Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 01:08 AM EST

PDB ID	:	3CZO
Title	:	Crystal Structure of Double Mutant Phenylalanine Ammonia-Lyase From Anabaena Variabilis
Authors	:	Stevens, R.C.; Wang, L.
Deposited on	:	2008-04-29
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

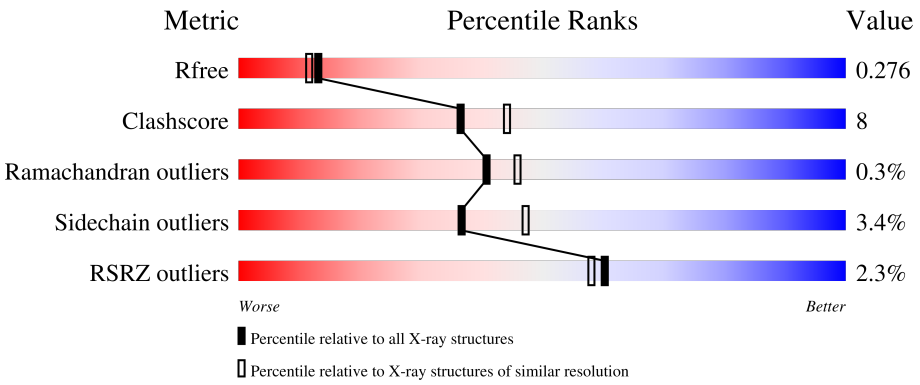
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	539	2% 80% 18% •
1	B	539	2% 83% 15% •
1	C	539	2% 87% 12% •
1	D	539	3% 82% 16% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17166 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 Histidine ammonia-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	537	4128	2600	726	783	4	15	0	0	0
1	B	539	4126	2602	723	782	4	15	0	1	0
1	C	537	4109	2595	718	777	4	15	0	1	0
1	D	537	4114	2596	720	779	4	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	SER	CYS	engineered mutation	UNP Q3M5Z3
A	565	SER	CYS	engineered mutation	UNP Q3M5Z3
B	503	SER	CYS	engineered mutation	UNP Q3M5Z3
B	565	SER	CYS	engineered mutation	UNP Q3M5Z3
C	503	SER	CYS	engineered mutation	UNP Q3M5Z3
C	565	SER	CYS	engineered mutation	UNP Q3M5Z3
D	503	SER	CYS	engineered mutation	UNP Q3M5Z3
D	565	SER	CYS	engineered mutation	UNP Q3M5Z3

- Molecule 2 is water.

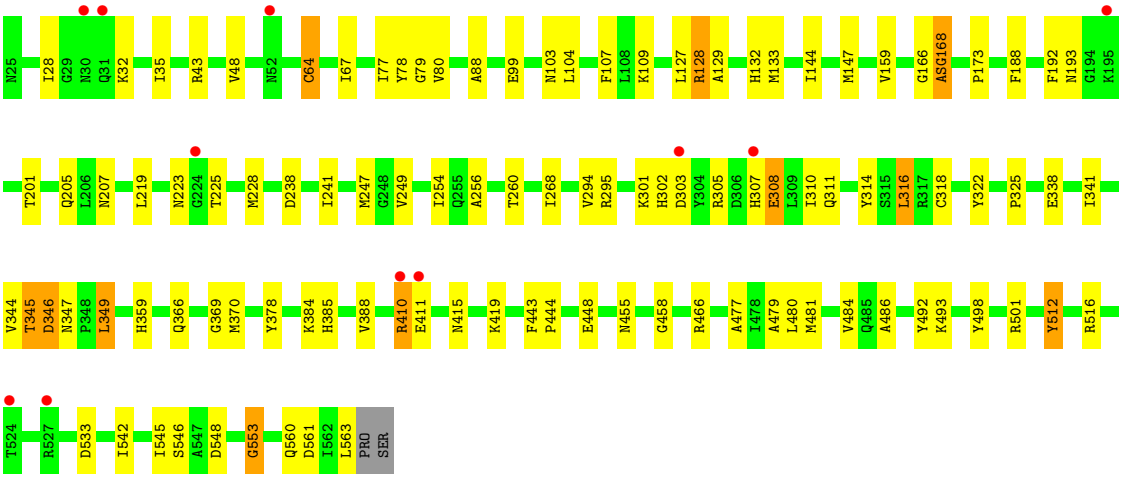
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	198	198	198	0	0
2	B	138	138	138	0	0
2	C	230	231	231	0	1
2	D	122	122	122	0	0

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.

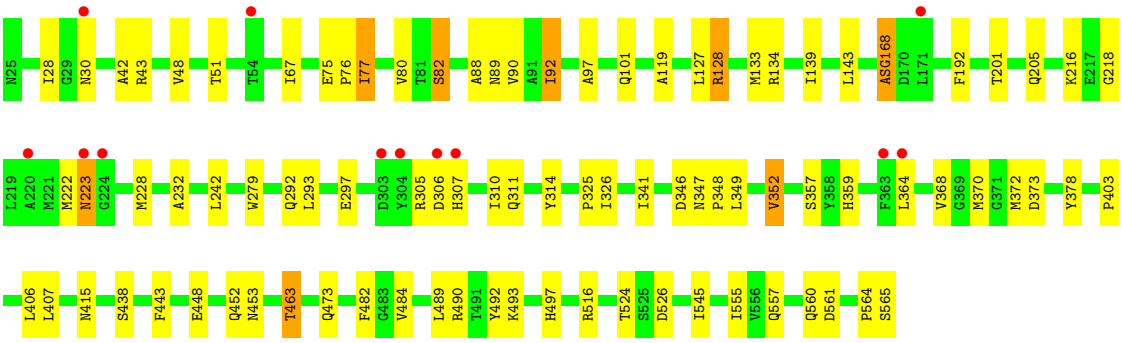
• Molecule 1: Histidine ammonia-lyase

Chain A:



