Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 07:25 AM EST

PDB ID	:	2RJS
Title	:	SgTAM bound to substrate mimic
Authors	:	Montavon, T.J.; Christianson, C.V.; Bruner, S.D.
Deposited on	:	2007-10-15
Resolution	:	2.40 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:

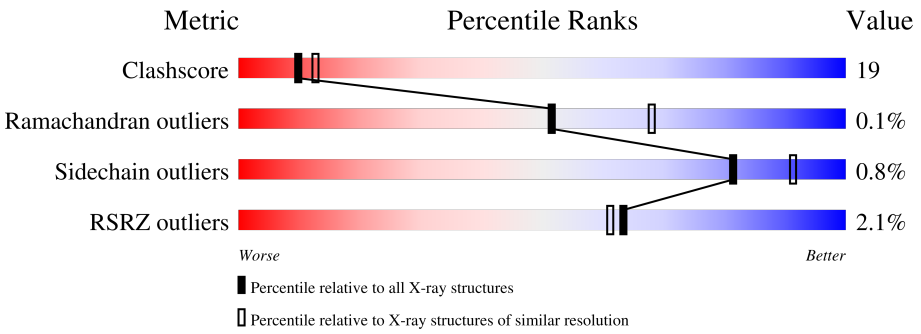
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	537	2% 66% 30% ··
1	B	537	2% 71% 27% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MDO	B	152	-	-	X	-
2	296	A	1001	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	296	B	1001	-	-	X	X

2 Entry composition (i)

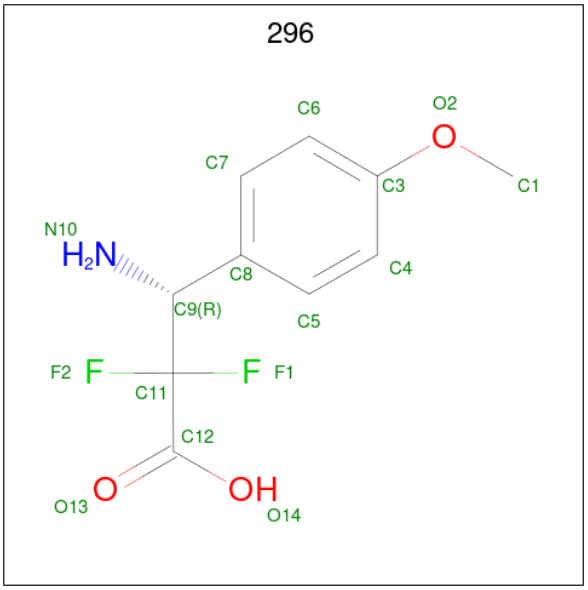
There are 3 unique types of molecules in this entry. The entry contains 8451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tyrosine aminomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	4007	2503	727	769	8	0	0	0
			Total	C	N	O	S			
1	B	527	4014	2508	728	770	8	0	0	0

- Molecule 2 is (3R)-3-amino-2,2-difluoro-3-(4-methoxyphenyl)propanoic acid (three-letter code: 296) (formula: $C_{10}H_{11}F_2NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	16	10	2	1	3	0	0
			Total	C	F	N	O		
2	B	1	16	10	2	1	3	0	0

- Molecule 3 is water.

