



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:29 PM UTC

PDB ID : 3U4J / pdb_00003u4j
Title : Crystal structure of NAD-dependent aldehyde dehydrogenase from *Sinorhizobium meliloti*
Authors : Eswaramoorthy, S.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYS-GRC)
Deposited on : 2011-10-08
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

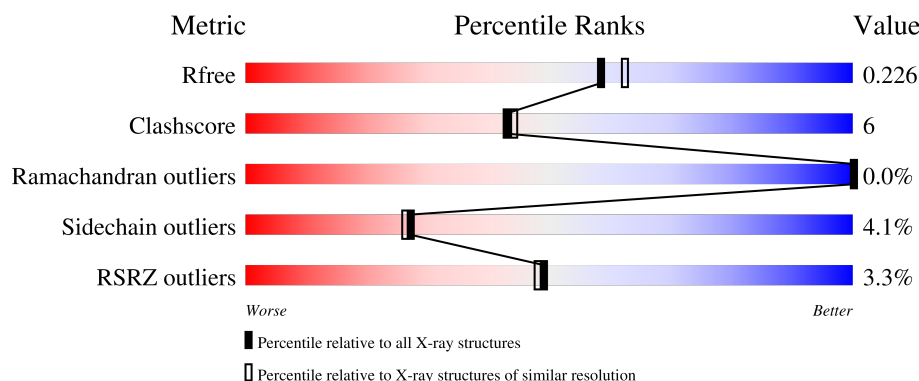
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	528	% 81% 13% • •
1	B	528	9% 80% 14% • 5%
1	C	528	2% 84% 11% • •
1	D	528	% 82% 12% • 5%

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15736 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 NAD-dependent aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	Se	0	0	0
			3785	2388	667	717	5	8			
1	B	502	Total	C	N	O	S	Se	0	0	0
			3765	2375	664	714	5	7			
1	C	505	Total	C	N	O	S	Se	0	0	0
			3791	2391	670	717	5	8			
1	D	503	Total	C	N	O	S	Se	0	0	0
			3776	2381	668	715	5	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q930S8
A	0	VAL	-	expression tag	UNP Q930S8
A	505	ALA	-	expression tag	UNP Q930S8
A	506	GLU	-	expression tag	UNP Q930S8
A	507	ASN	-	expression tag	UNP Q930S8
A	508	LEU	-	expression tag	UNP Q930S8
A	509	TYR	-	expression tag	UNP Q930S8
A	510	PHE	-	expression tag	UNP Q930S8
A	511	GLN	-	expression tag	UNP Q930S8
A	512	SER	-	expression tag	UNP Q930S8
A	513	HIS	-	expression tag	UNP Q930S8
A	514	HIS	-	expression tag	UNP Q930S8
A	515	HIS	-	expression tag	UNP Q930S8
A	516	HIS	-	expression tag	UNP Q930S8
A	517	HIS	-	expression tag	UNP Q930S8
A	518	HIS	-	expression tag	UNP Q930S8
A	519	TRP	-	expression tag	UNP Q930S8
A	520	SER	-	expression tag	UNP Q930S8
A	521	HIS	-	expression tag	UNP Q930S8
A	522	PRO	-	expression tag	UNP Q930S8
A	523	GLN	-	expression tag	UNP Q930S8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	524	PHE	-	expression tag	UNP Q930S8
A	525	GLU	-	expression tag	UNP Q930S8
A	526	LYS	-	expression tag	UNP Q930S8
B	-1	MSE	-	expression tag	UNP Q930S8
B	0	VAL	-	expression tag	UNP Q930S8
B	505	ALA	-	expression tag	UNP Q930S8
B	506	GLU	-	expression tag	UNP Q930S8
B	507	ASN	-	expression tag	UNP Q930S8
B	508	LEU	-	expression tag	UNP Q930S8
B	509	TYR	-	expression tag	UNP Q930S8
B	510	PHE	-	expression tag	UNP Q930S8
B	511	GLN	-	expression tag	UNP Q930S8
B	512	SER	-	expression tag	UNP Q930S8
B	513	HIS	-	expression tag	UNP Q930S8
B	514	HIS	-	expression tag	UNP Q930S8
B	515	HIS	-	expression tag	UNP Q930S8
B	516	HIS	-	expression tag	UNP Q930S8
B	517	HIS	-	expression tag	UNP Q930S8
B	518	HIS	-	expression tag	UNP Q930S8
B	519	TRP	-	expression tag	UNP Q930S8
B	520	SER	-	expression tag	UNP Q930S8
B	521	HIS	-	expression tag	UNP Q930S8
B	522	PRO	-	expression tag	UNP Q930S8
B	523	GLN	-	expression tag	UNP Q930S8
B	524	PHE	-	expression tag	UNP Q930S8
B	525	GLU	-	expression tag	UNP Q930S8
B	526	LYS	-	expression tag	UNP Q930S8
C	-1	MSE	-	expression tag	UNP Q930S8
C	0	VAL	-	expression tag	UNP Q930S8
C	505	ALA	-	expression tag	UNP Q930S8
C	506	GLU	-	expression tag	UNP Q930S8
C	507	ASN	-	expression tag	UNP Q930S8
C	508	LEU	-	expression tag	UNP Q930S8
C	509	TYR	-	expression tag	UNP Q930S8
C	510	PHE	-	expression tag	UNP Q930S8
C	511	GLN	-	expression tag	UNP Q930S8
C	512	SER	-	expression tag	UNP Q930S8
C	513	HIS	-	expression tag	UNP Q930S8
C	514	HIS	-	expression tag	UNP Q930S8
C	515	HIS	-	expression tag	UNP Q930S8
C	516	HIS	-	expression tag	UNP Q930S8
C	517	HIS	-	expression tag	UNP Q930S8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	518	HIS	-	expression tag	UNP Q930S8
C	519	TRP	-	expression tag	UNP Q930S8
C	520	SER	-	expression tag	UNP Q930S8
C	521	HIS	-	expression tag	UNP Q930S8
C	522	PRO	-	expression tag	UNP Q930S8
C	523	GLN	-	expression tag	UNP Q930S8
C	524	PHE	-	expression tag	UNP Q930S8
C	525	GLU	-	expression tag	UNP Q930S8
C	526	LYS	-	expression tag	UNP Q930S8
D	-1	MSE	-	expression tag	UNP Q930S8
D	0	VAL	-	expression tag	UNP Q930S8
D	505	ALA	-	expression tag	UNP Q930S8
D	506	GLU	-	expression tag	UNP Q930S8
D	507	ASN	-	expression tag	UNP Q930S8
D	508	LEU	-	expression tag	UNP Q930S8
D	509	TYR	-	expression tag	UNP Q930S8
D	510	PHE	-	expression tag	UNP Q930S8
D	511	GLN	-	expression tag	UNP Q930S8
D	512	SER	-	expression tag	UNP Q930S8
D	513	HIS	-	expression tag	UNP Q930S8
D	514	HIS	-	expression tag	UNP Q930S8
D	515	HIS	-	expression tag	UNP Q930S8
D	516	HIS	-	expression tag	UNP Q930S8
D	517	HIS	-	expression tag	UNP Q930S8
D	518	HIS	-	expression tag	UNP Q930S8
D	519	TRP	-	expression tag	UNP Q930S8
D	520	SER	-	expression tag	UNP Q930S8
D	521	HIS	-	expression tag	UNP Q930S8
D	522	PRO	-	expression tag	UNP Q930S8
D	523	GLN	-	expression tag	UNP Q930S8
D	524	PHE	-	expression tag	UNP Q930S8
D	525	GLU	-	expression tag	UNP Q930S8
D	526	LYS	-	expression tag	UNP Q930S8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