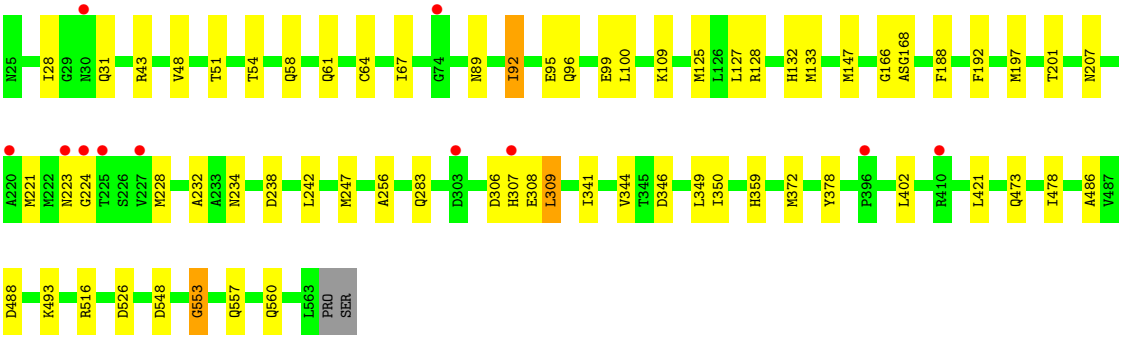
• Molecule 1: Histidine ammonia-lyase

Chain B:



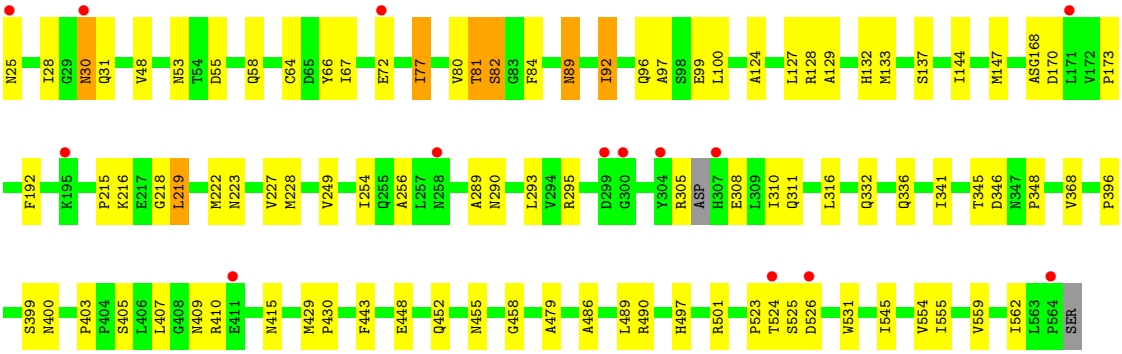
• Molecule 1: Histidine ammonia-lyase

Chain C:



- Molecule 1: Histidine ammonia-lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.15Å 78.05Å 156.76Å 90.00° 120.43° 90.00°	Depositor
Resolution (Å)	34.90 – 2.20 34.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (34.90-2.20) 92.6 (34.85-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.276 0.211 , 0.276	Depositor DCC
R_{free} test set	4763 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17166	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 46.22 % 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 1.1814e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.67	1/4175 (0.0%)	0.71	1/5643 (0.0%)
1	B	0.66	0/4177	0.73	1/5649 (0.0%)
1	C	0.65	0/4156	0.73	1/5617 (0.0%)
1	D	0.66	0/4161	0.72	0/5625
All	All	0.66	1/16669 (0.0%)	0.72	3/22534 (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	B	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	CYS	CB-SG	-5.12	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	C	309	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	128	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	82	SER	Peptide
1	D	82	SER	Peptide

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	4128	0	4102	92	0
1	B	4126	0	4091	72	0
1	C	4109	0	4074	51	0
1	D	4114	0	4084	69	0
2	A	198	0	0	7	0
2	B	138	0	0	6	0
2	C	231	0	0	9	0
2	D	122	0	0	1	0
All	All	17166	0	16351	260	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 8.

