%)	8 (2%)	1 (0%)	44	55
All	All	692/708 (98%)	672 (97%)	19 (3%)	1 (0%)	55	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/292 (102%)	291 (98%)	6 (2%)	60	77
1	B	297/292 (102%)	286 (96%)	11 (4%)	39	53
All	All	594/584 (102%)	577 (97%)	17 (3%)	48	64

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 [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

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	-	44,52,52	1.32	4 (9%)	51,80,80	1.53	5 (9%)
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	-	44,52,52	1.32	3 (6%)	51,80,80	1.58	6 (11%)
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	2.03	1.44	1.41
2	A	900	NAP	O4D-C1D	2.36	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	B	901	NAP	O4D-C1D	2.67	1.45	1.41
2	A	900	NAP	C4A-N3A	6.27	1.44	1.35
2	B	901	NAP	C4A-N3A	6.30	1.44	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAP	N3A-C2A-N1A	-6.50	123.20	128.86
2	A	900	NAP	N3A-C2A-N1A	-6.16	123.49	128.86
2	B	901	NAP	C4A-C5A-N7A	-3.72	105.81	109.41
2	A	900	NAP	C4A-C5A-N7A	-3.56	105.97	109.41
2	A	900	NAP	C3N-C7N-N7N	2.08	120.14	117.77
2	B	901	NAP	C4B-O4B-C1B	2.20	112.11	109.77
2	B	901	NAP	C2D-C3D-C4D	2.22	106.93	102.62
2	A	900	NAP	C2A-N1A-C6A	2.41	123.00	118.77
2	B	901	NAP	C2A-N1A-C6A	2.43	123.03	118.77
2	A	900	NAP	C1B-N9A-C4A	2.82	131.50	126.64
2	B	901	NAP	C3N-C7N-N7N	3.14	121.36	117.77

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/354 (95%)	2.85	234 (69%) 0 0	21, 34, 51, 56	0
1	B	338/354 (95%)	2.62	221 (65%) 0 0	22, 33, 48, 55	0
All	All	676/708 (95%)	2.74	455 (67%) 0 0	21, 33, 49, 56	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLY	11.9
1	B	63	PRO	10.8
1	B	53	ALA	9.0
1	A	84	VAL	8.5
1	A	230	VAL	8.0
1	A	81	PHE	8.0
1	A	226	LYS	7.6
1	B	76	PRO	7.6
1	B	72	ILE	7.5
1	A	44	ARG	7.3
1	B	73	PRO	7.3
1	A	280	LEU	7.1
1	A	104	ALA	6.9
1	A	53	ALA	6.8
1	A	147	TRP	6.6
1	B	70	VAL	6.5
1	A	70	VAL	6.3
1	B	207	ILE	6.3
1	B	95	LEU	6.0
1	A	263	GLU	6.0
1	A	99	PHE	6.0
1	B	99	PHE	5.9
1	A	267	ILE	5.9
1	B	47	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	77	LYS	5.8
1	B	71	VAL	5.8
1	B	9	ILE	5.6
1	B	152	ILE	5.6
1	A	286	ALA	5.5
1	B	20	VAL	5.5
1	A	289	ILE	5.5
1	A	56	TRP	5.4
1	A	354	ILE	5.4
1	A	98	LYS	5.4
1	B	226	LYS	5.4
1	A	237	ILE	5.2
1	B	225	LEU	5.2
1	A	162	ALA	5.2
1	B	274	PHE	5.2
1	B	45	SER	5.2
1	A	274	PHE	5.1
1	A	89	SER	5.0
1	B	49	LYS	5.0
1	A	43	GLU	5.0
1	A	31	HIS	4.9
1	B	314	VAL	4.9
1	B	91	LEU	4.9
1	A	353	TYR	4.9
1	A	169	ILE	4.8