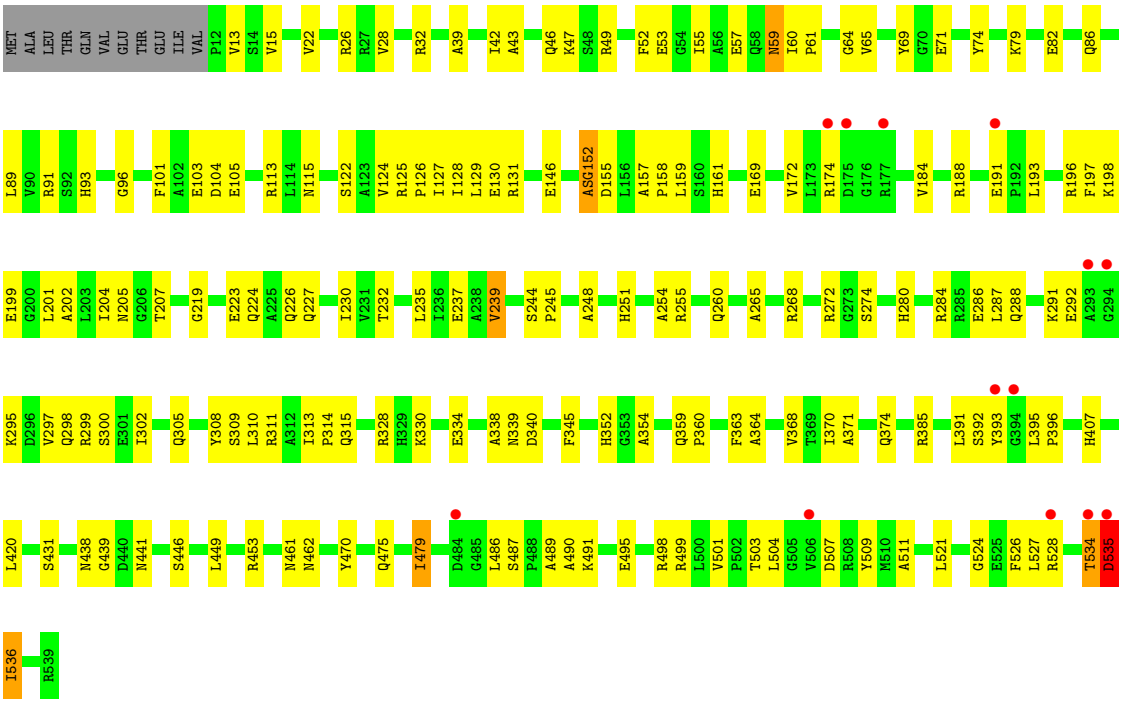
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	179	179	179	0	0
			Total	O		
3	B	219	219	219	0	0

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.

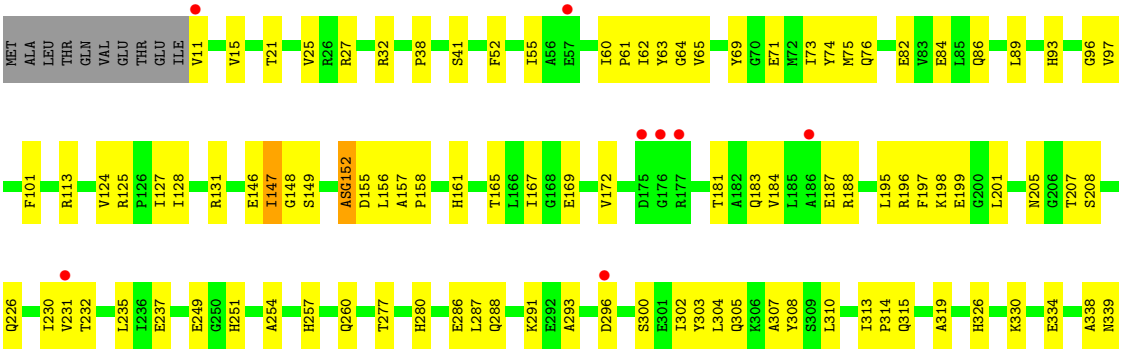
• Molecule 1: Tyrosine aminomutase

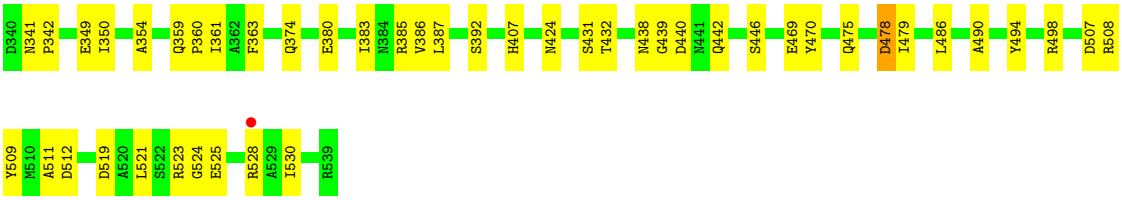
Chain A:



• Molecule 1: Tyrosine aminomutase

Chain B:




D340
N341
P342
E349
I350
A354
Q359
P360
I361
A362
F363
Q374
E380
I383
N384
R385
V386
L387
S392
H407
M424
S431
T432
M438
G439
D440
N441
Q442
S446
E469
Y470
Q475
D478
I479
L486
A490
Y494
R498
D507
R508
Y509
M510
A511
D512
D519
A520
L521
S522
R523
G524
E525
R528
A529
I530
R539

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.49Å 146.29Å 75.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (25.00-2.40) 93.1 (25.01-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.182 , 0.245 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8451	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.66% 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, 0.333 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: 296, 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	0.32	0/4053	0.61	2/5490 (0.0%)
1	B	0.34	0/4060	0.60	0/5501
All	All	0.33	0/8113	0.61	2/10991 (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	A	1	1
1	B	0	1
All	All	1	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	GLY	N-CA-C	-5.38	99.65	113.10
1	A	535	ASP	CB-CA-C	5.07	120.55	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	535	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	534	THR	Peptide
1	B	147	ILE	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	4007	0	4026	190	0
1	B	4014	0	4035	153	0
2	A	16	0	8	8	0
2	B	16	0	10	17	0
3	A	179	0	0	4	0
3	B	219	0	0	9	0
All	All	8451	0	8079	309	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 19.