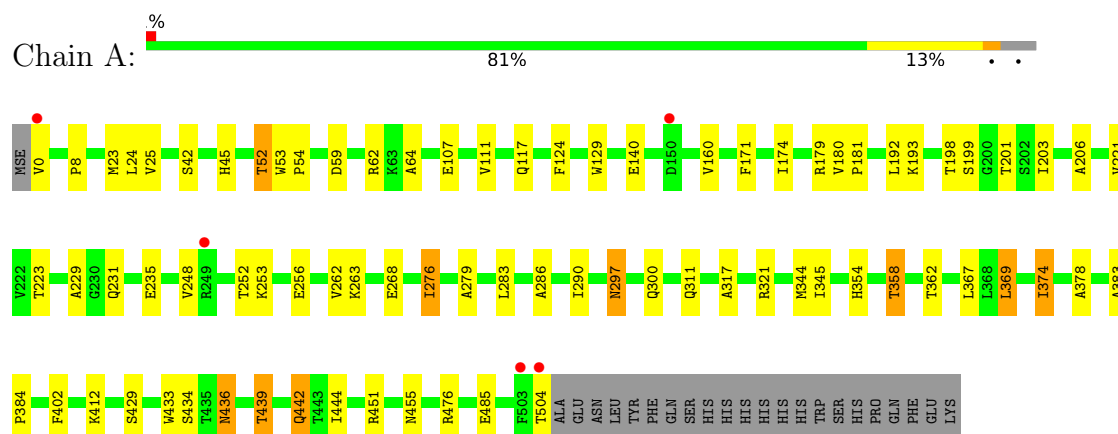
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total 193	O 193	0	0
3	B	108	Total 108	O 108	0	0
3	C	176	Total 176	O 176	0	0
3	D	141	Total 141	O 141	0	0

