



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 01:26 AM EDT

PDB ID : 3MY7  
Title : The Crystal Structure of the ACDH domain of an Alcohol Dehydrogenase from *Vibrio parahaemolyticus* to 2.25Å  
Authors : Stein, A.J.; Weger, A.; Volkart, L.; Gu, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : unknown  
Resolution : 2.30 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

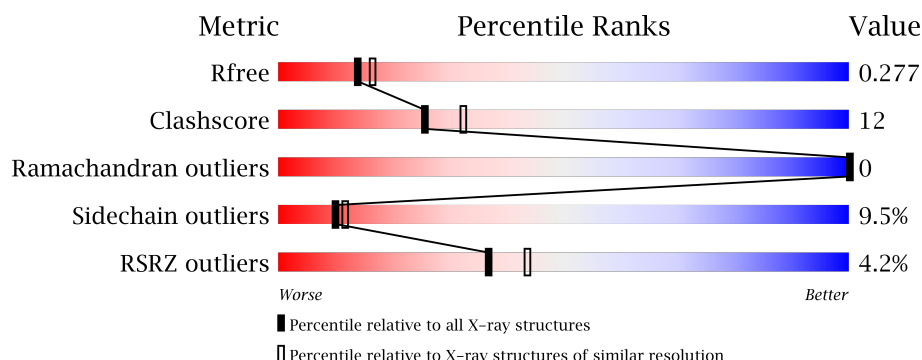
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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  $\geq 3$ , 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	452	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	452	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	452	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	452	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11963 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 Alcohol dehydrogenase/acetaldehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	Se	0	0	0
			2959	1870	502	573	3	11			
1	B	415	Total	C	N	O	S	Se	0	0	0
			2977	1879	510	575	2	11			
1	C	416	Total	C	N	O	S	Se	0	1	0
			3022	1907	518	583	3	11			
1	D	409	Total	C	N	O	S	Se	0	0	0
			2901	1824	502	562	2	11			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

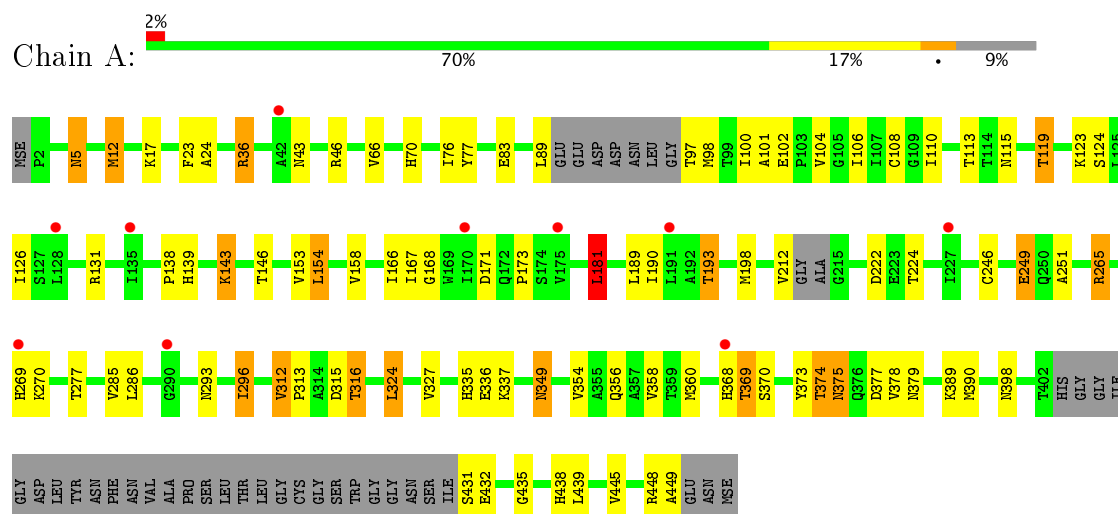
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	20	Total	O	0	0
			20	20		
3	C	30	Total	O	0	0
			30	30		
3	D	17	Total	O	0	0
			17	17		

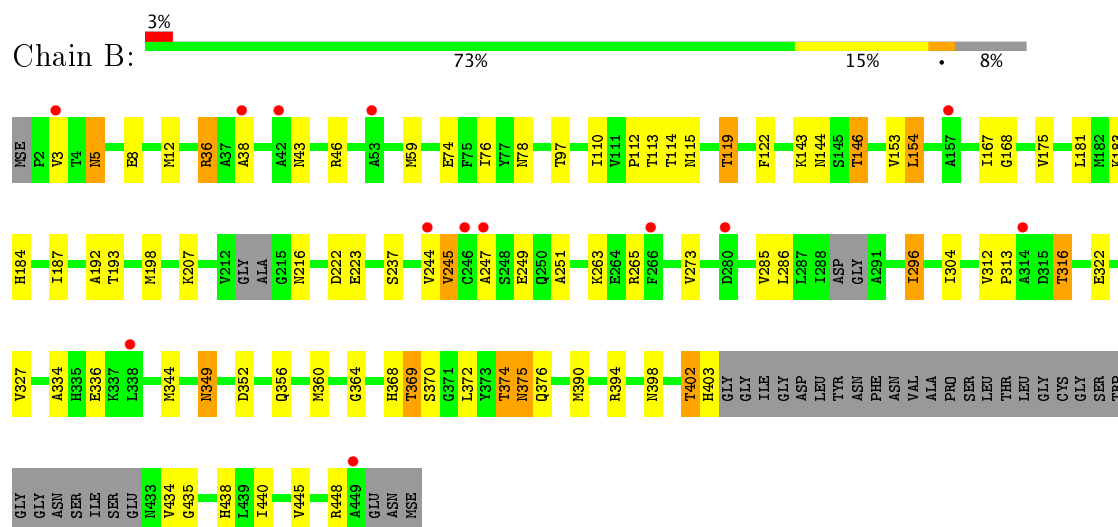
### 3 Residue-property plots

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.