All (309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MDO:HB21	2:B:1001:296:F2	1.31	1.14
1:B:152:MDO:HB22	2:B:1001:296:N10	0.80	1.12
1:B:152:MDO:HB22	2:B:1001:296:C9	1.83	1.05
1:A:534:THR:HG22	1:A:535:ASP:N	1.79	0.95
1:A:292:GLU:H	1:A:298:GLN:NE2	1.65	0.95
1:A:71:GLU:H	1:A:438:ASN:HD21	1.12	0.94
1:A:534:THR:HG22	1:A:535:ASP:H	1.27	0.94
1:B:152:MDO:CB2	2:B:1001:296:F2	2.05	0.93
1:B:152:MDO:HB22	2:B:1001:296:HN1A	1.34	0.92
1:A:248:ALA:HB2	1:A:268:ARG:NH1	1.86	0.91
1:A:292:GLU:N	1:A:298:GLN:HE22	1.70	0.89
1:A:152:MDO:HB21	2:A:1001:296:F2	1.57	0.88
1:A:526:PHE:O	1:A:527:LEU:HB3	1.73	0.88
1:A:59:ASN:HD21	1:A:79:LYS:H	1.21	0.88
1:B:71:GLU:H	1:B:438:ASN:HD21	1.25	0.81
1:A:292:GLU:H	1:A:298:GLN:HE22	0.85	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HE21	1:A:479:ILE:HD12	1.49	0.78
1:B:86:GLN:HG3	1:B:196:ARG:O	1.83	0.78
1:A:248:ALA:HB2	1:A:268:ARG:HH12	1.46	0.78
1:A:284:ARG:HD2	1:B:60:ILE:HD12	1.64	0.78
1:A:287:LEU:HD13	1:A:302:ILE:HB	1.65	0.77
1:A:122:SER:O	1:A:198:LYS:HE3	1.86	0.76
1:A:125:ARG:HD3	1:A:199:GLU:OE2	1.86	0.76
1:B:330:LYS:HA	1:B:330:LYS:HE2	1.68	0.76
1:B:152:MDO:CB2	2:B:1001:296:HN10	1.61	0.76
1:B:207:THR:H	1:B:339:ASN:HD22	1.33	0.76
1:B:251:HIS:HD2	1:B:260:GLN:HE21	1.34	0.76
1:B:235:LEU:HD11	1:B:386:VAL:HG11	1.68	0.75
1:B:172:VAL:HG21	1:B:184:VAL:HG21	1.69	0.74
1:A:86:GLN:HG3	1:A:196:ARG:O	1.88	0.74
1:A:198:LYS:O	1:A:198:LYS:HG2	1.88	0.74
1:A:39:ALA:HA	1:A:42:ILE:HG22	1.71	0.72
1:A:308:TYR:CZ	1:B:442:GLN:HG2	2.24	0.72
1:A:534:THR:CG2	1:A:535:ASP:N	2.53	0.72
1:B:251:HIS:CD2	1:B:260:GLN:HE21	2.07	0.71
1:A:71:GLU:N	1:A:438:ASN:HD21	1.86	0.70
1:A:93:HIS:NE2	2:A:1001:296:H6	2.06	0.70
1:A:96:GLY:H	1:A:161:HIS:HE1	1.39	0.70
1:A:126:PRO:O	1:A:130:GLU:HG3	1.90	0.70
1:A:491:LYS:O	1:A:495:GLU:HG2	1.90	0.70
1:B:235:LEU:HD11	1:B:386:VAL:CG1	2.22	0.70
1:A:534:THR:CG2	1:A:536:ILE:H	2.05	0.69
1:A:59:ASN:HD21	1:A:79:LYS:N	1.90	0.69
1:A:265:ALA:HA	1:A:268:ARG:HH21	1.57	0.68
1:A:359:GLN:NE2	1:B:374:GLN:HE21	1.90	0.68
1:B:55:ILE:HD11	1:B:60:ILE:HD11	1.74	0.68
1:A:232:THR:HG21	1:A:313:ILE:HG12	1.75	0.68
1:A:82:GLU:HG3	1:A:197:PHE:CD1	2.29	0.68
1:B:149:SER:HB2	1:B:155:ASP:HA	1.75	0.68
1:A:438:ASN:HD22	1:A:441:ASN:HB3	1.59	0.67