All (260) 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:481:MSE:HE1	1:A:542:ILE:HA	1.19	1.17
1:D:228:MSE:HE2	1:D:368:VAL:HB	1.20	1.14
1:D:228:MSE:CE	1:D:368:VAL:HB	1.86	1.05
1:D:228:MSE:HE2	1:D:368:VAL:CB	1.90	1.02
1:D:407:LEU:HD11	1:D:415:ASN:HB3	1.43	1.01
1:D:77:ILE:HG13	1:D:80:VAL:HB	1.44	1.00
1:A:359:HIS:HB3	1:B:311:GLN:HE21	1.26	1.00
1:A:481:MSE:HE2	1:A:545:ILE:HD12	1.47	0.94
1:D:77:ILE:HD11	1:D:80:VAL:HG21	1.50	0.94
1:B:77:ILE:HG13	1:B:80:VAL:HB	1.45	0.93
1:D:77:ILE:HD11	1:D:80:VAL:CG2	2.02	0.90
1:A:305:ARG:HE	1:A:308:GLU:CD	1.76	0.89
1:A:347:ASN:HD21	1:B:311:GLN:HE22	1.20	0.89
1:A:311:GLN:HE22	1:B:347:ASN:HD21	1.18	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:MSE:HE1	1:A:542:ILE:CA	2.03	0.87
1:D:77:ILE:CG1	1:D:80:VAL:HB	2.06	0.84
1:B:463:THR:HG21	2:B:679:HOH:O	1.79	0.81
1:A:127:LEU:HD22	1:A:341:ILE:HG23	1.62	0.81
1:B:77:ILE:CG1	1:B:80:VAL:HB	2.11	0.81
1:A:127:LEU:CD2	1:A:341:ILE:HG23	2.10	0.81
1:B:77:ILE:HD12	1:B:348:PRO:HG2	1.61	0.80
1:A:32:LYS:HD2	2:A:670:HOH:O	1.82	0.78
1:C:28:ILE:HG22	1:C:133:MSE:HG3	1.66	0.76
1:A:225:THR:H	1:A:345:THR:CG2	1.97	0.76
1:C:99:GLU:HG2	2:C:734:HOH:O	1.85	0.76
1:D:254:ILE:HG13	1:D:316:LEU:HD22	1.69	0.75
1:B:139:ILE:HD11	1:B:143:LEU:HD23	1.69	0.75
1:D:254:ILE:CG1	1:D:316:LEU:HD22	2.18	0.73
1:B:51:THR:HG22	1:B:133:MSE:HE2	1.71	0.72
1:D:223:ASN:O	1:D:346:ASP:HA	1.89	0.71
1:D:99:GLU:HG3	2:D:620:HOH:O	1.90	0.71
1:A:359:HIS:HB3	1:B:311:GLN:NE2	2.05	0.71
1:A:295:ARG:NH1	1:A:305:ARG:NH1	2.39	0.70
1:C:197:MSE:CE	1:C:201:THR:HG22	2.21	0.70
1:B:407:LEU:HD11	1:B:415:ASN:HB3	1.72	0.70
1:B:77:ILE:HD11	1:B:80:VAL:CG2	2.22	0.68
1:C:283:GLN:NE2	2:C:725:HOH:O	2.26	0.68
1:A:128:ARG:HH12	1:A:345:THR:HG22	1.59	0.68
1:B:407:LEU:CD1	1:B:415:ASN:HB3	2.25	0.67
1:A:481:MSE:CE	1:A:542:ILE:HA	2.13	0.67
1:D:293:LEU:HD22	1:D:490:ARG:HG3	1.76	0.67
1:A:225:THR:H	1:A:345:THR:HG23	1.58	0.66
1:C:223:ASN:O	1:C:346:ASP:HA	1.95	0.66
1:A:43:ARG:NH1	1:A:238:ASP:OD1	2.29	0.66
1:D:89:ASN:HD22	1:D:89:ASN:H	1.44	0.66
1:C:207:ASN:HD21	1:D:554:VAL:HG11	1.62	0.65
1:C:378:TYR:HB3	2:C:792:HOH:O	1.96	0.64
1:D:407:LEU:HD11	1:D:415:ASN:CB	2.25	0.64
1:A:128:ARG:NH1	1:A:345:THR:HG22	2.12	0.64
1:C:166:GLY:HA2	1:C:228:MSE:HE1	1.80	0.64
1:A:43:ARG:HH12	1:A:238:ASP:CG	2.01	0.64
1:B:77:ILE:HD11	1:B:80:VAL:HG21	1.80	0.63
1:A:207:ASN:ND2	2:A:682:HOH:O	2.25	0.63
1:A:166:GLY:HA2	1:A:228:MSE:HE1	1.81	0.63
1:A:359:HIS:CB	1:B:311:GLN:HE21	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:HD12	1:D:348:PRO:HG2	1.83	0.61
1:A:223:ASN:O	1:A:346:ASP:HA	2.00	0.61
1:D:81:THR:HG22	1:D:92:ILE:O	2.01	0.60
1:D:545:ILE:HG23	1:D:555:ILE:HD13	1.83	0.60
1:D:228:MSE:HE2	1:D:368:VAL:CG1	2.31	0.59
1:A:302:HIS:HE1	1:B:357:SER:O	1.85	0.59
1:C:197:MSE:HE2	1:C:201:THR:CG2	2.33	0.59
1:A:28:ILE:HG22	1:A:133:MSE:HG3	1.83	0.59
1:C:232:ALA:HB1	1:C:372:MSE:HE3	1.85	0.59
1:C:344:VAL:CG1	1:C:349:LEU:HD21	2.32	0.59
1:C:127:LEU:HD22	1:C:341:ILE:HG23	1.85	0.58