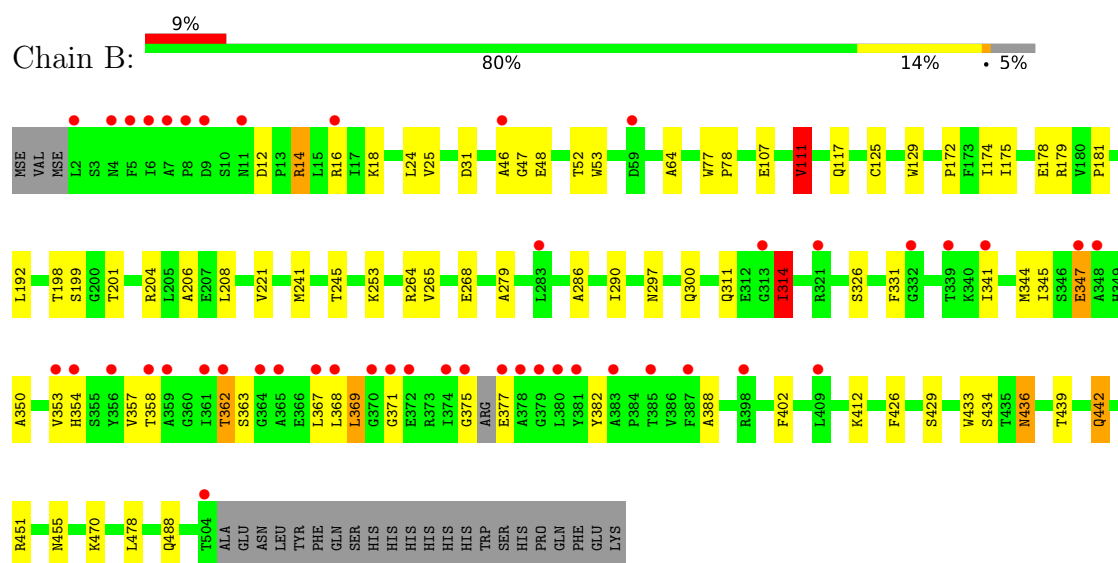
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

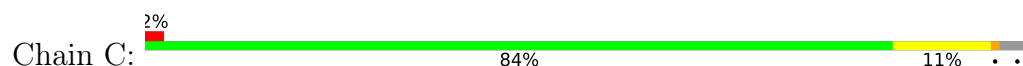
- Molecule 1: NAD-dependent aldehyde dehydrogenase

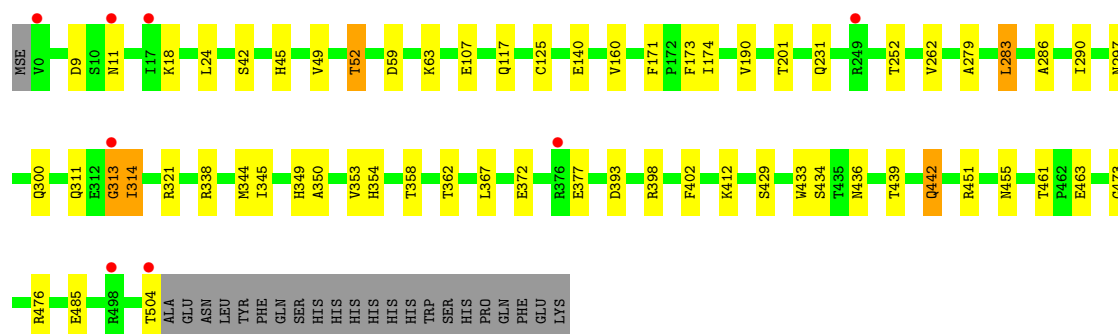


- Molecule 1: NAD-dependent aldehyde dehydrogenase

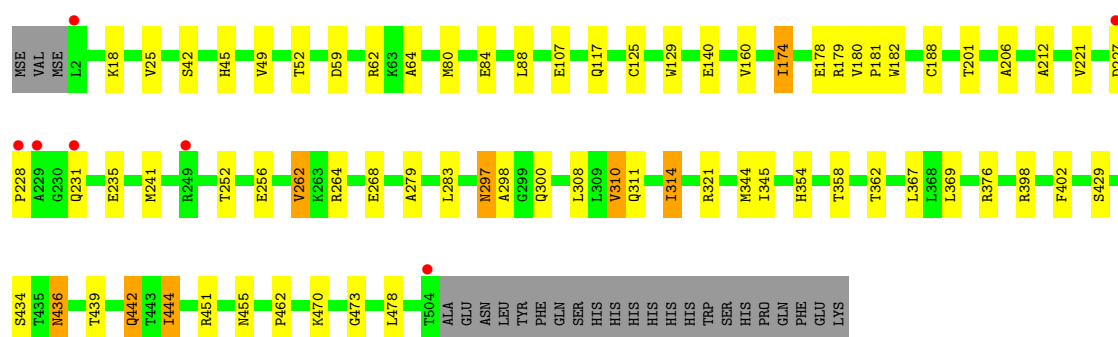
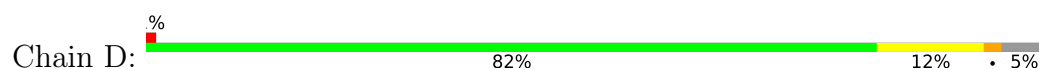