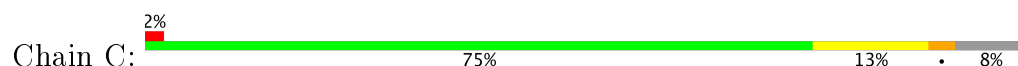
- Molecule 1: Alcohol dehydrogenase/acetaldehyde dehydrogenase

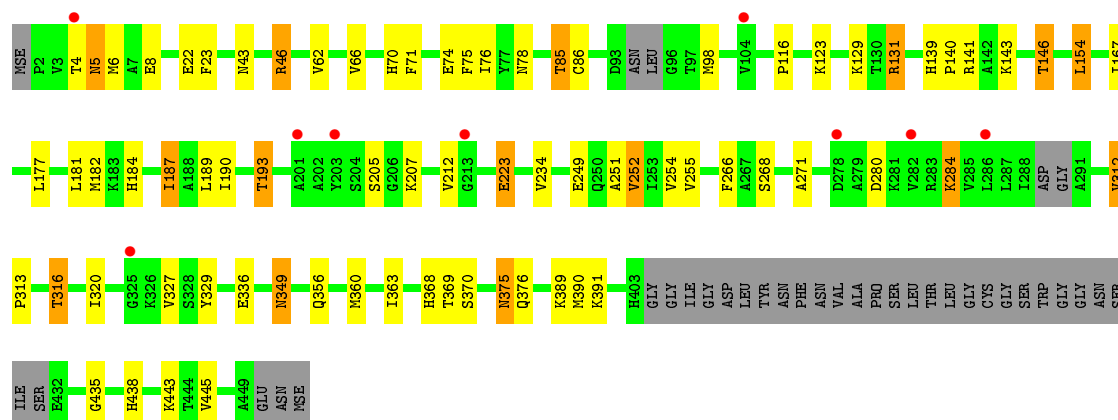


- Molecule 1: Alcohol dehydrogenase/acetaldehyde dehydrogenase

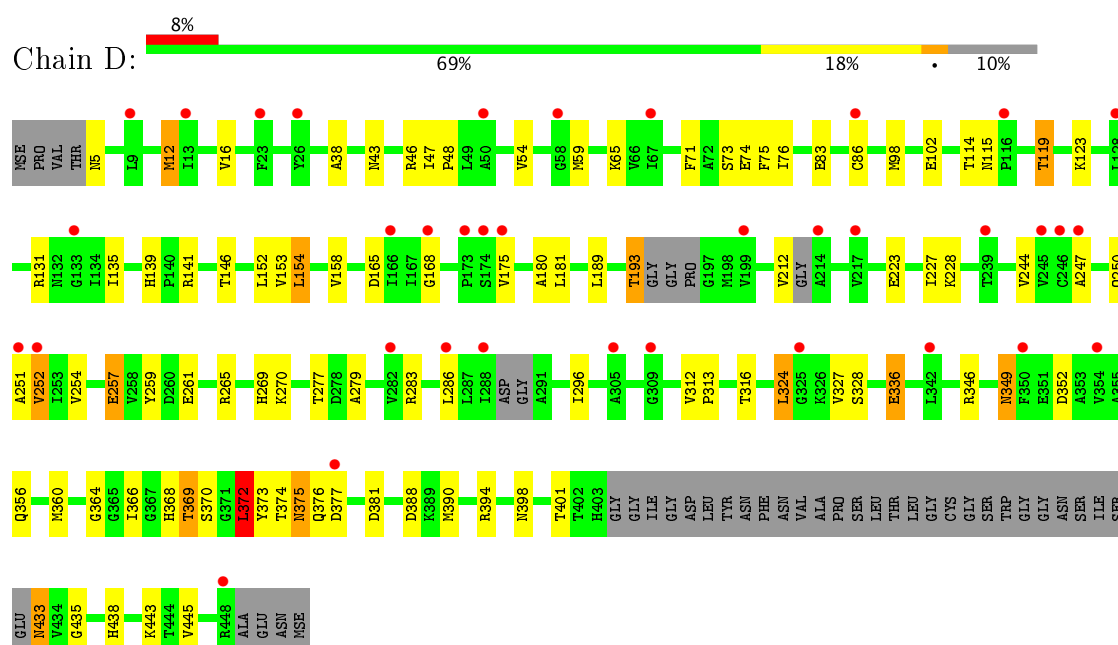


- Molecule 1: Alcohol dehydrogenase/acetaldehyde dehydrogenase





• Molecule 1: Alcohol dehydrogenase/acetaldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.65Å 145.49Å 91.99Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 46.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.30) 99.7 (46.44-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.229 , 0.281 0.229 , 0.277	Depositor DCC
$R_{free}$ test set	3748 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1929e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.67	0/2991	0.70	1/4055 (0.0%)
1	B	0.53	0/3008	0.65	0/4078
1	C	0.63	0/3057	0.69	0/4137
1	D	0.54	0/2927	0.64	1/3971 (0.0%)
All	All	0.60	0/11983	0.67	2/16241 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	372	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	181	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2959	0	2913	74	0
1	B	2977	0	2911	79	0
1	C	3022	0	2994	57	0
1	D	2901	0	2800	72	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	33	0	0	0	0
3	B	20	0	0	2	0
3	C	30	0	0	1	0
3	D	17	0	0	2	0
All	All	11963	0	11618	280	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 12.