1:A:184:VAL:O	1:A:188:ARG:HG3	1.92	0.67
1:A:207:THR:H	1:A:339:ASN:HD22	1.43	0.66
1:B:205:ASN:OD1	2:B:1001:296:N10	2.25	0.66
1:A:59:ASN:OD1	1:A:79:LYS:HG2	1.95	0.66
1:B:172:VAL:CG2	1:B:184:VAL:HG21	2.26	0.65
1:B:71:GLU:H	1:B:438:ASN:ND2	1.93	0.65
1:A:65:VAL:HG22	1:A:198:LYS:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:NE2	2:B:1001:296:H6	2.12	0.65
1:B:152:MDO:CB2	2:B:1001:296:C9	2.56	0.65
1:B:124:VAL:HG13	1:B:128:ILE:HD12	1.77	0.65
1:A:152:MDO:HB21	1:B:308:TYR:OH	1.96	0.65
1:A:64:GLY:HA3	1:A:201:LEU:HD22	1.80	0.64
1:B:152:MDO:CB2	2:B:1001:296:C11	2.76	0.64
1:B:167:ILE:HG13	1:B:169:GLU:HG3	1.78	0.63
1:A:308:TYR:CE2	1:B:442:GLN:HG2	2.33	0.63
1:A:32:ARG:HH22	1:A:103:GLU:HG2	1.62	0.63
1:B:15:VAL:HG23	1:B:15:VAL:O	1.99	0.63
1:B:96:GLY:H	1:B:161:HIS:HE1	1.46	0.62
1:A:32:ARG:NH2	1:A:103:GLU:HG2	2.14	0.62
1:A:251:HIS:HD2	1:A:260:GLN:HG2	1.62	0.62
1:A:53:GLU:O	1:A:57:GLU:HG2	1.98	0.62
1:A:198:LYS:O	1:A:198:LYS:CG	2.47	0.62
1:A:254:ALA:HB1	1:B:338:ALA:HB3	1.82	0.62
1:B:184:VAL:O	1:B:188:ARG:HG3	1.98	0.62
1:A:60:ILE:HA	1:B:288:GLN:OE1	1.99	0.61
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.65	0.61
1:B:152:MDO:HB22	2:B:1001:296:HN10	0.79	0.61
1:A:15:VAL:HG13	1:A:115:ASN:HD22	1.65	0.61
1:B:152:MDO:CB2	2:B:1001:296:HN1A	1.99	0.60
1:A:172:VAL:HG21	1:A:184:VAL:HG21	1.82	0.60
1:A:507:ASP:HB2	3:A:1090:HOH:O	2.00	0.60
1:A:128:ILE:HD11	1:A:199:GLU:CD	2.22	0.60
1:A:152:MDO:CB2	2:A:1001:296:F2	2.36	0.60
1:A:308:TYR:OH	1:B:152:MDO:HB21	2.00	0.60
1:A:534:THR:HG22	1:A:536:ILE:H	1.65	0.60
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.67	0.60
1:B:64:GLY:HA3	1:B:201:LEU:HD22	1.82	0.60
1:A:534:THR:HG21	1:A:536:ILE:HD12	1.83	0.59
1:A:235:LEU:HD22	1:A:310:LEU:HD21	1.82	0.59
1:A:534:THR:HG22	1:A:536:ILE:N	2.17	0.59
1:B:11:VAL:HG23	1:B:27:ARG:HH21	1.68	0.59
1:A:526:PHE:C	1:A:528:ARG:H	2.06	0.59
1:B:11:VAL:HG12	1:B:11:VAL:O	2.01	0.59
1:A:74:TYR:HB2	1:B:300:SER:O	2.02	0.59
1:A:534:THR:CG2	1:A:535:ASP:H	2.07	0.59
1:A:91:ARG:HD3	1:A:169:GLU:OE1	2.02	0.59
1:B:313:ILE:HD12	1:B:313:ILE:H	1.67	0.58
1:A:22:VAL:HG21	1:A:328:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:ARG:HG3	1:B:525:GLU:HG2	1.86	0.58