- Molecule 1: NAD-dependent aldehyde dehydrogenase





• Molecule 1: NAD-dependent aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.11Å 176.66Å 83.66Å 90.00° 98.49° 90.00°	Depositor
Resolution (Å)	47.98 – 2.00 47.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.98-2.00) 99.9 (47.98-2.00)	Depositor EDS
R_{merge}	0.92	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.187 , 0.224 0.190 , 0.226	Depositor DCC
R_{free} test set	7629 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15736	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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:
CA

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	0.82	1/3851 (0.0%)	0.89	0/5213
1	B	0.76	2/3831 (0.1%)	0.88	1/5186 (0.0%)
1	C	0.80	0/3857	0.89	2/5220 (0.0%)
1	D	0.80	1/3843 (0.0%)	0.90	2/5203 (0.0%)
All	All	0.79	4/15382 (0.0%)	0.89	5/20822 (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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	180	VAL	CA-CB	8.00	1.58	1.54
1	A	180	VAL	CA-CB	5.93	1.57	1.54
1	B	111	VAL	CA-CB	5.20	1.61	1.54
1	B	198	THR	CA-CB	5.20	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	212	ALA	N-CA-C	10.66	125.38	112.38
1	C	314	ILE	N-CA-C	-5.63	107.49	112.90
1	B	314	ILE	N-CA-C	-5.51	107.75	113.10
1	C	473	GLY	N-CA-C	5.39	118.45	110.63
1	D	473	GLY	N-CA-C	5.17	117.97	111.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	313	GLY	Peptide