All (280) 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:A:368:HIS:CD2	1:A:369:THR:HG22	1.53	1.43
1:A:368:HIS:HD2	1:A:369:THR:CG2	1.45	1.28
1:B:12:MSE:CE	1:B:168:GLY:HA3	1.69	1.22
1:B:368:HIS:CD2	1:B:369:THR:HG22	1.82	1.15
1:D:368:HIS:HD2	1:D:369:THR:HG22	1.13	1.10
1:B:12:MSE:HE1	1:B:168:GLY:HA3	1.23	1.09
1:D:12:MSE:HE3	1:D:168:GLY:HA3	1.21	1.08
1:B:368:HIS:HD2	1:B:369:THR:CG2	1.67	1.07
1:B:368:HIS:HD2	1:B:369:THR:HG22	0.90	1.07
1:A:110:ILE:HD13	1:A:198:MSE:HE2	1.43	0.99
1:D:368:HIS:CD2	1:D:369:THR:HG22	2.04	0.92
1:C:368:HIS:HD2	1:C:369:THR:OG1	1.50	0.92
1:A:368:HIS:HD2	1:A:369:THR:HG22	0.75	0.92
1:B:435:GLY:H	1:B:438:HIS:HD2	1.13	0.91
1:A:435:GLY:H	1:A:438:HIS:HD2	1.18	0.91
1:C:123:LYS:HZ1	1:C:193:THR:HG22	1.32	0.91
1:B:43:ASN:O	1:B:46:ARG:HG3	1.73	0.88
1:D:12:MSE:CE	1:D:168:GLY:HA3	2.04	0.88
1:B:12:MSE:HE3	1:B:168:GLY:HA3	1.56	0.87
1:C:85:THR:HG21	1:C:129:LYS:O	1.77	0.85
1:D:43:ASN:HD21	1:D:46:ARG:HH21	1.18	0.85
1:D:115:ASN:O	1:D:119:THR:HG23	1.76	0.84
1:A:327:VAL:H	1:A:356:GLN:HE21	1.24	0.83
1:A:368:HIS:CD2	1:A:369:THR:CG2	2.34	0.83
1:C:223:GLU:HG3	1:C:255:VAL:HG11	1.62	0.82
1:A:222:ASP:OD2	1:A:374:THR:HG23	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:PRO:O	1:A:316:THR:HG22	1.80	0.82
1:C:123:LYS:NZ	1:C:193:THR:HG22	1.95	0.81
1:D:364:GLY:C	1:D:366:ILE:H	1.79	0.81
1:A:110:ILE:CD1	1:A:198:MSE:HE2	2.11	0.81
1:C:368:HIS:CD2	1:C:369:THR:OG1	2.34	0.79
1:D:327:VAL:H	1:D:356:GLN:HE21	1.26	0.79
1:D:114:THR:OG1	1:D:244:VAL:HG13	1.83	0.79
1:B:435:GLY:H	1:B:438:HIS:CD2	2.01	0.77
1:B:76:ILE:HD13	1:B:122:PHE:HD1	1.49	0.77
1:D:193:THR:HB	1:D:212:VAL:HB	1.65	0.76
1:A:46:ARG:HG2	1:A:66:VAL:HG13	1.68	0.75
1:C:154:LEU:HG	1:C:167:ILE:HB	1.67	0.75
1:A:435:GLY:H	1:A:438:HIS:CD2	2.04	0.75
1:D:368:HIS:HD2	1:D:369:THR:CG2	1.96	0.74
1:B:322:GLU:HG2	1:B:344:MSE:HE3	1.69	0.74
1:A:189:LEU:HD23	1:A:190:ILE:N	2.03	0.73
1:C:6:MSE:HE2	1:C:177:LEU:HD23	1.70	0.73
1:D:43:ASN:ND2	1:D:46:ARG:HH21	1.87	0.73
1:C:435:GLY:H	1:C:438:HIS:HD2	1.34	0.73
1:B:375:ASN:HD22	1:B:375:ASN:C	1.90	0.72
1:B:263:LYS:HZ2	1:B:273:VAL:HG11	1.52	0.72
1:C:123:LYS:NZ	1:C:193:THR:CG2	2.51	0.72
1:D:327:VAL:H	1:D:356:GLN:NE2	1.87	0.72
1:C:139:HIS:HD2	1:C:141:ARG:H	1.35	0.72
1:D:12:MSE:HE2	1:D:16:VAL:CG2	2.20	0.72
1:D:86:CYS:SG	1:D:131:ARG:NH1	2.63	0.72
1:A:110:ILE:HD13	1:A:198:MSE:CE	2.20	0.71
1:A:265:ARG:HG2	1:A:265:ARG:HH21	1.54	0.71
1:B:12:MSE:HE1	1:B:168:GLY:CA	2.14	0.71
1:B:263:LYS:NZ	1:B:322:GLU:CD	2.45	0.70
1:C:327:VAL:H	1:C:356:GLN:HE21	1.37	0.70
1:A:115:ASN:O	1:A:119:THR:HG23	1.91	0.70
1:D:12:MSE:HE2	1:D:16:VAL:HG21	1.74	0.69
1:A:97:THR:HA	1:A:445:VAL:O	1.93	0.69
1:C:375:ASN:C	1:C:375:ASN:HD22	1.95	0.68
1:D:59:MSE:HE3	1:D:244:VAL:HG21	1.76	0.68
1:A:123:LYS:HZ2	1:A:193:THR:HG23	1.57	0.68
1:A:5:ASN:C	1:A:5:ASN:HD22	1.95	0.68
1:B:59:MSE:CE	1:B:114:THR:HA	2.23	0.68
1:D:364:GLY:C	1:D:366:ILE:N	2.47	0.67
1:B:368:HIS:CD2	1:B:369:THR:CG2	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASP:OD2	1:B:374:THR:HG22	1.96	0.66
1:C:146:THR:HG21	3:C:479:HOH:O	1.95	0.66
1:B:263:LYS:HZ3	1:B:322:GLU:CD	1.98	0.66
1:B:286:LEU:HD23	1:B:296:ILE:HD13	1.77	0.65
1:B:376:GLN:HG3	1:B:398:ASN:ND2	2.11	0.65
1:B:59:MSE:HE1	1:B:114:THR:HA	1.79	0.65
1:D:364:GLY:O	1:D:366:ILE:N	2.29	0.65
1:A:123:LYS:NZ	1:A:193:THR:CG2	2.60	0.64
1:A:89:LEU:HD11	1:A:101:ALA:HB2	1.79	0.64
1:B:112:PRO:HD3	1:B:193:THR:HB	1.80	0.64
1:A:313:PRO:O	1:A:316:THR:CG2	2.46	0.64
1:A:327:VAL:H	1:A:356:GLN:NE2	1.94	0.64
1:D:327:VAL:N	1:D:356:GLN:HE21	1.95	0.63
1:C:74[A]:GLU:HA	1:C:74[A]:GLU:OE1	1.98	0.63
1:D:59:MSE:HE1	1:D:114:THR:HA	1.80	0.63
1:A:375:ASN:C	1:A:375:ASN:HD22	2.00	0.63
1:B:285:VAL:HG12	1:B:296:ILE:HD12	1.81	0.63
1:A:43:ASN:O	1:A:46:ARG:HB2	1.99	0.62
1:D:251:ALA:HB3	1:D:360:MSE:HE1	1.81	0.62
1:A:154:LEU:HG	1:A:167:ILE:HB	1.81	0.62
1:A:286:LEU:HA	1:A:296:ILE:HD12	1.81	0.62
1:D:16:VAL:HG22	1:D:165:ASP:O	2.00	0.62
1:B:448:ARG:H	1:C:376:GLN:HE22	1.47	0.61
1:C:329:TYR:HA	1:C:363:ILE:HD11	1.83	0.60
1:B:184:HIS:O	1:B:207:LYS:NZ	2.32	0.60
1:A:113:THR:HG23	1:A:139:HIS:CG	2.37	0.60
1:B:76:ILE:CD1	1:B:122:PHE:HD1	2.12	0.60
1:D:251:ALA:HB3	1:D:360:MSE:SE	2.52	0.60
1:B:5:ASN:HD22	1:B:5:ASN:C	2.05	0.60
1:D:312:VAL:CG1	1:D:316:THR:HG21	2.32	0.60