1:C:557:GLN:HA	1:C:560:GLN:HG3	1.85	0.58
1:C:125:MSE:HG2	1:C:147:MSE:HE2	1.84	0.58
1:B:223:ASN:O	1:B:346:ASP:HA	2.03	0.58
1:D:127:LEU:HD22	1:D:341:ILE:HG23	1.86	0.58
1:A:268:ILE:HA	1:B:349:LEU:HD12	1.85	0.58
1:B:232:ALA:HB1	1:B:372:MSE:HE3	1.84	0.58
1:C:197:MSE:HE1	1:C:201:THR:HG22	1.86	0.58
1:C:51:THR:HG22	1:C:133:MSE:CE	2.34	0.58
1:D:332:GLN:O	1:D:336:GLN:HG3	2.04	0.58
1:B:545:ILE:HG23	1:B:555:ILE:HD13	1.86	0.57
1:B:352:VAL:HG22	2:B:660:HOH:O	2.03	0.57
1:D:92:ILE:HD12	1:D:96:GLN:HG2	1.86	0.57
1:B:77:ILE:CD1	1:B:348:PRO:HG2	2.31	0.57
1:A:166:GLY:HA2	1:A:228:MSE:CE	2.35	0.57
1:C:197:MSE:HE2	1:C:201:THR:HG22	1.87	0.57
1:B:43:ARG:HH21	1:B:43:ARG:HG3	1.69	0.57
1:D:228:MSE:CE	1:D:368:VAL:CG1	2.83	0.56
1:C:128:ARG:HH12	1:C:224:GLY:HA3	1.71	0.56
1:A:484:VAL:HG13	1:A:512:TYR:CD1	2.41	0.56
1:D:228:MSE:CE	1:D:368:VAL:CB	2.66	0.56
1:B:92:ILE:HD11	1:B:97:ALA:HA	1.88	0.55
1:D:137:SER:O	1:D:216:LYS:HE3	2.07	0.55
1:B:407:LEU:HD11	1:B:415:ASN:CB	2.36	0.55
1:D:89:ASN:HD22	1:D:89:ASN:N	2.03	0.55
1:D:218:GLY:O	1:D:222:MSE:HE3	2.07	0.54
1:A:305:ARG:HB2	1:A:308:GLU:HG3	1.88	0.54
1:B:293:LEU:HD22	1:B:490:ARG:HG3	1.89	0.54
1:C:166:GLY:HA2	1:C:228:MSE:CE	2.38	0.54
1:D:310:ILE:HG23	1:D:311:GLN:HG3	1.90	0.54
1:D:501:ARG:HD3	1:D:523:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ILE:HG22	1:D:133:MSE:HG3	1.90	0.53
1:A:347:ASN:ND2	1:B:311:GLN:HE22	1.97	0.53
1:A:314:TYR:OH	1:B:168:MDO:HB21	2.09	0.53
1:B:28:ILE:HG22	1:B:133:MSE:HG3	1.91	0.53
1:A:480:LEU:O	1:A:484:VAL:HG23	2.08	0.53
1:B:524:THR:HG22	1:B:526:ASP:H	1.73	0.53
1:C:256:ALA:HB1	1:C:486:ALA:HB1	1.90	0.53
1:A:310:ILE:HG22	1:B:88:ALA:HB1	1.90	0.52
1:D:403:PRO:HG2	1:D:489:LEU:HD13	1.92	0.52
1:B:326:ILE:HG23	1:B:378:TYR:HB3	1.90	0.52
1:C:207:ASN:ND2	2:C:694:HOH:O	2.40	0.52
1:D:128:ARG:NH1	1:D:345:THR:O	2.42	0.52
1:D:228:MSE:HE1	1:D:458:GLY:HA3	1.92	0.52
1:C:109:LYS:HE2	1:C:188:PHE:CE2	2.44	0.52
1:D:254:ILE:HG12	1:D:316:LEU:HD22	1.91	0.52
1:A:109:LYS:HE2	1:A:188:PHE:CE2	2.45	0.52
1:D:144:ILE:HA	1:D:147:MSE:HE3	1.92	0.52
1:A:35:ILE:HG13	1:A:338:GLU:HG2	1.92	0.52
1:B:51:THR:HG22	1:B:133:MSE:CE	2.39	0.52
1:C:344:VAL:HG11	1:C:349:LEU:HD21	1.91	0.51
1:C:359:HIS:HE1	2:C:798:HOH:O	1.93	0.51
1:B:242:LEU:HD11	1:B:473:GLN:HG3	1.91	0.51
1:A:104:LEU:HA	1:A:107:PHE:CE1	2.46	0.51
1:B:373:ASP:OD2	1:B:438:SER:HB2	2.11	0.51
1:A:225:THR:H	1:A:345:THR:HG21	1.73	0.51
1:A:370:MSE:SE	1:B:325:PRO:HB2	2.61	0.51
1:D:129:ALA:O	1:D:133:MSE:HG2	2.10	0.51
1:A:128:ARG:HG3	1:A:132:HIS:CE1	2.45	0.51
1:A:305:ARG:HB2	1:A:308:GLU:CG	2.41	0.51
1:A:78:TYR:H	1:A:359:HIS:CE1	2.29	0.50
1:C:344:VAL:HG11	1:C:349:LEU:CD2	2.41	0.50
1:A:166:GLY:CA	1:A:228:MSE:HE1	2.41	0.50
1:A:410:ARG:HH22	1:A:492:TYR:HE2	1.57	0.50
1:B:279:TRP:HE1	1:B:565:SER:HG	1.60	0.50
1:A:345:THR:O	1:A:346:ASP:HB2	2.10	0.50
1:A:347:ASN:HD21	1:B:311:GLN:NE2	1.99	0.50
1:D:443:PHE:HB2	1:D:455:ASN:OD1	2.12	0.50