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	3785	0	3777	53	0
1	B	3765	0	3753	52	0
1	C	3791	0	3788	40	0
1	D	3776	0	3767	45	0
2	A	1	0	0	0	0
3	A	193	0	0	6	0
3	B	108	0	0	1	0
3	C	176	0	0	4	0
3	D	141	0	0	4	0
All	All	15736	0	15085	188	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 (188) 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:344:MSE:HE1	1:B:353:VAL:HG21	1.34	1.05
1:C:344:MSE:HE1	1:C:353:VAL:HG21	1.45	0.98
1:D:80:MSE:HE3	1:D:84:GLU:HB3	1.46	0.96
1:C:279:ALA:H	1:C:311:GLN:HE21	1.12	0.94
1:A:279:ALA:H	1:A:311:GLN:HE21	1.11	0.90
1:D:279:ALA:H	1:D:311:GLN:HE21	1.19	0.87
1:A:231:GLN:O	1:A:235:GLU:HG2	1.76	0.86
1:B:442:GLN:HA	1:B:442:GLN:HE21	1.40	0.84
1:B:279:ALA:H	1:B:311:GLN:HE21	1.25	0.83
1:C:107:GLU:HG2	1:C:201:THR:HG21	1.60	0.82
1:A:374:ILE:HD13	1:A:383:ALA:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:THR:HG23	3:C:597:HOH:O	1.79	0.81
1:D:442:GLN:HE21	1:D:442:GLN:HA	1.46	0.80
1:A:279:ALA:H	1:A:311:GLN:NE2	1.79	0.80
1:B:344:MSE:HE1	1:B:353:VAL:CG2	2.13	0.79
1:D:283:LEU:HD21	1:D:321:ARG:HE	1.47	0.79
1:B:107:GLU:HG2	1:B:201:THR:HG21	1.65	0.78
1:B:347:GLU:H	1:B:347:GLU:CD	1.90	0.77
1:B:46:ALA:O	1:B:48:GLU:N	2.16	0.77
1:A:283:LEU:HD23	1:A:321:ARG:NH1	2.00	0.76
1:B:12:ASP:OD2	1:B:14:ARG:HD3	1.86	0.75
1:A:107:GLU:HG2	1:A:201:THR:HG21	1.68	0.74
1:D:283:LEU:CD2	1:D:321:ARG:HE	2.03	0.72
1:C:279:ALA:H	1:C:311:GLN:NE2	1.86	0.71
1:D:107:GLU:HG2	1:D:201:THR:HG21	1.71	0.71
1:C:344:MSE:HE1	1:C:353:VAL:CG2	2.19	0.71
1:B:434:SER:H	1:B:455:ASN:HD21	1.37	0.71
1:D:52:THR:HG23	3:D:540:HOH:O	1.91	0.71
1:C:436:ASN:HD22	1:C:439:THR:H	1.39	0.70
1:A:252:THR:O	1:A:256:GLU:HG3	1.93	0.69
1:A:434:SER:H	1:A:455:ASN:HD21	1.40	0.69
1:D:59:ASP:OD1	1:D:62:ARG:NH1	2.24	0.69
1:B:279:ALA:H	1:B:311:GLN:NE2	1.91	0.68
1:A:439:THR:HG21	3:A:557:HOH:O	1.95	0.67
1:B:279:ALA:HA	1:B:314:ILE:HG12	1.75	0.67
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.60	0.67
1:D:279:ALA:H	1:D:311:GLN:NE2	1.91	0.67
1:C:434:SER:H	1:C:455:ASN:HD21	1.43	0.67
1:C:442:GLN:HE21	1:C:442:GLN:HA	1.58	0.66
1:A:354:HIS:O	1:A:358:THR:HG23	1.95	0.65
1:D:231:GLN:O	1:D:235:GLU:HG2	1.97	0.64
1:A:42:SER:OG	1:A:45:HIS:HD2	1.81	0.63
1:D:279:ALA:HA	1:D:314:ILE:HG12	1.80	0.62
1:A:52:THR:HG23	3:A:617:HOH:O	2.00	0.61
1:A:248:VAL:O	1:A:252:THR:HG23	2.00	0.61
1:A:283:LEU:HD23	1:A:321:ARG:CZ	2.31	0.61
1:C:9:ASP:OD1	1:C:11:ASN:HB2	2.00	0.61
1:A:160:VAL:HG23	3:A:705:HOH:O	1.99	0.61
1:C:313:GLY:HA2	3:C:556:HOH:O	1.99	0.61
1:A:8:PRO:HG2	1:A:378:ALA:HB1	1.83	0.60
1:C:344:MSE:HE2	1:C:350:ALA:HA	1.84	0.60
1:D:80:MSE:CE	1:D:84:GLU:HB3	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LEU:HB3	1:C:321:ARG:NH1	2.18	0.59
1:B:46:ALA:O	1:B:48:GLU:HG2	2.02	0.59
1:C:59:ASP:OD2	1:C:63:LYS:NZ	2.35	0.58
1:D:434:SER:H	1:D:455:ASN:HD21	1.52	0.58
1:A:300:GLN:HE22	1:A:345:ILE:H	1.49	0.58
1:D:300:GLN:HE22	1:D:345:ILE:H	1.49	0.58
1:C:42:SER:OG	1:C:45:HIS:HD2	1.85	0.58