1:B:313:PRO:O	1:B:316:THR:HG23	2.03	0.59
1:B:376:GLN:HG3	1:B:398:ASN:HD22	1.68	0.59
1:D:369:THR:HB	1:D:394:ARG:HB2	1.84	0.59
1:B:222:ASP:OD2	1:B:374:THR:CG2	2.51	0.58
1:A:123:LYS:NZ	1:A:193:THR:HG23	2.18	0.58
1:C:139:HIS:CD2	1:C:141:ARG:H	2.19	0.58
1:B:251:ALA:HB3	1:B:360:MSE:SE	2.53	0.58
1:C:123:LYS:HZ2	1:C:193:THR:CG2	2.16	0.58
1:D:251:ALA:CB	1:D:360:MSE:HE1	2.34	0.58
1:B:369:THR:HB	1:B:394:ARG:HB2	1.86	0.58
1:D:71:PHE:O	1:D:75:PHE:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HG21	1:A:198:MSE:HG2	1.84	0.57
1:B:43:ASN:O	1:B:46:ARG:CG	2.49	0.57
1:B:154:LEU:HG	1:B:167:ILE:HB	1.86	0.57
1:B:76:ILE:HD13	1:B:122:PHE:CD1	2.36	0.57
1:C:266:PHE:CG	1:C:320:ILE:HD13	2.39	0.56
1:C:329:TYR:HA	1:C:363:ILE:CD1	2.35	0.56
1:A:143:LYS:HE2	1:A:171:ASP:O	2.06	0.56
1:C:6:MSE:CE	1:C:177:LEU:HD23	2.35	0.56
1:A:324:LEU:H	1:A:324:LEU:HD23	1.70	0.56
1:D:435:GLY:H	1:D:438:HIS:HD2	1.52	0.56
1:A:312:VAL:HG13	1:A:316:THR:CG2	2.36	0.56
1:C:5:ASN:C	1:C:5:ASN:HD22	2.09	0.56
1:B:296:ILE:HG12	1:B:304:ILE:HG12	1.88	0.56
1:C:313:PRO:O	1:C:316:THR:HG23	2.04	0.56
1:D:12:MSE:HE1	1:D:135:ILE:HG12	1.87	0.56
1:C:251:ALA:HB3	1:C:360:MSE:SE	2.56	0.55
1:B:5:ASN:ND2	1:B:8:GLU:H	2.03	0.55
1:B:12:MSE:HE3	1:B:168:GLY:CA	2.34	0.55
1:C:370:SER:CB	1:C:390:MSE:HE2	2.37	0.55
1:B:76:ILE:CD1	1:B:122:PHE:CD1	2.89	0.55
1:A:370:SER:CB	1:A:390:MSE:HE2	2.36	0.55
1:A:249:GLU:CD	1:A:249:GLU:H	2.10	0.55
1:A:46:ARG:HD2	1:A:70:HIS:HB2	1.89	0.55
1:B:237:SER:HB3	1:B:402:THR:HG22	1.89	0.55
1:A:123:LYS:HZ2	1:A:193:THR:CG2	2.19	0.54
1:B:115:ASN:O	1:B:119:THR:HG23	2.07	0.54
1:A:143:LYS:HD2	1:A:173:PRO:HD2	1.90	0.54
1:A:36:ARG:HG2	1:A:77:TYR:CZ	2.43	0.54
1:D:12:MSE:CE	1:D:16:VAL:HG21	2.38	0.54
1:D:327:VAL:N	1:D:356:GLN:NE2	2.56	0.53
1:B:376:GLN:HE21	1:B:398:ASN:HD22	1.54	0.53
1:A:12:MSE:HE1	1:A:168:GLY:HA3	1.91	0.53
1:D:247:ALA:O	1:D:401:THR:HG21	2.09	0.53
1:B:390:MSE:O	1:C:443:LYS:HE2	2.09	0.52
1:B:435:GLY:N	1:B:438:HIS:HD2	1.95	0.52
1:A:375:ASN:C	1:A:375:ASN:ND2	2.63	0.52
1:C:252:VAL:HG13	1:C:254:VAL:CG2	2.40	0.52
1:C:223:GLU:HG3	1:C:255:VAL:CG1	2.35	0.52
1:D:47:ILE:HB	1:D:48:PRO:HD3	1.92	0.52
1:C:266:PHE:CD2	1:C:320:ILE:HD13	2.46	0.51
1:B:376:GLN:HE21	1:B:398:ASN:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD22	1:A:158:VAL:HG23	1.92	0.51
1:A:375:ASN:ND2	1:A:377:ASP:H	2.09	0.51
1:A:435:GLY:N	1:A:438:HIS:HD2	1.99	0.51
1:B:59:MSE:HE2	1:B:114:THR:HA	1.93	0.50
1:D:313:PRO:O	1:D:316:THR:HG23	2.11	0.50
1:C:71:PHE:O	1:C:75:PHE:HB3	2.11	0.50
1:D:59:MSE:CE	1:D:114:THR:HA	2.40	0.50
1:A:293:ASN:HB3	1:A:296:ILE:HD13	1.93	0.50
1:D:252:VAL:HG13	1:D:254:VAL:HG23	1.93	0.50
1:B:3:VAL:HG21	1:B:12:MSE:HG3	1.93	0.50
1:B:247:ALA:HB1	1:B:369:THR:CG2	2.42	0.50
1:C:271:ALA:HB1	1:C:320:ILE:CD1	2.41	0.50
1:C:98:MSE:HG2	1:C:445:VAL:HB	1.92	0.50
1:D:349:ASN:ND2	1:D:352:ASP:H	2.10	0.50
1:B:12:MSE:CE	1:B:168:GLY:CA	2.64	0.49
1:C:187:ILE:O	1:C:207:LYS:HE2	2.11	0.49
1:B:434:VAL:HA	1:B:438:HIS:CD2	2.48	0.49
1:D:139:HIS:HD2	1:D:141:ARG:H	1.60	0.49
1:A:222:ASP:OD2	1:A:374:THR:CG2	2.55	0.49
1:A:138:PRO:HB3	1:A:146:THR:HG21	1.93	0.49
1:B:322:GLU:HG2	1:B:344:MSE:CE	2.40	0.49
1:D:251:ALA:HB3	1:D:360:MSE:CE	2.42	0.49
1:A:265:ARG:CG	1:A:265:ARG:HH21	2.25	0.49
1:A:448:ARG:O	1:A:449:ALA:O	2.30	0.48
1:A:270:LYS:HG2	1:A:315:ASP:O	2.12	0.48
1:C:5:ASN:ND2	1:C:8:GLU:H	2.11	0.48
1:B:349:ASN:ND2	1:B:352:ASP:H	2.11	0.48
1:B:143:LYS:HG3	1:B:144:ASN:N	2.29	0.48
1:D:324:LEU:H	1:D:324:LEU:HD23	1.78	0.48
1:B:184:HIS:HB3	1:B:187:ILE:HD13	1.94	0.48
1:C:193:THR:HB	1:C:212:VAL:HB	1.94	0.48
1:A:224:THR:HG21	1:A:379:ASN:HD21	1.79	0.48
1:B:244:VAL:C	1:B:245:VAL:CG2	2.82	0.48
1:D:250:GLN:HG3	1:D:336:GLU:HA	1.95	0.48
1:D:123:LYS:NZ	1:D:193:THR:CG2	2.77	0.47
1:D:312:VAL:HG12	1:D:316:THR:HG21	1.96	0.47
1:B:97:THR:HA	1:B:445:VAL:O	2.14	0.47
1:D:390:MSE:HA	3:D:459:HOH:O	2.14	0.47
1:D:98:MSE:HG3	1:D:445:VAL:HB	1.97	0.47
1:B:237:SER:HB3	1:B:402:THR:CG2	2.44	0.47
1:B:285:VAL:HG12	1:B:296:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ALA:HB1	1:B:369:THR:HG21	1.96	0.47
1:A:17:LYS:HA	1:A:106:ILE:HD11	1.96	0.47
1:C:184:HIS:O	1:C:207:LYS:NZ	2.35	0.47
1:D:286:LEU:HD23	1:D:296:ILE:HD13	1.97	0.47
1:D:327:VAL:HG23	1:D:356:GLN:HE21	1.79	0.47
