Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:43 AM GMT

PDB ID	:	2NYN
Title	:	Crystal structure of phenylalanine ammonia-lyase from Anabaena variabilis
Authors	:	Louie, G.V.; Moffitt, M.C.; Bowman, M.E.; Pence, J.; Noel, J.P.; Moore, B.S.
Deposited on	:	2006-11-21
Resolution	:	1.90 Å(reported)

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

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

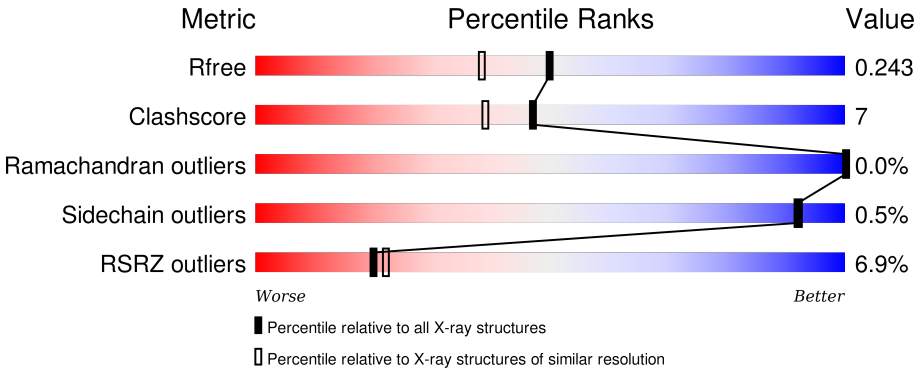
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	565	6% 75% 16% 9%
1	B	565	5% 73% 17% 9%
1	C	565	6% 75% 15% 9%
1	D	565	8% 76% 15% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16261 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 Phenylalanine/histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3930	2477	690	744	19			
1	B	512	Total	C	N	O	S	0	0	0
			3930	2477	690	744	19			
1	C	512	Total	C	N	O	S	0	0	0
			3930	2477	690	744	19			
1	D	512	Total	C	N	O	S	0	0	0
			3930	2477	690	744	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MDO	ALA	SEE REMARK 999	UNP Q3M5Z3
A	167	MDO	SER	SEE REMARK 999	UNP Q3M5Z3
A	167	MDO	GLY	SEE REMARK 999	UNP Q3M5Z3
B	167	MDO	ALA	SEE REMARK 999	UNP Q3M5Z3
B	167	MDO	SER	SEE REMARK 999	UNP Q3M5Z3
B	167	MDO	GLY	SEE REMARK 999	UNP Q3M5Z3
C	167	MDO	ALA	SEE REMARK 999	UNP Q3M5Z3
C	167	MDO	SER	SEE REMARK 999	UNP Q3M5Z3
C	167	MDO	GLY	SEE REMARK 999	UNP Q3M5Z3
D	167	MDO	ALA	SEE REMARK 999	UNP Q3M5Z3
D	167	MDO	SER	SEE REMARK 999	UNP Q3M5Z3
D	167	MDO	GLY	SEE REMARK 999	UNP Q3M5Z3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	131	Total	O	0	0
			131	131		

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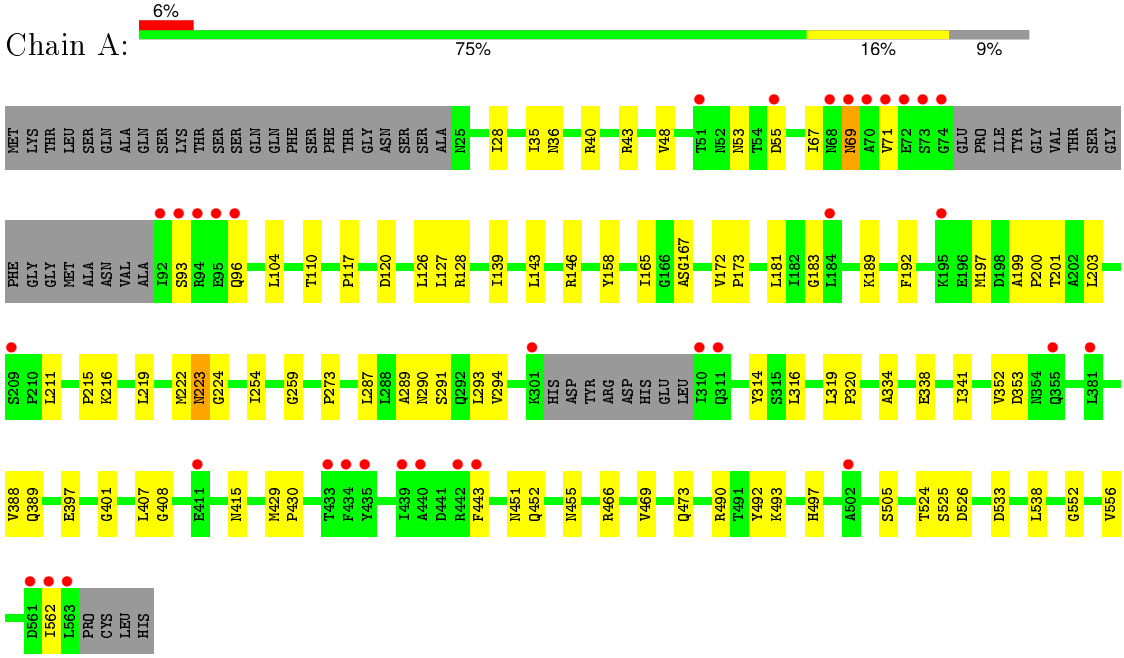
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	143	Total O 143 143	0	0
2	D	125	Total O 125 125	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