1	B	59	ASP	4.8
1	A	227	ASP	4.8
1	A	50	TYR	4.7
1	A	253	SER	4.7
1	A	28	LEU	4.7
1	B	335	ILE	4.7
1	A	277	LEU	4.7
1	B	68	ASP	4.6
1	A	143	GLU	4.6
1	A	189	ALA	4.6
1	A	225	LEU	4.6
1	A	87	VAL	4.6
1	A	68	ASP	4.6
1	B	163	VAL	4.6
1	A	91	LEU	4.6
1	B	93	SER	4.5
1	B	74	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	235	PHE	4.5
1	B	130	VAL	4.5
1	A	9	ILE	4.5
1	A	101	PRO	4.5
1	B	40	ALA	4.4
1	B	162	ALA	4.4
1	A	349	PHE	4.4
1	B	189	ALA	4.4
1	A	8	LYS	4.4
1	A	341	ALA	4.4
1	B	285	TYR	4.3
1	B	123	VAL	4.3
1	B	312	ILE	4.3
1	B	265	GLU	4.3
1	A	75	ASP	4.3
1	A	80	GLU	4.2
1	A	109	LEU	4.2
1	A	194	VAL	4.2
1	B	153	THR	4.2
1	A	59	ASP	4.2
1	A	25	VAL	4.2
1	B	103	PHE	4.1
1	B	54	CYS	4.1
1	B	120	GLU	4.1
1	A	62	ILE	4.1
1	A	63	PRO	4.1
1	A	148	ASP	4.1
1	B	334	THR	4.1
1	A	350	VAL	4.1
1	A	42	SER	4.1
1	A	140	ILE	4.0
1	A	142	ARG	4.0
1	A	151	ILE	4.0
1	B	192	ASN	4.0
1	A	177	ALA	4.0
1	B	178	VAL	4.0
1	B	17	THR	4.0
1	B	187	SER	4.0
1	B	221	LEU	4.0
1	B	150	ALA	4.0
1	A	278	LYS	4.0
1	B	161	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	4.0
1	A	76	PRO	4.0
1	A	96	ALA	4.0
1	B	101	PRO	4.0
1	A	36	LEU	3.9
1	A	232	LEU	3.9
1	A	34	PHE	3.9
1	B	34	PHE	3.9
1	B	232	LEU	3.9
1	A	82	GLU	3.8
1	B	174	GLY	3.8
1	B	270	VAL	3.8
1	A	74	THR	3.8
1	B	117	TYR	3.8
1	A	240	SER	3.8
1	B	338	ALA	3.8
1	A	37	THR	3.8
1	A	246	VAL	3.8
1	A	223	GLY	3.8
1	B	343	VAL	3.8
1	B	251	THR	3.8
1	A	285	TYR	3.8
1	A	327	TYR	3.8
1	A	348	TYR	3.8
1	B	56	TRP	3.7
1	A	54	CYS	3.7
1	A	72	ILE	3.7
1	A	94	ASP	3.7
1	A	158	SER	3.7
1	A	11	VAL	3.7
1	A	204	ILE	3.7
1	B	102	GLU	3.7
1	A	27	LEU	3.7
1	B	14	LEU	3.7
1	A	270	VAL	3.7
1	A	314	VAL	3.7
1	B	336	ARG	3.7
1	A	199	ILE	3.7
1	A	88	PHE	3.6
1	A	118	ARG	3.6
1	B	151	ILE	3.6
1	A	73	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLU	3.6
1	A	251	THR	3.6
1	B	180	ILE	3.6
1	B	198	ALA	3.5
1	A	191	TYR	3.5
1	B	195	PRO	3.5
1	A	339	ALA	3.5
1	B	96	ALA	3.5
1	A	129	GLU	3.5
1	A	282	LEU	3.5
1	B	191	TYR	3.5
1	B	341	ALA	3.5
1	B	143	GLU	3.5
1	A	313	VAL	3.5
1	A	198	ALA	3.5
1	B	158	SER	3.5
1	A	105	LYS	3.5
1	A	273	LYS	3.5
1	A	264	PRO	3.5
1	B	204	ILE	3.5
1	B	114	ALA	3.5
1	B	245	ALA	3.5
1	A	145	ARG	3.5
1	B	110	ILE	3.4
1	A	112	SER	3.4
1	A	161	CYS	3.4
1	A	207	ILE	3.4
1	B	212	GLU	3.4
1	A	160	ILE	3.4
1	B	348	TYR	3.4
1	B	181	ALA	3.4
1	B	254	ILE	3.4
1	B	209	ASN	3.4
1	B	353	TYR	3.4
1	A	322	ILE	3.4
1	B	36	LEU	3.4
1	B	16	ALA	3.4
1	A	110	ILE	3.4
1	B	86	ILE	3.4
1	B	237	ILE	3.4
1	B	349	PHE	3.4