1:A:311:GLN:HE21	1:B:359:HIS:HB3	1.75	0.50
1:A:144:ILE:HA	1:A:147:MSE:HE3	1.93	0.49
1:A:254:ILE:HG12	1:A:316:LEU:CD1	2.42	0.49
1:D:218:GLY:C	1:D:222:MSE:HE3	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:VAL:HG13	1:B:453:ASN:ND2	2.28	0.49
1:B:43:ARG:HG3	1:B:43:ARG:NH2	2.26	0.49
1:A:415:ASN:HA	1:A:533:ASP:OD2	2.12	0.49
1:A:388:VAL:CG1	1:B:453:ASN:ND2	2.76	0.49
1:B:42:ALA:HB1	1:B:119:ALA:O	2.13	0.48
1:C:92:ILE:HD12	1:C:100:LEU:HD22	1.94	0.48
1:D:289:ALA:O	1:D:290:ASN:HB2	2.12	0.48
1:A:201:THR:O	1:A:205:GLN:HG3	2.14	0.48
1:C:128:ARG:HH12	1:C:224:GLY:CA	2.25	0.48
1:C:128:ARG:HH12	1:C:224:GLY:N	2.11	0.48
1:D:30:ASN:HD22	1:D:31:GLN:H	1.61	0.48
1:A:359:HIS:HD2	2:B:574:HOH:O	1.95	0.48
1:D:216:LYS:O	1:D:216:LYS:HG3	2.13	0.48
1:D:249:VAL:HG11	1:D:479:ALA:HB1	1.96	0.48
1:A:256:ALA:HB1	1:A:486:ALA:HB1	1.95	0.48
1:C:378:TYR:CB	2:C:792:HOH:O	2.60	0.48
1:D:228:MSE:CE	1:D:458:GLY:HA3	2.44	0.48
1:D:308:GLU:OE2	1:D:400:ASN:ND2	2.47	0.48
1:A:260:THR:HB	1:A:295:ARG:NH1	2.29	0.47
1:D:89:ASN:H	1:D:89:ASN:ND2	2.11	0.47
1:C:51:THR:HG22	1:C:133:MSE:HE2	1.96	0.47
1:D:170:ASP:OD2	1:D:228:MSE:HG2	2.15	0.47
1:C:109:LYS:HE2	1:C:188:PHE:CZ	2.49	0.47
1:A:254:ILE:HG12	1:A:316:LEU:HD12	1.95	0.47
1:B:292:GLN:NE2	2:B:666:HOH:O	2.47	0.47
1:A:484:VAL:HG11	1:A:516:ARG:HD3	1.96	0.47
1:A:67:ILE:HD13	1:A:67:ILE:HA	1.76	0.47
1:C:128:ARG:NH1	1:C:224:GLY:HA3	2.30	0.47
1:D:524:THR:HG22	1:D:526:ASP:H	1.80	0.46
1:C:67:ILE:HD11	1:C:350:ILE:HD11	1.97	0.46
1:A:168:MDO:HB21	1:B:314:TYR:OH	2.14	0.46
1:A:173:PRO:HA	2:A:691:HOH:O	2.15	0.46
1:B:228:MSE:HG3	1:B:368:VAL:HG11	1.97	0.46
1:D:409:ASN:HB2	1:D:531:TRP:CE2	2.51	0.46
1:D:84:PHE:HE2	1:D:219:LEU:HG	1.80	0.46
1:D:170:ASP:O	1:D:173:PRO:HD2	2.16	0.46
1:D:219:LEU:HD22	1:D:223:ASN:HB2	1.97	0.46
1:B:92:ILE:O	1:B:92:ILE:HG13	2.12	0.46
1:C:96:GLN:NE2	2:C:734:HOH:O	2.27	0.46
1:D:256:ALA:HB1	1:D:486:ALA:HB1	1.98	0.46
1:D:497:HIS:HB2	1:D:525:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:GLN:HA	1:B:560:GLN:HG3	1.99	0.45
1:A:419:LYS:HA	2:A:617:HOH:O	2.15	0.45
1:C:128:ARG:HD2	1:C:132:HIS:CE1	2.51	0.45
1:B:484:VAL:HG11	1:B:516:ARG:HD3	1.99	0.45
1:C:95:GLU:HG2	2:C:763:HOH:O	2.17	0.45
1:A:384:LYS:HG2	1:B:443:PHE:CZ	2.51	0.45
1:A:303:ASP:HA	1:B:76:PRO:HG2	1.99	0.45
1:C:147:MSE:HE3	1:C:221:MSE:HE1	1.99	0.45
1:C:242:LEU:HD11	1:C:473:GLN:HG3	1.99	0.44
1:D:82:SER:O	1:D:100:LEU:HD21	2.18	0.44
1:A:129:ALA:O	1:A:133:MSE:HG2	2.17	0.44
1:A:295:ARG:NH1	1:A:305:ARG:HH12	2.14	0.44
1:A:443:PHE:HA	1:A:444:PRO:HD3	1.91	0.44
1:A:501:ARG:HG3	1:A:512:TYR:HE2	1.82	0.44
1:D:128:ARG:HG3	1:D:132:HIS:CE1	2.52	0.44
1:D:295:ARG:NH1	1:D:305:ARG:CZ	2.81	0.44
1:A:88:ALA:HB1	1:B:310:ILE:HG22	1.99	0.44
1:A:378:TYR:HB3	2:A:763:HOH:O	2.17	0.44
1:C:147:MSE:CE	1:C:221:MSE:HE1	2.47	0.44
1:A:345:THR:HG22	1:A:345:THR:O	2.17	0.44
1:C:548:ASP:OD2	1:C:553:GLY:HA3	2.18	0.44
1:D:429:MSE:SE	1:D:429:MSE:C	3.06	0.44
1:D:545:ILE:HG23	1:D:555:ILE:CD1	2.45	0.44