1:C:46:ARG:HD3	1:C:70:HIS:HB2	1.96	0.46
1:B:296:ILE:HD11	1:B:304:ILE:HG23	1.96	0.46
1:C:280:ASP:O	1:C:284:LYS:HG2	2.14	0.46
1:C:375:ASN:ND2	1:C:375:ASN:C	2.67	0.46
1:D:227:ILE:HG21	1:D:261:GLU:HG2	1.98	0.46
1:C:312:VAL:HG13	1:C:316:THR:CG2	2.46	0.46
1:C:435:GLY:N	1:C:438:HIS:HD2	2.09	0.46
1:A:24:ALA:O	1:A:131:ARG:NH2	2.49	0.46
1:B:244:VAL:O	1:B:244:VAL:HG12	2.15	0.46
1:D:123:LYS:HZ1	1:D:193:THR:HG22	1.81	0.46
1:B:375:ASN:ND2	1:B:375:ASN:C	2.64	0.45
1:B:146:THR:HG21	3:B:469:HOH:O	2.14	0.45
1:D:154:LEU:O	1:D:158:VAL:HG23	2.16	0.45
1:A:375:ASN:HD22	1:A:377:ASP:H	1.64	0.45
1:D:114:THR:OG1	1:D:244:VAL:CG1	2.62	0.45
1:B:36:ARG:HD3	1:B:36:ARG:HA	1.73	0.45
1:B:74:GLU:OE2	1:B:78:ASN:OD1	2.34	0.45
1:D:252:VAL:HG13	1:D:254:VAL:CG2	2.47	0.45
1:A:108:CYS:SG	1:A:181:LEU:HD13	2.57	0.45
1:D:73:SER:OG	1:D:74:GLU:N	2.50	0.45
1:B:349:ASN:HD22	1:B:352:ASP:H	1.63	0.44
1:C:190:ILE:HD12	1:C:205:SER:OG	2.17	0.44
1:B:110:ILE:HB	1:B:192:ALA:HA	2.00	0.44
1:A:251:ALA:HB3	1:A:360:MSE:SE	2.68	0.44
1:C:349:ASN:C	1:C:349:ASN:HD22	2.20	0.44
1:C:43:ASN:OD1	1:C:70:HIS:HD2	2.00	0.44
1:D:257:GLU:O	1:D:257:GLU:HG3	2.18	0.44
1:C:370:SER:HB2	1:C:390:MSE:HE2	1.99	0.44
1:A:349:ASN:HD22	1:A:349:ASN:C	2.20	0.44
1:A:5:ASN:C	1:A:5:ASN:ND2	2.68	0.44
1:C:193:THR:HA	1:C:212:VAL:O	2.18	0.44
1:D:370:SER:CB	1:D:390:MSE:HE2	2.48	0.43
1:A:36:ARG:HG2	1:A:77:TYR:CE1	2.53	0.43
1:D:12:MSE:HE2	1:D:16:VAL:HG23	1.96	0.43
1:D:433:ASN:HD22	1:D:433:ASN:HA	1.61	0.43
1:B:375:ASN:HD22	1:B:376:GLN:N	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ASN:HD22	1:D:375:ASN:C	2.22	0.43
1:C:312:VAL:HG13	1:C:316:THR:HG21	1.99	0.43
1:A:12:MSE:HE1	1:A:168:GLY:CA	2.48	0.43
1:B:38:ALA:HB1	1:B:153:VAL:HG13	2.01	0.43
1:A:126:ILE:HD12	1:A:439:LEU:HD11	2.00	0.43
1:B:376:GLN:NE2	1:B:398:ASN:HD22	2.17	0.43
1:D:38:ALA:HB1	1:D:153:VAL:HG13	2.01	0.43
1:D:54:VAL:HG23	1:D:65:LYS:HD2	2.01	0.43
1:C:182:MSE:HG2	1:C:190:ILE:HD13	2.01	0.43
1:C:271:ALA:HB1	1:C:320:ILE:HD12	2.01	0.43
1:A:193:THR:HB	1:A:212:VAL:HB	2.01	0.42
1:C:62:VAL:O	1:C:66:VAL:HG23	2.19	0.42
1:D:228:LYS:HG2	1:D:265:ARG:CZ	2.49	0.42
1:B:327:VAL:H	1:B:356:GLN:HE21	1.67	0.42
1:C:249:GLU:CD	1:C:249:GLU:H	2.22	0.42
1:D:269:HIS:O	1:D:270:LYS:HB2	2.19	0.42
1:A:98:MSE:HE3	1:A:100:ILE:HD11	2.02	0.42
1:C:327:VAL:H	1:C:356:GLN:NE2	2.11	0.42
1:D:259:TYR:CD1	1:D:346:ARG:HG3	2.54	0.42
1:C:284:LYS:HG2	1:C:284:LYS:H	1.62	0.42
1:B:168:GLY:HA2	3:B:458:HOH:O	2.19	0.42
1:B:370:SER:HB2	1:B:390:MSE:HE2	2.02	0.42
1:D:123:LYS:HZ2	1:D:193:THR:HG23	1.84	0.42
1:D:376:GLN:NE2	1:D:398:ASN:HD22	2.17	0.42
1:A:370:SER:HB3	1:A:390:MSE:HE2	2.00	0.42
1:B:244:VAL:O	1:B:245:VAL:HG22	2.19	0.42
1:A:124:SER:HB3	1:A:153:VAL:HG11	2.02	0.41
1:A:312:VAL:HG13	1:A:316:THR:HG21	2.02	0.41
1:A:312:VAL:HG22	1:A:316:THR:HG21	2.02	0.41
1:C:116:PRO:HB2	1:C:146:THR:HG22	2.02	0.41
1:C:271:ALA:HB1	1:C:320:ILE:HD11	2.01	0.41
1:A:222:ASP:OD1	1:A:224:THR:OG1	2.35	0.41
1:A:269:HIS:O	1:A:270:LYS:HB2	2.19	0.41
1:A:373:TYR:HA	1:A:398:ASN:OD1	2.20	0.41
1:D:102:GLU:HB2	1:D:443:LYS:HE2	2.03	0.41
1:B:263:LYS:NZ	1:B:322:GLU:OE1	2.46	0.41
1:B:370:SER:CB	1:B:390:MSE:HE2	2.51	0.41
1:D:373:TYR:CD1	1:D:398:ASN:HA	2.56	0.41
1:A:354:VAL:O	1:A:358:VAL:HG23	2.21	0.41
1:A:154:LEU:HD22	1:A:158:VAL:CG2	2.51	0.40
1:D:372:LEU:HD13	1:D:374:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HG23	1:A:167:ILE:HG13	2.03	0.40
1:C:86:CYS:SG	1:C:131:ARG:HD2	2.61	0.40
1:D:180:ALA:O	3:D:458:HOH:O	2.21	0.40
1:B:216:ASN:HB2	1:B:364:GLY:HA3	2.03	0.40
1:D:46:ARG:HG3	1:D:47:ILE:HG13	2.02	0.40
1:A:335:HIS:O	1:A:337:LYS:HG3	2.22	0.40
1:B:334:ALA:O	1:B:360:MSE:HE3	2.21	0.40
1:D:279:ALA:O	1:D:283:ARG:HB2	2.22	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	403/452 (89%)	390 (97%)	13 (3%)	0	100	100
1	B	407/452 (90%)	393 (97%)	14 (3%)	0	100	100
1	C	409/452 (90%)	400 (98%)	9 (2%)	0	100	100
1	D	399/452 (88%)	384 (96%)	15 (4%)	0	100	100
All	All	1618/1808 (90%)	1567 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	300/346 (87%)	269 (90%)	31 (10%)	8	9
1	B	297/346 (86%)	271 (91%)	26 (9%)	12	14
1	C	307/346 (89%)	278 (91%)	29 (9%)	10	12
1	D	284/346 (82%)	257 (90%)	27 (10%)	10	12
All	All	1188/1384 (86%)	1075 (90%)	113 (10%)	10	12