1	A	188	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	243	ARG	3.3
1	A	141	GLN	3.3
1	B	250	HIS	3.3
1	A	236	LYS	3.3
1	A	260	GLU	3.3
1	B	46	ALA	3.3
1	A	332	HIS	3.3
1	A	312	ILE	3.3
1	B	57	PHE	3.3
1	B	13	VAL	3.3
1	B	61	ASP	3.3
1	A	228	GLY	3.3
1	A	344	LEU	3.3
1	B	125	LEU	3.3
1	A	66	ILE	3.3
1	A	164	ILE	3.3
1	B	109	LEU	3.2
1	A	111	PHE	3.2
1	A	71	VAL	3.2
1	A	58	GLN	3.2
1	B	85	ASP	3.2
1	A	39	LEU	3.2
1	A	180	ILE	3.2
1	B	317	ILE	3.2
1	A	29	ALA	3.2
1	A	283	PRO	3.2
1	A	163	VAL	3.2
1	A	334	THR	3.2
1	A	51	LYS	3.2
1	B	132	ALA	3.2
1	A	24	PHE	3.2
1	B	319	LYS	3.2
1	A	244	VAL	3.2
1	A	269	GLU	3.2
1	B	176	GLU	3.2
1	B	164	ILE	3.1
1	B	84	VAL	3.1
1	B	228	GLY	3.1
1	A	187	SER	3.1
1	A	342	SER	3.1
1	A	173	PHE	3.1
1	B	206	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	350	VAL	3.1
1	B	337	GLY	3.1
1	A	297	ARG	3.1
1	A	291	ILE	3.1
1	B	155	PRO	3.1
1	B	179	PHE	3.1
1	B	194	VAL	3.1
1	A	49	LYS	3.1
1	B	244	VAL	3.1
1	A	284	THR	3.1
1	B	327	TYR	3.0
1	B	135	LEU	3.0
1	A	315	GLY	3.0
1	A	132	ALA	3.0
1	A	126	VAL	3.0
1	A	238	SER	3.0
1	B	82	GLU	3.0
1	B	44	ARG	3.0
1	A	290	VAL	3.0
1	A	300	PRO	3.0
1	A	57	PHE	3.0
1	A	103	PHE	3.0
1	B	196	SER	3.0
1	B	223	GLY	3.0
1	B	83	ASP	3.0
1	B	279	ASP	3.0
1	B	11	VAL	3.0
1	B	156	ASN	3.0
1	A	100	GLU	2.9
1	B	200	LEU	2.9
1	A	157	CYS	2.9
1	B	233	ALA	2.9
1	B	231	GLU	2.9
1	A	235	PHE	2.9
1	A	13	VAL	2.9
1	A	153	THR	2.9
1	B	24	PHE	2.9
1	B	342	SER	2.9
1	B	229	LYS	2.9
1	B	88	PHE	2.9
1	A	203	LEU	2.9
1	B	66	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	182	THR	2.9
1	B	218	SER	2.9
1	A	156	ASN	2.9
1	B	121	GLU	2.9
1	A	206	PHE	2.8
1	A	255	PHE	2.8
1	A	116	ALA	2.8
1	B	62	ILE	2.8
1	B	354	ILE	2.8
1	A	185	ALA	2.8
1	B	27	LEU	2.8
1	B	38	ALA	2.8
1	B	147	TRP	2.8
1	B	89	SER	2.8
1	A	121	GLU	2.8
1	A	265	GLU	2.8
1	A	166	LEU	2.8
1	B	276	PRO	2.8
1	B	65	ASN	2.8
1	B	115	SER	2.8
1	A	117	TYR	2.8
1	B	126	VAL	2.8
1	A	65	ASN	2.8
1	B	30	ASP	2.7
1	B	230	VAL	2.7
1	A	352	LYS	2.7
1	B	252	GLU	2.7
1	B	256	VAL	2.7
1	B	8	LYS	2.7
1	A	295	ILE	2.7
1	B	39	LEU	2.7
1	B	263	GLU	2.7
1	B	248	ASP	2.7
1	A	15	GLY	2.7
1	B	149	GLY	2.7
1	B	41	ALA	2.7
1	B	177	ALA	2.7
1	A	192	ASN	2.7
1	B	290	VAL	2.7
1	A	60	ARG	2.6
1	B	157	CYS	2.6
1	B	32	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	291	ILE	2.6
1	A	159	THR	2.6
1	B	173	PHE	2.6
1	B	309	GLY	2.6
1	B	87	VAL	2.6
1	B	352	LYS	2.6
1	B	127	ILE	2.6
1	A	146	GLY	2.6
1	A	331	GLU	2.6
1	B	199	ILE	2.6
1	B	344	LEU	2.6
1	A	256	VAL	2.6
1	A	134	HIS	2.6
1	A	41	ALA	2.6
1	A	335	ILE	2.6