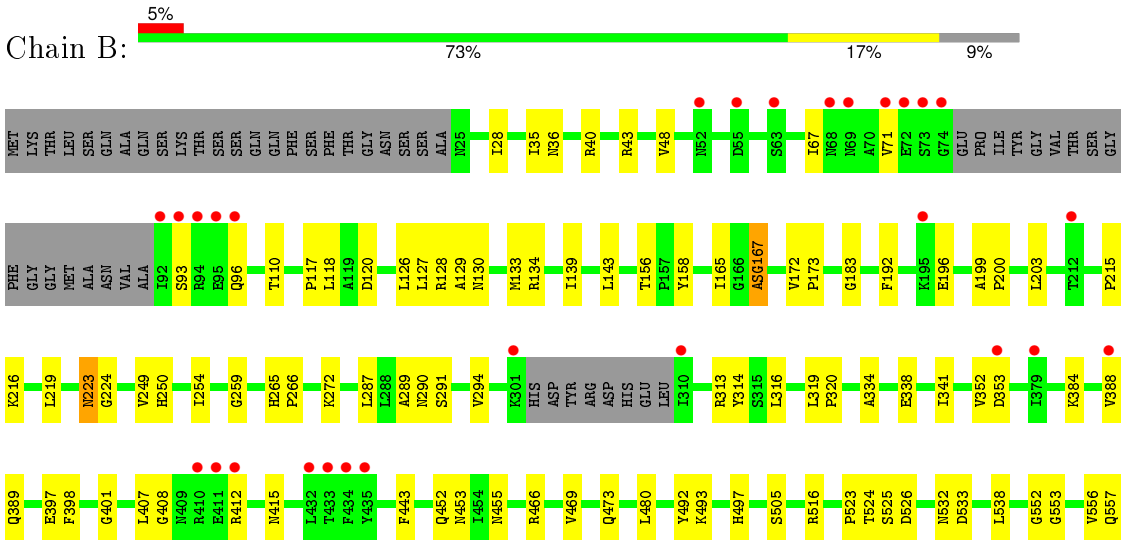
- Molecule 1: Phenylalanine/histidine ammonia-lyase

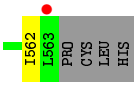
Chain A:



- Molecule 1: Phenylalanine/histidine ammonia-lyase

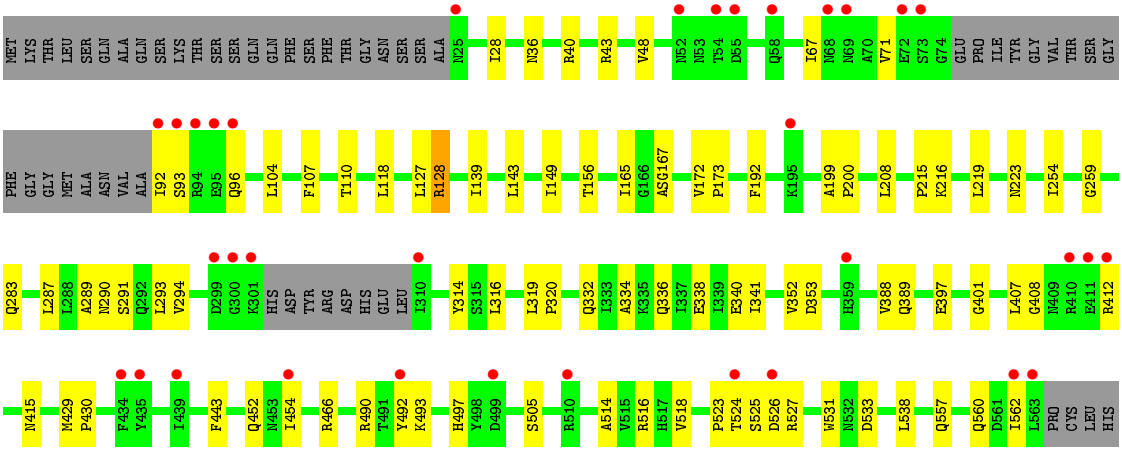
Chain B:





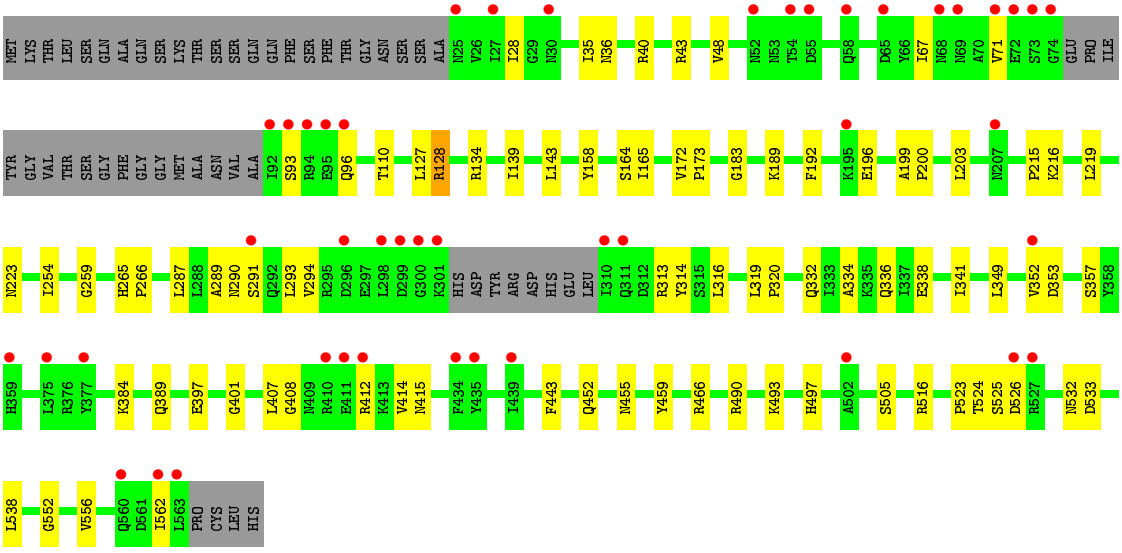
• Molecule 1: Phenylalanine/histidine ammonia-lyase