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	MSE
1	A	23	PHE
1	A	36	ARG
1	A	76	ILE
1	A	83	GLU
1	A	102	GLU
1	A	104	VAL
1	A	119	THR
1	A	143	LYS
1	A	154	LEU
1	A	181	LEU
1	A	193	THR
1	A	246	CYS
1	A	249	GLU
1	A	265	ARG
1	A	277	THR
1	A	285	VAL
1	A	296	ILE
1	A	312	VAL
1	A	316	THR
1	A	324	LEU
1	A	336	GLU
1	A	349	ASN
1	A	369	THR
1	A	374	THR
1	A	375	ASN
1	A	378	VAL
1	A	389	LYS
1	A	431	SER
1	A	432	GLU
1	B	5	ASN
1	B	36	ARG

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Mol	Chain	Res	Type
1	B	113	THR
1	B	119	THR
1	B	146	THR
1	B	154	LEU
1	B	175	VAL
1	B	181	LEU
1	B	183	LYS
1	B	198	MSE
1	B	223	GLU
1	B	245	VAL
1	B	249	GLU
1	B	265	ARG
1	B	296	ILE
1	B	312	VAL
1	B	316	THR
1	B	336	GLU
1	B	349	ASN
1	B	369	THR
1	B	372	LEU
1	B	374	THR
1	B	375	ASN
1	B	402	THR
1	B	403	HIS
1	B	440	ILE
1	C	4	THR
1	C	5	ASN
1	C	22	GLU
1	C	23	PHE
1	C	46	ARG
1	C	76	ILE
1	C	78	ASN
1	C	85	THR
1	C	131	ARG
1	C	140	PRO
1	C	143	LYS
1	C	146	THR
1	C	154	LEU
1	C	181	LEU
1	C	187	ILE
1	C	189	LEU
1	C	193	THR
1	C	223	GLU