1	A	128	PRO	2.6
1	A	250	HIS	2.6
1	B	278	LYS	2.6
1	A	221	LEU	2.5
1	A	133	ASP	2.5
1	A	231	GLU	2.5
1	B	224	THR	2.5
1	A	131	ASN	2.5
1	A	245	ALA	2.5
1	A	61	ASP	2.5
1	A	14	LEU	2.5
1	A	323	PHE	2.5
1	B	234	ASN	2.5
1	A	22	GLN	2.5
1	A	85	ASP	2.5
1	A	241	CYS	2.5
1	A	124	PRO	2.5
1	B	298	PRO	2.5
1	A	254	ILE	2.5
1	B	325	VAL	2.5
1	A	351	LYS	2.5
1	A	102	GLU	2.4
1	A	205	PRO	2.4
1	A	233	ALA	2.4
1	B	42	SER	2.4
1	B	167	LYS	2.4
1	B	166	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	2.4
1	A	333	ASN	2.4
1	B	284	THR	2.4
1	B	303	ASP	2.4
1	A	55	TYR	2.4
1	B	220	LYS	2.4
1	A	298	PRO	2.4
1	A	224	THR	2.4
1	A	347	GLU	2.4
1	A	127	ILE	2.4
1	B	31	HIS	2.4
1	B	185	ALA	2.4
1	A	259	LYS	2.3
1	B	148	ASP	2.3
1	A	293	GLU	2.3
1	A	184	GLN	2.3
1	B	112	SER	2.3
1	B	81	PHE	2.3
1	A	268	LYS	2.3
1	B	295	ILE	2.3
1	A	137	LEU	2.3
1	B	52	ASP	2.3
1	A	20	VAL	2.3
1	A	343	VAL	2.3
1	A	190	GLY	2.3
1	B	105	LYS	2.3
1	B	283	PRO	2.3
1	B	351	LYS	2.3
1	B	111	PHE	2.3
1	A	150	ALA	2.3
1	A	179	PHE	2.3
1	B	124	PRO	2.3
1	A	262	ALA	2.3
1	B	247	ILE	2.3
1	A	302	LEU	2.2
1	B	145	ARG	2.2
1	B	144	LYS	2.2
1	A	106	GLU	2.2
1	B	90	ALA	2.2
1	B	37	THR	2.2
1	A	171	ASP	2.2
1	A	234	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	43	GLU	2.2
1	B	269	GLU	2.2
1	A	213	LYS	2.2
1	B	311	SER	2.2
1	B	64	GLU	2.2
1	B	113	ASN	2.2
1	B	159	THR	2.2
1	A	167	LYS	2.2
1	A	219	LEU	2.2
1	B	205	PRO	2.2
1	A	266	GLU	2.2
1	B	48	LYS	2.2
1	B	273	LYS	2.2
1	A	144	LYS	2.1
1	A	305	ASN	2.1
1	B	50	TYR	2.1
1	A	301	ARG	2.1
1	A	114	ALA	2.1
1	B	339	ALA	2.1
1	A	152	ILE	2.1
1	B	160	ILE	2.1
1	B	267	ILE	2.1
1	B	330	LEU	2.1
1	A	195	PRO	2.1
1	B	184	GLN	2.1
1	B	213	LYS	2.1
1	A	196	SER	2.1
1	A	311	SER	2.1
1	B	92	PRO	2.1
1	A	325	VAL	2.1
1	B	202	ASN	2.1
1	B	79	GLU	2.1
1	A	209	ASN	2.1
1	A	292	ARG	2.1
1	A	67	LYS	2.1
1	B	98	LYS	2.1
1	B	239	ALA	2.1
1	B	262	ALA	2.1
1	B	287	LYS	2.1
1	B	315	GLY	2.1
1	A	79	GLU	2.0
1	B	100	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	75	ASP	2.0
1	A	86	ILE	2.0
1	A	155	PRO	2.0
1	A	95	LEU	2.0
1	A	35	GLU	2.0
1	B	190	GLY	2.0
1	B	253	SER	2.0
1	B	175	LEU	2.0
1	B	249	GLY	2.0
1	B	60	ARG	2.0
1	B	346	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MLA	B	902	7/7	0.46	0.62	7.30	101,101,102,102	0
3	MLA	A	904	7/7	0.72	0.40	2.04	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	0.31	0.50	72,86,96,96	0
3	MLA	B	905	7/7	0.47	0.31	-0.24	35,35,35,35	0
3	MLA	A	903	7/7	0.74	0.23	-0.91	30,31,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.