Chain C:



• Molecule 1: Phenylalanine/histidine ammonia-lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.19Å 88.52Å 90.06Å 103.52° 97.82° 116.24°	Depositor
Resolution (Å)	100.00 – 1.90 48.56 – 1.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-1.90) 77.6 (48.56-1.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.74Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.242 0.223 , 0.243	Depositor DCC
R_{free} test set	7619 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 174523 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16261	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.33	0/3984	0.57	0/5406
1	B	0.33	0/3984	0.56	0/5406
1	C	0.33	0/3984	0.56	0/5406
1	D	0.33	0/3984	0.56	0/5406
All	All	0.33	0/15936	0.56	0/21624

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	MDO	Mainchain
1	B	167	MDO	Mainchain

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	3930	0	3927	63	0
1	B	3930	0	3926	70	0
1	C	3930	0	3927	63	0
1	D	3930	0	3927	59	0
2	A	142	0	0	1	0
2	B	131	0	0	5	0
2	C	143	0	0	1	0
2	D	125	0	0	5	0
All	All	16261	0	15707	235	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 (235) 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:D:287:LEU:HD21	1:D:562:ILE:HD11	1.39	1.04
1:C:287:LEU:HD21	1:C:562:ILE:HD11	1.46	0.98
1:A:287:LEU:HD21	1:A:562:ILE:HD11	1.45	0.98
1:C:110:THR:HG22	1:D:538:LEU:HB2	1.51	0.92
1:B:287:LEU:HD21	1:B:562:ILE:HD11	1.51	0.91
1:C:538:LEU:HB2	1:D:110:THR:HG22	1.56	0.88
1:B:128:ARG:HH12	1:B:224:GLY:HA3	1.41	0.84
1:D:128:ARG:HA	1:D:128:ARG:HE	1.45	0.81
1:A:538:LEU:HB2	1:B:110:THR:HG22	1.63	0.80
1:C:128:ARG:HE	1:C:128:ARG:HA	1.48	0.78
1:D:524:THR:HG22	1:D:526:ASP:H	1.49	0.78
1:C:127:LEU:HD22	1:C:341:ILE:HG23	1.65	0.77
1:A:110:THR:HG22	1:B:538:LEU:HB2	1.65	0.77
1:A:524:THR:HG22	1:A:526:ASP:H	1.50	0.77
1:C:524:THR:HG22	1:C:526:ASP:H	1.52	0.74
1:B:524:THR:HG22	1:B:526:ASP:H	1.50	0.74
1:D:127:LEU:HD22	1:D:341:ILE:HG23	1.72	0.70
1:C:28:ILE:HD11	1:C:48:VAL:HG11	1.72	0.69
1:A:128:ARG:HH12	1:A:224:GLY:HA3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:GLN:HG2	1:C:314:TYR:CE2	2.29	0.67
1:D:414:VAL:HG13	2:D:1393:HOH:O	1.95	0.66
1:C:557:GLN:HA	1:C:560:GLN:HG3	1.79	0.65
1:B:128:ARG:NH1	1:B:224:GLY:HA3	2.11	0.64
1:A:452:GLN:HG2	1:D:314:TYR:CE2	2.33	0.63
1:D:316:LEU:HD23	1:D:389:GLN:HE22	1.63	0.63
1:C:316:LEU:HD23	1:C:389:GLN:HE22	1.64	0.62
1:A:69:ASN:N	1:A:69:ASN:HD22	1.96	0.62
1:C:407:LEU:HD12	1:C:408:GLY:N	2.15	0.62
1:C:407:LEU:HD12	1:C:408:GLY:H	1.65	0.61
1:D:352:VAL:HG22	2:D:1509:HOH:O	1.99	0.61
1:B:165:ILE:HD11	1:B:452:GLN:OE1	2.01	0.61
1:B:199:ALA:HB3	1:B:200:PRO:HD3	1.83	0.60
1:A:314:TYR:CE2	1:D:452:GLN:HG2	2.36	0.60
1:D:172:VAL:HB	1:D:173:PRO:HD3	1.83	0.59
1:A:127:LEU:HD22	1:A:341:ILE:HG23	1.84	0.59
1:A:291:SER:HB2	1:A:505:SER:HB3	1.85	0.59
1:A:452:GLN:HG2	1:D:314:TYR:CZ	2.38	0.59
1:D:219:LEU:O	1:D:223:ASN:HB2	2.03	0.59
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.86	0.58