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Mol	Chain	Res	Type
1	C	234	VAL
1	C	252	VAL
1	C	268	SER
1	C	284	LYS
1	C	312	VAL
1	C	316	THR
1	C	336	GLU
1	C	349	ASN
1	C	375	ASN
1	C	389	LYS
1	C	391	LYS
1	D	5	ASN
1	D	12	MSE
1	D	76	ILE
1	D	83	GLU
1	D	119	THR
1	D	146	THR
1	D	152	LEU
1	D	154	LEU
1	D	175	VAL
1	D	181	LEU
1	D	189	LEU
1	D	193	THR
1	D	223	GLU
1	D	252	VAL
1	D	257	GLU
1	D	277	THR
1	D	324	LEU
1	D	328	SER
1	D	336	GLU
1	D	349	ASN
1	D	369	THR
1	D	372	LEU
1	D	375	ASN
1	D	377	ASP
1	D	381	ASP
1	D	388	ASP
1	D	433	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	30	GLN
1	A	43	ASN
1	A	69	ASN
1	A	70	HIS
1	A	349	ASN
1	A	356	GLN
1	A	368	HIS
1	A	375	ASN
1	A	376	GLN
1	A	379	ASN
1	A	438	HIS
1	B	5	ASN
1	B	52	GLN
1	B	69	ASN
1	B	78	ASN
1	B	139	HIS
1	B	349	ASN
1	B	356	GLN
1	B	368	HIS
1	B	375	ASN
1	B	376	GLN
1	B	379	ASN
1	B	438	HIS
1	C	5	ASN
1	C	30	GLN
1	C	52	GLN
1	C	69	ASN
1	C	70	HIS
1	C	139	HIS
1	C	349	ASN
1	C	356	GLN
1	C	368	HIS
1	C	375	ASN
1	C	376	GLN
1	C	438	HIS
1	D	43	ASN
1	D	52	GLN
1	D	69	ASN
1	D	70	HIS
1	D	139	HIS
1	D	349	ASN
1	D	356	GLN