1:D:448:GLU:HB3	1:D:452:GLN:HG3	1.99	0.44
1:B:218:GLY:O	1:B:222:MSE:HE3	2.17	0.43
1:B:306:ASP:HA	1:B:307:HIS:HA	1.45	0.43
1:C:306:ASP:HA	1:C:308:GLU:H	1.83	0.43
1:D:66:TYR:CD2	1:D:66:TYR:C	2.91	0.43
1:D:124:ALA:HB2	1:D:227:VAL:HA	1.99	0.43
1:A:378:TYR:CB	2:A:763:HOH:O	2.65	0.43
1:A:501:ARG:HG3	1:A:512:TYR:CE2	2.52	0.43
1:D:215:PRO:O	1:D:216:LYS:HB3	2.18	0.43
1:D:559:VAL:HB	1:D:562:ILE:HD12	1.99	0.43
1:A:492:TYR:HB2	1:A:498:TYR:CE2	2.53	0.43
1:A:322:TYR:CE1	1:A:385:HIS:HB2	2.54	0.43
1:B:134:ARG:NE	2:B:567:HOH:O	2.44	0.43
1:C:166:GLY:CA	1:C:228:MSE:HE1	2.49	0.43
1:A:366:GLN:HG3	1:A:370:MSE:SE	2.69	0.42
1:A:548:ASP:OD2	1:A:553:GLY:HA3	2.19	0.42
1:B:201:THR:O	1:B:205:GLN:HG3	2.19	0.42
1:A:241:ILE:HA	1:A:563:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:SER:HA	1:B:90:VAL:O	2.18	0.42
1:D:295:ARG:HH12	1:D:305:ARG:CZ	2.31	0.42
1:A:225:THR:N	1:A:345:THR:HG23	2.30	0.42
1:A:318:CYS:HB3	1:B:364:LEU:HD22	2.01	0.42
1:A:325:PRO:HB2	1:B:370:MSE:SE	2.69	0.42
1:A:443:PHE:HB2	1:A:455:ASN:OD1	2.19	0.42
1:B:77:ILE:HD11	1:B:80:VAL:HG23	1.99	0.42
1:B:448:GLU:HB3	1:B:452:GLN:HG3	2.02	0.42
1:B:101:GLN:NE2	1:B:216:LYS:H	2.17	0.42
1:B:127:LEU:HD22	1:B:341:ILE:HG23	2.02	0.42
1:C:247:MSE:CE	1:C:283:GLN:HB2	2.50	0.42
1:C:306:ASP:HA	1:C:308:GLU:N	2.35	0.42
1:B:168:MDO:O2	1:B:223:ASN:ND2	2.48	0.42
1:A:77:ILE:HB	1:A:80:VAL:HB	2.01	0.41
1:A:477:ALA:O	1:A:481:MSE:HE3	2.19	0.41
1:C:43:ARG:HH12	1:C:238:ASP:CG	2.24	0.41
1:D:92:ILE:HD11	1:D:97:ALA:HA	2.02	0.41
1:A:344:VAL:HG12	1:A:349:LEU:HD11	2.01	0.41
1:A:249:VAL:HG11	1:A:479:ALA:HB1	2.03	0.41
1:C:43:ARG:HH11	1:C:234:ASN:HB3	1.85	0.41
1:A:247:MSE:HE2	1:A:247:MSE:HB2	1.99	0.41
1:B:134:ARG:NH2	2:B:567:HOH:O	2.45	0.41
1:A:103:ASN:HB3	2:A:601:HOH:O	2.19	0.41
1:A:302:HIS:CE1	1:B:357:SER:O	2.70	0.41
1:B:492:TYR:HA	1:B:497:HIS:O	2.21	0.41
1:A:369:GLY:HA2	1:A:458:GLY:HA2	2.01	0.41
1:B:406:LEU:HD12	1:B:482:PHE:HD2	1.86	0.41
1:C:359:HIS:CE1	2:C:798:HOH:O	2.71	0.41
1:C:421:LEU:HG	1:C:478:ILE:HG23	2.02	0.41
1:C:488:ASP:OD2	1:C:516:ARG:NH1	2.41	0.41
1:A:359:HIS:CD2	1:B:311:GLN:HG2	2.56	0.41
1:C:128:ARG:HA	1:C:128:ARG:HD3	1.89	0.40
1:D:396:PRO:HA	1:D:399:SER:OG	2.21	0.40
1:A:159:VAL:CG1	1:A:173:PRO:HB3	2.50	0.40
1:C:61:GLN:O	1:C:64:CYS:HB3	2.21	0.40
1:A:79:GLY:HA3	1:A:219:LEU:HD22	2.04	0.40
1:D:429:MSE:HB3	1:D:430:PRO:HD3	2.02	0.40
1:B:297:GLU:OE1	1:B:305:ARG:NH2	2.55	0.40
1:B:403:PRO:HG2	1:B:489:LEU:HD13	2.04	0.40
1:B:560:GLN:O	1:B:564:PRO:HD3	2.22	0.40
1:D:28:ILE:O	1:D:133:MSE:HE2	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	532/539 (99%)	510 (96%)	18 (3%)	4 (1%)	19	19
1	B	535/539 (99%)	517 (97%)	17 (3%)	1 (0%)	47	55
1	C	533/539 (99%)	514 (96%)	18 (3%)	1 (0%)	47	55
1	D	530/539 (98%)	510 (96%)	19 (4%)	1 (0%)	47	55
All	All	2130/2156 (99%)	2051 (96%)	72 (3%)	7 (0%)	41	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	ASN
1	D	405	SER
1	A	193	ASN
1	A	346	ASP
1	C	553	GLY
1	A	448	GLU
1	A	553	GLY