1:B:172:VAL:HB	1:B:173:PRO:HD3	1.86	0.58
1:B:127:LEU:HD22	1:B:341:ILE:HG23	1.86	0.57
1:C:43:ARG:HH21	1:C:43:ARG:HG3	1.69	0.57
1:D:28:ILE:HD11	1:D:48:VAL:HG11	1.86	0.57
1:C:92:ILE:O	1:C:93:SER:HB3	2.03	0.57
1:C:497:HIS:HB2	1:C:525:SER:HB2	1.86	0.57
1:A:172:VAL:HB	1:A:173:PRO:HD3	1.87	0.57
1:B:139:ILE:HD11	1:B:143:LEU:HD23	1.86	0.57
1:A:43:ARG:HG3	1:A:43:ARG:HH21	1.69	0.57
1:C:516:ARG:NH2	1:C:523:PRO:HA	2.20	0.57
1:B:452:GLN:HG2	1:C:314:TYR:CZ	2.41	0.56
1:D:139:ILE:HD11	1:D:143:LEU:HD23	1.87	0.56
1:C:219:LEU:O	1:C:223:ASN:HB2	2.05	0.56
1:C:199:ALA:HB3	1:C:200:PRO:HD3	1.86	0.56
1:A:139:ILE:HD11	1:A:143:LEU:HD23	1.87	0.56
1:C:36:ASN:O	1:C:40:ARG:HG3	2.06	0.55
1:B:314:TYR:CE2	1:C:452:GLN:HG2	2.41	0.55
1:A:28:ILE:HD11	1:A:126:LEU:HD12	1.88	0.55
1:A:67:ILE:O	1:A:71:VAL:HG23	2.06	0.55
1:C:93:SER:HB3	1:C:96:GLN:HB3	1.89	0.55
1:B:28:ILE:HD11	1:B:48:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASN:O	1:A:40:ARG:HG3	2.06	0.55
1:D:36:ASN:O	1:D:40:ARG:HG3	2.07	0.55
1:C:67:ILE:O	1:C:71:VAL:HG23	2.07	0.55
1:C:291:SER:HB2	1:C:505:SER:HB3	1.90	0.54
1:B:407:LEU:HD12	1:B:408:GLY:N	2.22	0.54
1:C:139:ILE:HD11	1:C:143:LEU:HD23	1.89	0.54
1:D:67:ILE:O	1:D:71:VAL:HG23	2.07	0.54
1:B:314:TYR:CZ	1:C:452:GLN:HG2	2.43	0.54
1:A:314:TYR:CZ	1:D:452:GLN:HG2	2.43	0.54
1:B:407:LEU:HD12	1:B:408:GLY:H	1.73	0.54
1:A:165:ILE:HD11	1:A:452:GLN:OE1	2.07	0.54
1:D:334:ALA:O	1:D:338:GLU:HG3	2.08	0.54
1:D:254:ILE:HG12	1:D:316:LEU:HD22	1.90	0.53
1:A:289:ALA:O	1:A:290:ASN:HB2	2.09	0.53
1:D:128:ARG:NE	1:D:128:ARG:HA	2.20	0.53
1:C:514:ALA:O	1:C:518:VAL:HG23	2.09	0.53
1:C:334:ALA:O	1:C:338:GLU:HG3	2.09	0.53
1:B:36:ASN:O	1:B:40:ARG:HG3	2.08	0.53
1:A:316:LEU:HD23	1:A:389:GLN:HE22	1.74	0.53
1:C:110:THR:HG22	1:D:538:LEU:CB	2.29	0.53
1:C:289:ALA:O	1:C:290:ASN:HB2	2.08	0.53
1:B:319:LEU:HB3	1:B:320:PRO:HD3	1.90	0.52
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.90	0.52
1:B:289:ALA:O	1:B:290:ASN:HB2	2.10	0.52
1:C:172:VAL:HB	1:C:173:PRO:HD3	1.91	0.52
1:D:407:LEU:HD12	1:D:408:GLY:H	1.75	0.52
1:A:407:LEU:HD12	1:A:408:GLY:N	2.25	0.52
1:A:183:GLY:HA3	1:A:203:LEU:HD12	1.91	0.51
1:A:319:LEU:HB3	1:A:320:PRO:HD3	1.91	0.51
1:D:401:GLY:HA3	1:D:493:LYS:HE3	1.91	0.51
1:D:43:ARG:HH21	1:D:43:ARG:HG3	1.76	0.51
1:C:319:LEU:HB3	1:C:320:PRO:HD3	1.93	0.51
1:A:429:MET:HB3	1:A:430:PRO:HD3	1.93	0.51
1:D:407:LEU:HD12	1:D:408:GLY:N	2.26	0.51
1:B:43:ARG:HH21	1:B:43:ARG:HG3	1.75	0.51
1:D:165:ILE:HD11	1:D:452:GLN:OE1	2.11	0.51
1:B:67:ILE:O	1:B:71:VAL:HG23	2.10	0.51
1:A:497:HIS:HB2	1:A:525:SER:HB2	1.91	0.51
1:D:516:ARG:NH2	1:D:523:PRO:HA	2.26	0.50
1:D:291:SER:HB2	1:D:505:SER:HB3	1.93	0.50
1:A:28:ILE:HD11	1:A:48:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ARG:HB2	1:C:415:ASN:ND2	2.27	0.50
1:D:259:GLY:O	1:D:294:VAL:HG13	2.12	0.50
1:A:407:LEU:HD12	1:A:408:GLY:H	1.77	0.49
1:C:562:ILE:HG22	1:C:562:ILE:O	2.13	0.49
1:A:562:ILE:O	1:A:562:ILE:HG22	2.12	0.49