1:A:436:ASN:HB3	1:A:439:THR:HG23	1.86	0.57
1:B:344:MSE:HE2	1:B:350:ALA:HA	1.85	0.57
1:A:52:THR:CG2	3:A:617:HOH:O	2.51	0.57
1:A:117:GLN:HE22	1:A:297:ASN:HD22	1.52	0.57
1:A:276:ILE:HD12	1:A:276:ILE:N	2.19	0.57
1:B:117:GLN:HE22	1:B:297:ASN:HD22	1.52	0.57
1:B:344:MSE:CE	1:B:353:VAL:HG21	2.22	0.57
1:C:117:GLN:HE22	1:C:297:ASN:HD22	1.54	0.56
1:D:252:THR:O	1:D:256:GLU:HG3	2.06	0.56
1:C:283:LEU:HB3	1:C:321:ARG:HH11	1.70	0.55
1:A:279:ALA:N	1:A:311:GLN:HE21	1.94	0.55
1:A:140:GLU:HG2	3:A:641:HOH:O	2.07	0.55
1:B:344:MSE:CE	1:B:350:ALA:HA	2.38	0.55
1:C:344:MSE:HE3	1:C:349:HIS:CD2	2.42	0.54
1:B:436:ASN:HD22	1:B:439:THR:H	1.54	0.54
1:D:298:ALA:HB1	1:D:344:MSE:CE	2.38	0.54
1:D:298:ALA:HB1	1:D:344:MSE:HE1	1.90	0.54
1:B:300:GLN:HE22	1:B:345:ILE:N	2.06	0.54
1:C:358:THR:O	1:C:362:THR:HG23	2.07	0.53
1:C:173:PHE:CD1	1:C:201:THR:HB	2.43	0.53
1:C:140:GLU:HG2	3:C:692:HOH:O	2.07	0.53
1:D:227:ASP:HB2	1:D:228:PRO:HD3	1.91	0.52
1:B:18:LYS:HE2	3:B:584:HOH:O	2.08	0.52
1:C:354:HIS:O	1:C:358:THR:HG23	2.09	0.52
1:B:354:HIS:HB2	1:B:382:TYR:HE1	1.75	0.52
1:C:262:VAL:HG22	1:D:252:THR:HG22	1.90	0.52
1:B:358:THR:O	1:B:362:THR:HG23	2.10	0.52
1:C:344:MSE:HE3	1:C:349:HIS:HD2	1.75	0.51
1:B:433:TRP:HA	1:B:455:ASN:ND2	2.25	0.51
1:B:300:GLN:HE22	1:B:345:ILE:H	1.57	0.51
1:B:12:ASP:OD2	1:B:14:ARG:CD	2.57	0.51
1:C:393:ASP:HA	1:C:398:ARG:HH21	1.75	0.50
1:B:442:GLN:HA	1:B:442:GLN:NE2	2.20	0.50
1:D:160:VAL:HG12	1:D:188:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ALA:N	1:B:311:GLN:HE21	2.01	0.49
1:C:436:ASN:ND2	1:C:439:THR:H	2.09	0.49
1:A:436:ASN:HD22	1:A:439:THR:H	1.60	0.49
1:A:129:TRP:CE2	1:A:181:PRO:HG3	2.48	0.49
1:A:369:LEU:HD13	1:A:384:PRO:O	2.13	0.49
1:D:436:ASN:ND2	1:D:439:THR:H	2.11	0.49
1:A:59:ASP:OD1	1:A:62:ARG:NH1	2.46	0.49
1:C:300:GLN:HE22	1:C:345:ILE:H	1.61	0.48
1:B:192:LEU:HB3	1:B:221:VAL:HG22	1.95	0.48
1:C:372:GLU:OE1	3:C:642:HOH:O	2.20	0.48
1:D:179:ARG:NH2	1:D:268:GLU:HG3	2.29	0.48
1:D:308:LEU:HG	1:D:310:VAL:HG22	1.96	0.48
1:A:374:ILE:CD1	1:A:383:ALA:HB2	2.37	0.48
1:B:175:ILE:HD13	1:B:245:THR:HG21	1.95	0.48
1:C:429:SER:HA	1:C:451:ARG:O	2.13	0.48
1:D:436:ASN:HD22	1:D:439:THR:H	1.62	0.48
1:A:286:ALA:O	1:A:290:ILE:HG12	2.13	0.48
1:A:111:VAL:HG22	1:A:198:THR:HG21	1.94	0.47
1:A:124:PHE:HE2	3:A:584:HOH:O	1.96	0.47
1:C:279:ALA:HA	1:C:314:ILE:HG21	1.96	0.47
1:B:178:GLU:HG2	1:B:478:LEU:HD21	1.96	0.47
1:D:80:MSE:HE1	1:D:88:LEU:HD12	1.97	0.47
1:B:436:ASN:ND2	1:B:439:THR:H	2.13	0.47
1:C:252:THR:HG22	1:D:262:VAL:HG22	1.97	0.47
1:D:429:SER:HA	1:D:451:ARG:O	2.14	0.47
1:D:117:GLN:HE22	1:D:297:ASN:HD22	1.62	0.47
1:B:107:GLU:OE1	1:B:172:PRO:HD2	2.15	0.46
1:A:358:THR:O	1:A:362:THR:HG23	2.15	0.46
1:A:283:LEU:HB3	1:A:321:ARG:HH11	1.80	0.46
1:B:129:TRP:CE2	1:B:181:PRO:HG3	2.50	0.46
1:C:344:MSE:CE	1:C:353:VAL:HG21	2.31	0.46
1:A:300:GLN:HE22	1:A:345:ILE:N	2.13	0.46
1:A:476:ARG:O	1:A:485:GLU:CG	2.63	0.46
1:C:433:TRP:HA	1:C:455:ASN:ND2	2.30	0.46
1:A:193:LYS:HG3	1:A:229:ALA:HB1	1.98	0.46