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Mol	Chain	Res	Type
1	D	368	HIS
1	D	375	ASN
1	D	376	GLN
1	D	379	ASN
1	D	433	ASN
1	D	438	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 ⓘ

Of 4 ligands modelled in this entry, 4 are 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/452 (88%)	0.30	10 (2%) 58 65	26, 42, 62, 89	0
1	B	404/452 (89%)	0.26	13 (3%) 48 55	30, 47, 66, 89	0
1	C	405/452 (89%)	0.27	9 (2%) 62 69	26, 42, 60, 80	0
1	D	398/452 (88%)	0.58	36 (9%) 10 14	34, 53, 77, 91	0
All	All	1607/1808 (88%)	0.35	68 (4%) 37 44	26, 46, 68, 91	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	286	LEU	6.2
1	D	252	VAL	5.5
1	C	286	LEU	5.2
1	B	246	CYS	5.1
1	D	23	PHE	4.6
1	D	354	VAL	4.6
1	C	325	GLY	4.5
1	B	247	ALA	4.3
1	C	213	GLY	4.3
1	D	377	ASP	4.1
1	B	314	ALA	4.0
1	A	170	ILE	3.9
1	D	325	GLY	3.8
1	D	214	ALA	3.6
1	D	9	LEU	3.6
1	D	50	ALA	3.4
1	B	449	ALA	3.3
1	D	199	VAL	3.3
1	D	245	VAL	3.2
1	C	282	VAL	3.1
1	B	244	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	128	LEU	2.9
1	B	38	ALA	2.9
1	D	251	ALA	2.9
1	A	227	ILE	2.9
1	C	104	VAL	2.8
1	D	246	CYS	2.8
1	D	217	VAL	2.8
1	D	26	TYR	2.8
1	D	342	LEU	2.7
1	D	288	ILE	2.7
1	D	166	ILE	2.7
1	D	174	SER	2.7
1	D	305	ALA	2.7
1	D	247	ALA	2.6
1	B	42	ALA	2.6
1	C	278	ASP	2.5
1	C	4	THR	2.5
1	D	86	CYS	2.5
1	D	13	ILE	2.5
1	D	173	PRO	2.5
1	D	175	VAL	2.4
1	D	239	THR	2.4
1	A	191	LEU	2.4
1	D	282	VAL	2.4
1	C	203	TYR	2.3
1	D	448	ARG	2.3
1	D	67	ILE	2.3
1	D	133	GLY	2.3
1	B	280	ASP	2.3
1	A	368	HIS	2.3
1	B	3	VAL	2.2
1	D	350	PHE	2.2
1	A	135	ILE	2.2
1	A	290	GLY	2.2
1	A	175	VAL	2.2
1	A	128	LEU	2.2
1	B	338	LEU	2.2
1	D	58	GLY	2.2
1	B	53	ALA	2.1
1	B	157	ALA	2.1
1	D	168	GLY	2.1
1	B	266	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	116	PRO	2.1
1	D	309	GLY	2.1
1	A	42	ALA	2.1
1	A	269	HIS	2.0
1	C	201	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CL	A	453	1/1	0.92	0.12	-1.45	52,52,52,52	0
2	CL	B	453	1/1	0.88	0.11	-1.99	56,56,56,56	0
2	CL	C	453	1/1	0.98	0.09	-2.01	51,51,51,51	0
2	CL	D	453	1/1	0.96	0.05	-2.70	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.