1:B:291:SER:HB2	1:B:505:SER:HB3	1.94	0.49
1:C:283:GLN:NE2	2:C:1406:HOH:O	2.44	0.49
1:A:215:PRO:O	1:A:216:LYS:HB3	2.13	0.49
1:A:397:GLU:HG2	1:C:397:GLU:HB3	1.95	0.49
1:A:197:MET:HE3	1:A:201:THR:HG22	1.95	0.49
1:D:497:HIS:HB2	1:D:525:SER:HB2	1.94	0.48
1:B:334:ALA:O	1:B:338:GLU:HG3	2.13	0.48
1:B:316:LEU:HD23	1:B:389:GLN:HE22	1.78	0.48
1:D:215:PRO:O	1:D:216:LYS:HB3	2.14	0.48
1:B:516:ARG:NH2	1:B:523:PRO:HA	2.29	0.48
1:A:43:ARG:NH2	1:A:43:ARG:HG3	2.28	0.47
1:A:254:ILE:HG12	1:A:316:LEU:HD22	1.95	0.47
1:B:28:ILE:HD11	1:B:126:LEU:HD12	1.96	0.47
1:B:35:ILE:HG13	1:B:338:GLU:HG2	1.96	0.47
1:B:497:HIS:HB2	1:B:525:SER:HB2	1.95	0.47
1:D:93:SER:CB	1:D:96:GLN:HE21	2.28	0.47
1:A:104:LEU:HD23	1:A:222:MET:HE3	1.95	0.47
1:B:401:GLY:HA3	1:B:493:LYS:HE3	1.96	0.47
1:D:293:LEU:HD22	1:D:490:ARG:HG3	1.96	0.47
1:A:334:ALA:O	1:A:338:GLU:HG3	2.15	0.47
1:D:562:ILE:O	1:D:562:ILE:HG22	2.15	0.47
1:D:35:ILE:HG13	1:D:338:GLU:HG2	1.96	0.47
1:D:319:LEU:HB3	1:D:320:PRO:HD3	1.97	0.47
1:B:352:VAL:HG23	1:B:353:ASP:N	2.30	0.47
1:A:146:ARG:HG3	1:A:181:LEU:HD22	1.96	0.46
1:C:332:GLN:O	1:C:336:GLN:HG3	2.15	0.46
1:B:183:GLY:HA3	1:B:203:LEU:HD12	1.97	0.46
1:A:492:TYR:HA	1:A:497:HIS:O	2.16	0.46
1:B:249:VAL:HG22	1:B:480:LEU:HD23	1.97	0.46
1:C:127:LEU:CD2	1:C:341:ILE:HG23	2.42	0.46
1:B:412:ARG:NE	2:B:1390:HOH:O	2.47	0.46
1:B:93:SER:CB	1:B:96:GLN:HE21	2.29	0.46
1:C:43:ARG:NH2	1:C:43:ARG:HG3	2.29	0.46
1:C:429:MET:HB3	1:C:430:PRO:HD3	1.98	0.46
1:B:562:ILE:O	1:B:562:ILE:HG22	2.16	0.46
1:B:259:GLY:O	1:B:294:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:NH1	1:A:224:GLY:HA3	2.27	0.45
1:C:215:PRO:O	1:C:216:LYS:HB3	2.16	0.45
1:D:43:ARG:HG3	1:D:43:ARG:NH2	2.31	0.45
1:A:293:LEU:HD22	1:A:490:ARG:HG3	1.97	0.45
1:D:289:ALA:O	1:D:290:ASN:HB2	2.17	0.45
1:B:167:MDO:HB21	1:C:314:TYR:OH	2.17	0.45
1:B:388:VAL:HG13	2:B:1120:HOH:O	2.15	0.45
1:A:219:LEU:O	1:A:223:ASN:HB2	2.16	0.45
1:B:117:PRO:HD2	1:B:120:ASP:OD2	2.17	0.45
1:B:492:TYR:HA	1:B:497:HIS:O	2.16	0.45
1:D:415:ASN:HA	1:D:533:ASP:OD2	2.16	0.45
1:B:469:VAL:O	1:B:473:GLN:HG3	2.17	0.45
1:C:165:ILE:HD11	1:C:452:GLN:OE1	2.17	0.45
1:A:469:VAL:O	1:A:473:GLN:HG3	2.17	0.45
1:D:332:GLN:O	1:D:336:GLN:HG3	2.17	0.45
1:D:412:ARG:HD2	1:D:532:ASN:OD1	2.17	0.44
1:C:254:ILE:HG12	1:C:316:LEU:HD22	1.99	0.44
1:B:412:ARG:CZ	2:B:1390:HOH:O	2.65	0.44
1:C:352:VAL:HG23	1:C:353:ASP:N	2.33	0.44
1:A:259:GLY:O	1:A:294:VAL:HG13	2.16	0.44
1:D:134:ARG:HD3	2:D:1278:HOH:O	2.17	0.44
1:D:352:VAL:HG23	1:D:353:ASP:N	2.33	0.44
1:A:466:ARG:HD3	1:A:466:ARG:O	2.18	0.44
1:B:552:GLY:HA2	1:B:556:VAL:HG21	2.00	0.44
1:C:415:ASN:HA	1:C:533:ASP:OD2	2.17	0.44
1:C:407:LEU:HD13	1:C:415:ASN:HB3	1.99	0.44
1:B:412:ARG:HD2	1:B:532:ASN:OD1	2.17	0.44
1:C:466:ARG:HD3	1:C:466:ARG:O	2.18	0.43
1:D:466:ARG:HD3	1:D:466:ARG:O	2.17	0.43
1:A:415:ASN:HA	1:A:533:ASP:OD2	2.17	0.43
1:C:28:ILE:HD11	1:C:48:VAL:CG1	2.46	0.43
1:C:407:LEU:CD1	1:C:415:ASN:HB3	2.49	0.43
1:B:415:ASN:HA	1:B:533:ASP:OD2	2.17	0.43