1:D:140:GLU:HG2	3:D:570:HOH:O	2.16	0.46
1:B:241:MSE:SE	1:B:264:ARG:HD2	2.66	0.46
1:B:433:TRP:HA	1:B:455:ASN:HD22	1.80	0.46
1:B:206:ALA:HB2	1:B:221:VAL:CG2	2.47	0.45
1:B:107:GLU:O	1:B:111:VAL:HG13	2.16	0.45
1:B:426:PHE:O	1:B:470:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:TRP:HA	1:A:455:ASN:ND2	2.31	0.45
1:C:461:THR:HB	1:C:463:GLU:OE2	2.16	0.45
1:A:429:SER:HA	1:A:451:ARG:O	2.15	0.45
1:A:25:VAL:HG13	1:A:64:ALA:HA	1.99	0.45
1:A:476:ARG:O	1:A:485:GLU:HG3	2.17	0.45
1:D:18:LYS:HD2	1:D:49:VAL:O	2.17	0.44
1:D:25:VAL:HG13	1:D:64:ALA:HA	2.00	0.44
1:A:206:ALA:HB2	1:A:221:VAL:CG2	2.47	0.44
1:C:286:ALA:O	1:C:290:ILE:HG12	2.18	0.44
1:D:206:ALA:HB2	1:D:221:VAL:HG23	1.98	0.44
1:C:171:PHE:HB3	1:C:174:ILE:HB	1.99	0.44
1:B:429:SER:HA	1:B:451:ARG:O	2.18	0.44
1:B:179:ARG:NH2	1:B:268:GLU:HG3	2.33	0.44
1:A:53:TRP:CD2	1:A:199:SER:HB2	2.53	0.44
1:B:357:VAL:HG11	1:B:371:GLY:HA2	1.99	0.44
1:D:125:CYS:SG	1:D:174:ILE:HA	2.58	0.43
1:B:125:CYS:SG	1:B:174:ILE:HA	2.58	0.43
1:B:331:PHE:CB	1:B:341:ILE:HB	2.48	0.43
1:C:18:LYS:HD3	1:C:49:VAL:O	2.18	0.43
1:B:25:VAL:HG13	1:B:64:ALA:HA	2.00	0.43
1:D:42:SER:OG	1:D:45:HIS:HD2	2.02	0.43
1:D:182:TRP:CH2	1:D:478:LEU:HD22	2.53	0.43
1:A:344:MSE:HE2	1:A:344:MSE:HA	2.01	0.43
1:C:125:CYS:SG	1:C:174:ILE:HA	2.59	0.42
1:D:129:TRP:CE2	1:D:181:PRO:HG3	2.54	0.42
1:A:206:ALA:HB2	1:A:221:VAL:HG23	2.01	0.42
1:C:344:MSE:CE	1:C:349:HIS:CD2	3.02	0.42
1:A:300:GLN:NE2	1:A:345:ILE:H	2.17	0.42
1:D:462:PRO:HA	1:D:478:LEU:HD13	2.01	0.42
1:B:206:ALA:HB2	1:B:221:VAL:HG23	2.02	0.42
1:B:368:LEU:HD11	1:B:388:ALA:HB2	2.02	0.42
1:B:326:SER:HB3	1:B:369:LEU:HD12	2.00	0.42
1:B:354:HIS:O	1:B:358:THR:HG23	2.20	0.41
1:D:470:LYS:HE3	3:D:562:HOH:O	2.20	0.41
1:A:203:ILE:HD11	1:A:223:THR:HG21	2.02	0.41
1:A:436:ASN:ND2	1:A:439:THR:H	2.17	0.41
1:C:476:ARG:O	1:C:485:GLU:CG	2.69	0.41
1:D:241:MSE:SE	1:D:264:ARG:HD2	2.69	0.41
1:A:171:PHE:HB3	1:A:174:ILE:HB	2.02	0.41
1:B:77:TRP:HB3	1:B:78:PRO:HD3	2.02	0.41
1:A:283:LEU:HD21	1:A:317:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLN:HE22	1:D:297:ASN:ND2	2.19	0.41
1:A:23:MSE:HG3	1:A:54:PRO:HG2	2.02	0.41
1:B:204:ARG:O	1:B:208:LEU:HG	2.20	0.41
1:B:375:GLY:C	1:B:377:GLU:HA	2.45	0.41
1:D:376:ARG:HG3	3:D:608:HOH:O	2.21	0.41
1:A:179:ARG:NH2	1:A:268:GLU:HG3	2.36	0.40
1:A:192:LEU:HB3	1:A:221:VAL:HG22	2.03	0.40
1:B:286:ALA:O	1:B:290:ILE:HG12	2.21	0.40
1:D:354:HIS:O	1:D:358:THR:HG23	2.21	0.40
1:B:53:TRP:CD2	1:B:199:SER:HB2	2.56	0.40
1:D:358:THR:O	1:D:362:THR:HG23	2.21	0.40
1:D:444:ILE:HD12	1:D:444:ILE:HA	1.96	0.40
1:D:178:GLU:HG2	1:D:478:LEU:HD21	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	503/528 (95%)	490 (97%)	13 (3%)	0	100	100
1	B	498/528 (94%)	482 (97%)	15 (3%)	1 (0%)	43	42
1	C	503/528 (95%)	490 (97%)	13 (3%)	0	100	100
1	D	501/528 (95%)	486 (97%)	15 (3%)	0	100	100
All	All	2005/2112 (95%)	1948 (97%)	56 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	GLY