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	443/430 (103%)	424 (96%)	19 (4%)	29	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	441/430 (103%)	428 (97%)	13 (3%)	42	54
1	C	438/430 (102%)	426 (97%)	12 (3%)	44	57
1	D	440/430 (102%)	424 (96%)	16 (4%)	35	45
All	All	1762/1720 (102%)	1702 (97%)	60 (3%)	37	47

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	A	64	CYS
1	A	99	GLU
1	A	128	ARG
1	A	192	PHE
1	A	294	VAL
1	A	301	LYS
1	A	307	HIS
1	A	308	GLU
1	A	316	LEU
1	A	345	THR
1	A	349	LEU
1	A	410	ARG
1	A	411	GLU
1	A	493	LYS
1	A	512	TYR
1	A	546	SER
1	A	560	GLN
1	A	561	ASP
1	B	48	VAL
1	B	67	ILE
1	B	75	GLU
1	B	77	ILE
1	B	89	ASN
1	B	92	ILE
1	B	128	ARG
1	B	192	PHE
1	B	223	ASN
1	B	352	VAL
1	B	463	THR
1	B	493	LYS
1	B	561	ASP
1	C	31	GLN

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Mol	Chain	Res	Type
1	C	48	VAL
1	C	54	THR
1	C	58	GLN
1	C	89	ASN
1	C	92	ILE
1	C	192	PHE
1	C	307	HIS
1	C	309	LEU
1	C	402	LEU
1	C	493	LYS
1	C	526	ASP
1	D	25	ASN
1	D	30	ASN
1	D	48	VAL
1	D	53	ASN
1	D	55	ASP
1	D	58	GLN
1	D	64	CYS
1	D	67	ILE
1	D	72	GLU
1	D	77	ILE
1	D	81	THR
1	D	89	ASN
1	D	92	ILE
1	D	192	PHE
1	D	219	LEU
1	D	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	240	GLN
1	A	283	GLN
1	A	311	GLN
1	A	359	HIS
1	B	58	GLN
1	B	89	ASN
1	B	132	HIS
1	B	240	GLN
1	B	283	GLN
1	B	302	HIS