1:A:352:VAL:HG23	1:A:353:ASP:N	2.33	0.43
1:C:92:ILE:O	1:C:93:SER:CB	2.66	0.43
1:B:412:ARG:HB2	1:B:415:ASN:ND2	2.34	0.43
1:B:466:ARG:O	1:B:466:ARG:HD3	2.19	0.43
1:B:28:ILE:CG2	1:B:130:ASN:HA	2.48	0.43
1:B:397:GLU:HB3	1:D:397:GLU:HG2	2.01	0.43
1:D:349:LEU:O	1:D:357:SER:HA	2.19	0.43
1:B:219:LEU:O	1:B:223:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TYR:CD2	1:A:189:LYS:HB2	2.54	0.43
1:B:28:ILE:CD1	1:B:48:VAL:HG11	2.49	0.43
1:C:443:PHE:CE2	1:C:454:ILE:HA	2.54	0.43
1:B:553:GLY:O	1:B:557:GLN:HG3	2.19	0.43
1:B:43:ARG:NH2	1:B:43:ARG:HG3	2.33	0.43
1:C:401:GLY:HA3	1:C:493:LYS:HE3	2.00	0.43
1:A:69:ASN:N	1:A:69:ASN:ND2	2.67	0.42
1:A:117:PRO:HD2	1:A:120:ASP:OD2	2.18	0.42
1:B:215:PRO:O	1:B:216:LYS:HB3	2.18	0.42
1:B:407:LEU:HD13	1:B:415:ASN:HB3	2.01	0.42
1:B:134:ARG:NH2	2:B:1176:HOH:O	2.53	0.42
1:B:250:HIS:O	1:B:254:ILE:HG13	2.20	0.42
1:A:28:ILE:HD11	1:A:126:LEU:CD1	2.49	0.42
1:D:158:TYR:CD2	1:D:189:LYS:HB2	2.55	0.42
1:D:158:TYR:CE2	1:D:196:GLU:HG3	2.55	0.42
1:D:443:PHE:HB2	1:D:455:ASN:OD1	2.19	0.42
1:A:93:SER:CB	1:A:96:GLN:HE21	2.33	0.42
1:A:146:ARG:NH2	1:A:211:LEU:HD11	2.35	0.42
1:C:527:ARG:HD2	1:C:531:TRP:CD2	2.55	0.42
1:B:265:HIS:HA	1:B:266:PRO:HD3	1.86	0.41
1:A:388:VAL:HG13	2:D:1091:HOH:O	2.20	0.41
1:B:314:TYR:OH	1:C:167:MDO:HB21	2.20	0.41
1:A:552:GLY:HA2	1:A:556:VAL:HG21	2.02	0.41
1:B:129:ALA:O	1:B:133:MET:HG2	2.21	0.41
1:C:293:LEU:HD22	1:C:490:ARG:HG3	2.03	0.41
1:A:443:PHE:HB2	1:A:455:ASN:OD1	2.21	0.41
1:A:35:ILE:HG13	1:A:338:GLU:HG2	2.02	0.41
1:B:384:LYS:HE3	2:B:1326:HOH:O	2.21	0.41
1:D:265:HIS:HA	1:D:266:PRO:HD3	1.90	0.41
1:D:266:PRO:HG3	2:D:1210:HOH:O	2.19	0.41
1:A:451:ASN:OD1	1:D:313:ARG:NH2	2.53	0.41
1:A:28:ILE:CD1	1:A:48:VAL:HG11	2.51	0.41
1:A:319:LEU:HD23	1:A:319:LEU:C	2.41	0.41
1:A:104:LEU:HB3	1:A:222:MET:HE1	2.03	0.41
1:B:313:ARG:NH1	1:B:398:PHE:HD1	2.19	0.41
1:D:552:GLY:HA2	1:D:556:VAL:HG21	2.03	0.41
1:C:149:ILE:HG21	1:C:208:LEU:HD11	2.01	0.41
1:A:53:ASN:OD1	1:A:55:ASP:HB2	2.21	0.41
1:B:158:TYR:CE2	1:B:196:GLU:HG3	2.56	0.41
1:C:259:GLY:O	1:C:294:VAL:HG13	2.21	0.41
1:D:183:GLY:HA3	1:D:203:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LYS:HE3	1:C:340:GLU:OE1	2.21	0.40
1:B:443:PHE:HB2	1:B:455:ASN:OD1	2.21	0.40
1:C:492:TYR:HA	1:C:497:HIS:O	2.21	0.40
1:B:407:LEU:CD1	1:B:415:ASN:HB3	2.51	0.40
1:D:164:SER:HB3	1:D:459:TYR:CG	2.57	0.40
1:C:104:LEU:HD12	1:C:107:PHE:CE1	2.57	0.40
1:C:118:LEU:HD22	1:C:156:THR:HB	2.03	0.40
2:A:1225:HOH:O	1:D:384:LYS:HE3	2.22	0.40
1:B:453:ASN:ND2	1:C:388:VAL:CG1	2.85	0.40
1:A:401:GLY:HA3	1:A:493:LYS:HE3	2.03	0.40
1:B:118:LEU:HD22	1:B:156:THR:HB	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	505/565 (89%)	484 (96%)	20 (4%)	1 (0%)	52	42
1	B	505/565 (89%)	486 (96%)	19 (4%)	0	100	100
1	C	505/565 (89%)	484 (96%)	21 (4%)	0	100	100
1	D	505/565 (89%)	485 (96%)	20 (4%)	0	100	100
All	All	2020/2260 (89%)	1939 (96%)	80 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	PRO