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	387/401 (96%)	368 (95%)	19 (5%)	22	20
1	B	385/401 (96%)	366 (95%)	19 (5%)	22	20
1	C	388/401 (97%)	375 (97%)	13 (3%)	32	33
1	D	386/401 (96%)	374 (97%)	12 (3%)	35	37
All	All	1546/1604 (96%)	1483 (96%)	63 (4%)	27	26

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

Mol	Chain	Res	Type
1	A	0	VAL
1	A	24	LEU
1	A	52	THR
1	A	253	LYS
1	A	262	VAL
1	A	263	LYS
1	A	276	ILE
1	A	297	ASN
1	A	358	THR
1	A	367	LEU
1	A	369	LEU
1	A	374	ILE
1	A	402	PHE
1	A	412	LYS
1	A	436	ASN
1	A	439	THR
1	A	442	GLN
1	A	444	ILE
1	A	504	THR
1	B	14	ARG
1	B	16	ARG
1	B	24	LEU
1	B	31	ASP
1	B	52	THR

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Mol	Chain	Res	Type
1	B	111	VAL
1	B	253	LYS
1	B	265	VAL
1	B	314	ILE
1	B	347	GLU
1	B	362	THR
1	B	363	SER
1	B	367	LEU
1	B	369	LEU
1	B	402	PHE
1	B	412	LYS
1	B	436	ASN
1	B	442	GLN
1	B	488	GLN
1	C	24	LEU
1	C	52	THR
1	C	160	VAL
1	C	190	VAL
1	C	231	GLN
1	C	283	LEU
1	C	338	ARG
1	C	367	LEU
1	C	377	GLU
1	C	402	PHE
1	C	412	LYS
1	C	442	GLN
1	C	504	THR
1	D	174	ILE
1	D	262	VAL
1	D	297	ASN
1	D	310	VAL
1	D	314	ILE
1	D	367	LEU
1	D	369	LEU
1	D	398	ARG
1	D	402	PHE
1	D	436	ASN
1	D	442	GLN
1	D	444	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	297	ASN
1	A	300	GLN
1	A	311	GLN
1	A	436	ASN
1	A	442	GLN
1	A	455	ASN
1	A	488	GLN
1	B	22	GLN
1	B	296	HIS
1	B	297	ASN
1	B	300	GLN
1	B	311	GLN
1	B	436	ASN
1	B	442	GLN
1	B	455	ASN
1	B	488	GLN
1	C	45	HIS
1	C	135	GLN
1	C	231	GLN
1	C	297	ASN
1	C	300	GLN
1	C	311	GLN
1	C	349	HIS
1	C	436	ASN
1	C	442	GLN
1	C	455	ASN
1	C	488	GLN
1	D	45	HIS
1	D	135	GLN
1	D	142	GLN
1	D	296	HIS
1	D	297	ASN
1	D	300	GLN
1	D	311	GLN
1	D	436	ASN
1	D	442	GLN
1	D	455	ASN
1	D	488	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	497/528 (94%)	-0.44	5 (1%) 79 79	7, 13, 24, 41	0
1	B	495/528 (93%)	0.30	46 (9%) 14 13	7, 19, 41, 57	0
1	C	497/528 (94%)	-0.32	8 (1%) 70 70	6, 14, 27, 39	0
1	D	496/528 (93%)	-0.11	7 (1%) 73 73	9, 17, 29, 43	0
All	All	1985/2112 (93%)	-0.14	66 (3%) 49 48	6, 15, 33, 57	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	ALA	7.5
1	D	227	ASP	5.1
1	B	378	ALA	4.0
1	B	375	GLY	3.9
1	B	2	LEU	3.8
1	B	347	GLU	3.7
1	B	381	TYR	3.7
1	D	228	PRO	3.6
1	B	367	LEU	3.4
1	B	374	ILE	3.4
1	B	359	ALA	3.4
1	C	504	THR	3.1
1	B	7	ALA	3.1
1	B	365	ALA	3.1
1	B	283	LEU	3.0
1	B	353	VAL	3.0
1	C	0	VAL	3.0
1	C	17	ILE	2.9
1	B	6	ILE	2.9
1	B	379	GLY	2.9
1	A	504	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	249	ARG	2.8
1	B	383	ALA	2.7
1	B	358	THR	2.7
1	B	16	ARG	2.7
1	A	150	ASP	2.7
1	B	380	LEU	2.7
1	B	4	ASN	2.7
1	B	361	ILE	2.7
1	B	321	ARG	2.7
1	B	371	GLY	2.7
1	B	504	THR	2.6
1	C	249	ARG	2.6
1	B	370	GLY	2.6
1	C	313	GLY	2.6
1	D	231	GLN	2.5
1	B	409	LEU	2.4
1	B	364	GLY	2.4
1	B	377	GLU	2.4
1	D	2	LEU	2.4
1	B	332	GLY	2.4
1	D	229	ALA	2.3
1	A	503	PHE	2.3
1	A	0	VAL	2.3
1	B	356	TYR	2.3
1	B	8	PRO	2.3
1	B	368	LEU	2.3
1	B	5	PHE	2.3
1	B	339	THR	2.3
1	B	362	THR	2.2
1	B	11	ASN	2.2
1	B	398	ARG	2.2
1	B	387	PHE	2.2
1	D	504	THR	2.2
1	C	376	ARG	2.2
1	C	11	ASN	2.2
1	C	498	ARG	2.2
1	A	249	ARG	2.1
1	B	372	GLU	2.1
1	B	385	THR	2.1
1	B	9	ASP	2.1
1	B	59	ASP	2.1
1	B	341	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	354	HIS	2.0
1	B	348	ALA	2.0
1	B	313	GLY	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	601	1/1	0.99	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.