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Mol	Chain	Res	Type
1	B	311	GLN
1	B	474	ASN
1	B	560	GLN
1	C	69	ASN
1	C	89	ASN
1	C	207	ASN
1	C	240	GLN
1	C	283	GLN
1	C	292	GLN
1	C	474	ASN
1	D	25	ASN
1	D	89	ASN
1	D	240	GLN
1	D	258	ASN
1	D	283	GLN
1	D	292	GLN
1	D	400	ASN
1	D	474	ASN
1	D	560	GLN

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	C	168	1	12,13,14	3.80	4 (33%)	15,18,20	7.65	10 (66%)
1	MDO	A	168	1	12,13,14	3.80	4 (33%)	15,18,20	7.15	8 (53%)
1	MDO	D	168	1	12,13,14	3.90	4 (33%)	15,18,20	7.21	10 (66%)
1	MDO	B	168	1	12,13,14	3.77	3 (25%)	15,18,20	8.03	10 (66%)

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	C	168	1	-	2/4/23/24	0/1/1/1
1	MDO	A	168	1	-	1/4/23/24	0/1/1/1
1	MDO	D	168	1	-	0/4/23/24	0/1/1/1
1	MDO	B	168	1	-	1/4/23/24	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	MDO	O2-C2	12.26	1.49	1.23
1	A	168	MDO	O2-C2	11.90	1.48	1.23
1	C	168	MDO	O2-C2	11.66	1.47	1.23
1	B	168	MDO	O2-C2	11.44	1.47	1.23
1	B	168	MDO	C1-N2	4.38	1.38	1.32
1	C	168	MDO	C1-N2	3.86	1.37	1.32
1	D	168	MDO	C1-N2	3.64	1.37	1.32
1	B	168	MDO	C2-N3	-3.46	1.31	1.39
1	A	168	MDO	C1-N2	3.44	1.37	1.32
1	A	168	MDO	C2-N3	-2.99	1.32	1.39
1	D	168	MDO	C2-N3	-2.95	1.32	1.39
1	C	168	MDO	C2-N3	-2.84	1.33	1.39
1	C	168	MDO	CA2-C2	-2.48	1.38	1.43
1	D	168	MDO	CA2-C2	-2.17	1.38	1.43
1	A	168	MDO	CA2-C2	-2.08	1.39	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	168	MDO	CA2-C2-N3	25.21	115.29	103.37
1	C	168	MDO	CA2-C2-N3	23.33	114.40	103.37
1	A	168	MDO	CA2-C2-N3	22.30	113.91	103.37
1	D	168	MDO	CA2-C2-N3	21.96	113.75	103.37
1	C	168	MDO	O2-C2-CA2	-11.06	124.75	130.96
1	B	168	MDO	C2-CA2-N2	-10.51	101.57	108.93
1	D	168	MDO	O2-C2-CA2	-10.35	125.15	130.96
1	A	168	MDO	C2-CA2-N2	-9.14	102.53	108.93
1	C	168	MDO	C2-CA2-N2	-8.90	102.70	108.93
1	B	168	MDO	O2-C2-CA2	-8.85	125.99	130.96
1	D	168	MDO	C2-CA2-N2	-8.73	102.81	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	MDO	O2-C2-CA2	-8.10	126.41	130.96
1	C	168	MDO	C2-N3-C1	-7.33	104.26	107.97
1	B	168	MDO	C2-N3-C1	-6.92	104.46	107.97
1	D	168	MDO	C2-N3-C1	-6.09	104.88	107.97
1	A	168	MDO	C2-N3-C1	-6.07	104.90	107.97
1	B	168	MDO	CA2-N2-C1	5.34	110.23	105.40
1	A	168	MDO	CA2-N2-C1	5.19	110.10	105.40
1	D	168	MDO	CA2-N2-C1	4.95	109.88	105.40
1	C	168	MDO	CA2-N2-C1	4.91	109.84	105.40
1	A	168	MDO	CB2-CA2-C2	4.44	130.88	122.76
1	B	168	MDO	N3-C1-N2	-4.42	108.39	111.45
1	A	168	MDO	N3-C1-N2	-4.21	108.54	111.45
1	D	168	MDO	N3-C1-N2	-4.02	108.67	111.45
1	C	168	MDO	N3-C1-N2	-3.85	108.79	111.45
1	B	168	MDO	CB2-CA2-C2	3.80	129.72	122.76
1	B	168	MDO	CA3-N3-C1	3.58	131.46	127.16
1	C	168	MDO	CB2-CA2-C2	3.56	129.28	122.76
1	D	168	MDO	CB2-CA2-C2	3.37	128.93	122.76
1	C	168	MDO	CA3-N3-C1	3.22	131.03	127.16
1	D	168	MDO	CA3-N3-C1	3.02	130.79	127.16
1	B	168	MDO	O2-C2-N3	-2.85	118.68	124.35
1	C	168	MDO	O3-C3-CA3	-2.55	118.69	126.39
1	A	168	MDO	O2-C2-N3	-2.36	119.66	124.35
1	D	168	MDO	CA1-C1-N3	2.34	127.56	124.75
1	D	168	MDO	O3-C3-CA3	-2.25	119.59	126.39
1	C	168	MDO	CA1-C1-N3	2.11	127.27	124.75
1	B	168	MDO	C1-CA1-N1	2.05	115.21	109.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	168	MDO	N2-C1-CA1-CB
1	C	168	MDO	N2-C1-CA1-CB
1	A	168	MDO	N3-C1-CA1-CB
1	C	168	MDO	N3-C1-CA1-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	168	MDO	1	0
1	B	168	MDO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	521/539 (96%)	-0.08	11 (2%)	63	61	16, 30, 46, 58	0
1	B	523/539 (97%)	-0.06	12 (2%)	60	58	18, 30, 46, 58	0
1	C	521/539 (96%)	-0.05	11 (2%)	63	61	18, 30, 47, 55	0
1	D	521/539 (96%)	-0.07	14 (2%)	54	52	17, 30, 46, 59	0
All	All	2086/2156 (96%)	-0.07	48 (2%)	60	58	16, 30, 46, 59	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	HIS	6.1
1	C	307	HIS	6.1
1	A	30	ASN	4.0
1	D	307	HIS	3.8
1	B	306	ASP	3.4
1	A	52	ASN	3.4
1	C	74	GLY	3.2
1	B	30	ASN	3.0
1	C	224	GLY	2.9
1	D	411	GLU	2.9
1	B	307	HIS	2.8
1	C	227	VAL	2.7
1	A	410	ARG	2.7
1	D	299	ASP	2.7
1	B	363	PHE	2.7
1	D	564	PRO	2.6
1	C	303	ASP	2.6
1	B	223	ASN	2.6
1	B	364	LEU	2.5
1	C	30	ASN	2.5
1	B	224	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	225	THR	2.4
1	C	410	ARG	2.4
1	C	223	ASN	2.4
1	D	25	ASN	2.4
1	D	30	ASN	2.4
1	D	258	ASN	2.4
1	B	171	LEU	2.3
1	A	224	GLY	2.3
1	B	54	THR	2.3
1	A	303	ASP	2.3
1	D	72	GLU	2.2
1	D	300	GLY	2.2
1	A	524	THR	2.1
1	C	220	ALA	2.1
1	D	304	TYR	2.1
1	D	524	THR	2.1
1	C	396	PRO	2.1
1	A	411	GLU	2.1
1	D	526	ASP	2.1
1	A	195	LYS	2.1
1	B	304	TYR	2.1
1	A	527	ARG	2.1
1	B	220	ALA	2.1
1	B	303	ASP	2.0
1	D	195	LYS	2.0
1	D	171	LEU	2.0
1	A	31	GLN	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. 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(Å^2)	Q<0.9
1	MDO	B	168	13/14	0.90	0.22	25,27,28,29	0
1	MDO	A	168	13/14	0.91	0.15	26,28,29,30	0
1	MDO	D	168	13/14	0.92	0.18	26,30,31,33	0
1	MDO	C	168	13/14	0.94	0.18	25,29,30,30	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.