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	423/468 (90%)	420 (99%)	3 (1%)	88	88
1	B	423/468 (90%)	421 (100%)	2 (0%)	92	92
1	C	423/468 (90%)	421 (100%)	2 (0%)	92	92
1	D	423/468 (90%)	421 (100%)	2 (0%)	92	92
All	All	1692/1872 (90%)	1683 (100%)	9 (0%)	92	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	192	PHE
1	A	223	ASN
1	B	192	PHE
1	B	223	ASN
1	C	128	ARG
1	C	192	PHE
1	D	128	ARG
1	D	192	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	68	ASN
1	A	69	ASN
1	A	96	GLN
1	A	205	GLN
1	A	207	ASN
1	A	223	ASN
1	A	240	GLN
1	A	258	ASN
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	292	GLN
1	A	474	ASN
1	B	44	ASN
1	B	68	ASN
1	B	96	GLN
1	B	205	GLN
1	B	207	ASN
1	B	223	ASN
1	B	240	GLN
1	B	258	ASN
1	B	283	GLN
1	B	292	GLN
1	B	474	ASN
1	C	44	ASN
1	C	68	ASN
1	C	207	ASN
1	C	240	GLN
1	C	258	ASN
1	C	283	GLN
1	C	292	GLN
1	C	474	ASN
1	D	44	ASN
1	D	68	ASN
1	D	96	GLN
1	D	205	GLN
1	D	207	ASN
1	D	240	GLN
1	D	258	ASN
1	D	283	GLN
1	D	292	GLN
1	D	474	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MDO	A	167	1	11,13,14	2.19	2 (18%)	13,18,20	3.71	5 (38%)
1	MDO	B	167	1	11,13,14	2.19	2 (18%)	13,18,20	3.71	5 (38%)
1	MDO	C	167	1	11,13,14	2.22	3 (27%)	13,18,20	3.79	5 (38%)
1	MDO	D	167	1	11,13,14	2.24	2 (18%)	13,18,20	3.78	5 (38%)

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
1	MDO	A	167	1	-	0/4/23/24	0/1/1/1
1	MDO	B	167	1	-	0/4/23/24	0/1/1/1
1	MDO	C	167	1	-	0/4/23/24	0/1/1/1
1	MDO	D	167	1	-	0/4/23/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	167	MDO	C2-N3	-3.82	1.31	1.39
1	A	167	MDO	C2-N3	-3.80	1.31	1.39
1	C	167	MDO	C2-N3	-3.73	1.31	1.39
1	B	167	MDO	C2-N3	-3.56	1.32	1.39
1	C	167	MDO	C1-N2	2.10	1.35	1.32
1	A	167	MDO	O2-C2	5.04	1.33	1.23
1	C	167	MDO	O2-C2	5.04	1.33	1.23
1	B	167	MDO	O2-C2	5.13	1.34	1.23
1	D	167	MDO	O2-C2	5.16	1.34	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	167	MDO	O2-C2-CA2	-5.11	128.18	130.95
1	D	167	MDO	O2-C2-CA2	-5.08	128.20	130.95
1	B	167	MDO	O2-C2-CA2	-4.78	128.36	130.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	MDO	O2-C2-CA2	-4.53	128.50	130.95
1	A	167	MDO	C2-CA2-N2	-3.44	106.17	108.91
1	D	167	MDO	C2-CA2-N2	-3.37	106.22	108.91
1	B	167	MDO	C2-CA2-N2	-3.36	106.23	108.91
1	C	167	MDO	C2-CA2-N2	-3.22	106.34	108.91
1	D	167	MDO	N3-C1-N2	-3.04	109.21	111.56
1	A	167	MDO	N3-C1-N2	-2.99	109.25	111.56
1	B	167	MDO	N3-C1-N2	-2.98	109.26	111.56
1	C	167	MDO	N3-C1-N2	-2.90	109.32	111.56
1	D	167	MDO	CA2-N2-C1	2.03	107.70	105.35
1	A	167	MDO	CA2-N2-C1	2.15	107.85	105.35
1	C	167	MDO	CA-C1-N2	2.17	126.81	123.83
1	B	167	MDO	CA2-N2-C1	2.23	107.94	105.35
1	B	167	MDO	CA2-C2-N3	11.21	109.24	103.39
1	A	167	MDO	CA2-C2-N3	11.21	109.25	103.39
1	D	167	MDO	CA2-C2-N3	11.37	109.33	103.39
1	C	167	MDO	CA2-C2-N3	11.48	109.39	103.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	167	MDO	1	0
1	C	167	MDO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	511/565 (90%)	0.56	34 (6%)	21	23	13, 28, 53, 88	0
1	B	511/565 (90%)	0.51	29 (5%)	27	30	13, 28, 53, 87	0
1	C	511/565 (90%)	0.49	34 (6%)	21	23	14, 28, 51, 88	0
1	D	511/565 (90%)	0.55	45 (8%)	12	14	14, 27, 53, 88	0
All	All	2044/2260 (90%)	0.53	142 (6%)	20	22	13, 28, 53, 88	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	ILE	11.6
1	C	310	ILE	10.5
1	C	92	ILE	10.3
1	D	310	ILE	9.7
1	A	92	ILE	9.1
1	B	71	VAL	7.9
1	D	92	ILE	7.8
1	B	310	ILE	7.7
1	C	301	LYS	7.0
1	D	301	LYS	6.7
1	B	92	ILE	6.6
1	C	72	GLU	6.0
1	B	301	LYS	6.0
1	A	73	SER	5.8
1	D	68	ASN	5.7
1	D	73	SER	5.6
1	D	93	SER	5.0
1	A	301	LYS	4.8
1	B	96	GLN	4.7
1	B	73	SER	4.7
1	D	72	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	93	SER	4.4
1	C	300	GLY	4.4
1	D	300	GLY	4.4
1	B	95	GLU	4.3
1	A	195	LYS	4.2
1	A	68	ASN	4.1
1	A	72	GLU	4.0
1	C	68	ASN	4.0
1	C	96	GLN	3.9
1	A	93	SER	3.8
1	C	95	GLU	3.8
1	C	73	SER	3.7
1	D	55	ASP	3.7
1	C	52	ASN	3.7
1	D	96	GLN	3.6
1	C	299	ASP	3.6
1	B	410	ARG	3.5
1	B	72	GLU	3.5
1	A	563	LEU	3.5
1	D	69	ASN	3.4
1	D	563	LEU	3.4
1	C	439	ILE	3.4
1	D	439	ILE	3.3
1	D	299	ASP	3.3
1	B	195	LYS	3.3
1	D	71	VAL	3.3
1	C	94	ARG	3.3
1	D	52	ASN	3.2
1	A	94	ARG	3.1
1	A	96	GLN	3.1
1	D	95	GLU	3.1
1	A	74	GLY	3.1
1	A	71	VAL	3.1
1	B	563	LEU	3.0
1	D	410	ARG	3.0
1	A	69	ASN	3.0
1	D	562	ILE	3.0
1	D	195	LYS	2.9
1	A	311	GLN	2.9
1	B	69	ASN	2.9
1	C	69	ASN	2.9
1	A	439	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	560	GLN	2.9
1	C	55	ASP	2.9
1	B	434	PHE	2.9
1	C	410	ARG	2.9
1	A	433	THR	2.8
1	C	563	LEU	2.8
1	D	94	ARG	2.8
1	A	440	ALA	2.8
1	C	93	SER	2.8
1	C	411	GLU	2.8
1	D	434	PHE	2.8
1	C	562	ILE	2.8
1	D	58	GLN	2.8
1	A	55	ASP	2.8
1	D	65	ASP	2.8
1	A	355	GLN	2.8
1	D	30	ASN	2.7
1	C	412	ARG	2.7
1	C	435	TYR	2.7
1	D	54	THR	2.7
1	B	94	ARG	2.7
1	B	63	SER	2.7
1	C	434	PHE	2.7
1	B	68	ASN	2.6
1	D	411	GLU	2.6
1	B	435	TYR	2.6
1	D	359	HIS	2.6
1	B	433	THR	2.6
1	B	55	ASP	2.6
1	C	58	GLN	2.6
1	C	524	THR	2.6
1	B	74	GLY	2.5
1	D	296	ASP	2.5
1	A	443	PHE	2.5
1	C	499	ASP	2.5
1	A	562	ILE	2.5
1	A	51	THR	2.5
1	A	209	SER	2.5
1	A	435	TYR	2.4
1	D	74	GLY	2.4
1	B	432	LEU	2.4
1	A	442	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	207	ASN	2.3
1	A	411	GLU	2.3
1	A	434	PHE	2.3
1	C	195	LYS	2.3
1	B	411	GLU	2.3
1	C	526	ASP	2.3
1	A	95	GLU	2.3
1	B	379	ILE	2.3
1	D	527	ARG	2.2
1	C	54	THR	2.2
1	A	70	ALA	2.2
1	D	377	TYR	2.2
1	D	352	VAL	2.2
1	D	311	GLN	2.2
1	A	184	LEU	2.2
1	B	212	THR	2.2
1	C	510	ARG	2.2
1	B	353	ASP	2.1
1	D	435	TYR	2.1
1	C	359	HIS	2.1
1	C	454	ILE	2.1
1	D	526	ASP	2.1
1	D	298	LEU	2.1
1	D	412	ARG	2.1
1	B	388	VAL	2.1
1	B	412	ARG	2.1
1	A	381	LEU	2.1
1	A	502	ALA	2.1
1	A	561	ASP	2.1
1	D	375	LEU	2.1
1	D	502	ALA	2.1
1	C	25	ASN	2.1
1	B	52	ASN	2.0
1	D	25	ASN	2.0
1	D	291	SER	2.0
1	C	492	TYR	2.0
1	D	27	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MDO	C	167	13/14	0.90	0.12	-	25,27,30,32	0
1	MDO	A	167	13/14	0.89	0.12	-	22,27,30,31	0
1	MDO	D	167	13/14	0.88	0.12	-	25,28,29,30	0
1	MDO	B	167	13/14	0.90	0.12	-	23,26,27,29	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.