1:B:232:THR:HG21	1:B:313:ILE:HG12	1.84	0.58
1:A:420:LEU:HD22	1:A:461:ASN:HB3	1.86	0.58
1:A:93:HIS:HE2	2:A:1001:296:C3	2.17	0.57
1:A:101:PHE:CE1	1:A:146:GLU:HG2	2.39	0.57
1:A:172:VAL:CG2	1:A:184:VAL:HG21	2.34	0.57
1:A:224:GLN:NE2	1:A:462:ASN:HD22	2.02	0.57
1:A:345:PHE:CE2	1:B:249:GLU:HG3	2.39	0.57
1:A:359:GLN:HE22	1:B:374:GLN:HE21	1.53	0.57
1:A:82:GLU:HG3	1:A:197:PHE:CE1	2.40	0.56
1:A:534:THR:O	1:A:535:ASP:CB	2.54	0.56
1:B:207:THR:H	1:B:339:ASN:ND2	2.01	0.56
1:A:305:GLN:HE22	1:B:341:ASN:HD21	1.51	0.56
1:A:127:ILE:HD12	1:A:127:ILE:C	2.26	0.56
1:A:311:ARG:NH2	2:B:1001:296:O14	2.39	0.55
1:B:147:ILE:CG2	1:B:148:GLY:N	2.69	0.55
1:B:407:HIS:HD2	1:B:507:ASP:H	1.55	0.55
1:A:69:TYR:CZ	1:A:89:LEU:HD22	2.42	0.54
1:A:205:ASN:O	1:A:340:ASP:HA	2.07	0.54
1:A:534:THR:O	1:A:535:ASP:HB3	2.07	0.54
1:B:55:ILE:HD12	3:B:1026:HOH:O	2.07	0.54
1:B:494:TYR:CZ	1:B:498:ARG:HG3	2.42	0.54
1:B:231:VAL:HG21	1:B:469:GLU:HG2	1.90	0.54
1:B:470:TYR:CE1	1:B:521:LEU:HD21	2.43	0.54
1:A:359:GLN:N	1:A:360:PRO:HD2	2.23	0.54
1:A:52:PHE:HZ	1:A:65:VAL:HG21	1.71	0.54
1:A:244:SER:HB3	1:A:245:PRO:HD3	1.90	0.54
1:B:82:GLU:HG3	1:B:197:PHE:CD1	2.43	0.54
1:B:237:GLU:HG2	1:B:277:THR:HG23	1.89	0.54
1:B:152:MDO:O3	1:B:156:LEU:N	2.40	0.53
1:A:39:ALA:HA	1:A:42:ILE:CG2	2.37	0.53
1:A:280:HIS:HD2	1:B:349:GLU:HG3	1.72	0.53
1:B:334:GLU:HG3	1:B:361:ILE:CG1	2.38	0.53
1:B:313:ILE:HD12	1:B:313:ILE:N	2.24	0.53
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.90	0.53
1:B:392:SER:HA	3:B:1045:HOH:O	2.07	0.53
1:B:11:VAL:HG23	1:B:27:ARG:NH2	2.23	0.53
1:B:124:VAL:CG1	1:B:128:ILE:HB	2.38	0.53
1:A:486:LEU:HB3	1:A:490:ALA:HB3	1.91	0.53
1:A:345:PHE:CD2	1:B:249:GLU:HG3	2.44	0.52
1:B:359:GLN:N	1:B:360:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:NE	1:A:125:ARG:HG3	2.24	0.52
1:A:224:GLN:HE22	1:A:462:ASN:HD22	1.56	0.52
1:B:69:TYR:CZ	1:B:89:LEU:HD22	2.44	0.52
1:A:509:TYR:CE2	1:A:511:ALA:HB3	2.44	0.52
1:A:392:SER:O	1:A:393:TYR:HB2	2.10	0.52
1:A:39:ALA:CA	1:A:42:ILE:HG22	2.39	0.52
1:B:11:VAL:N	1:B:27:ARG:HH22	2.08	0.52
1:B:286:GLU:HG2	1:B:302:ILE:HD13	1.91	0.52
1:B:528:ARG:NH2	3:B:1083:HOH:O	2.43	0.51
1:A:43:ALA:O	1:A:47:LYS:HG3	2.10	0.51
1:A:65:VAL:CG2	1:A:198:LYS:HB2	2.41	0.51
1:A:127:ILE:HD12	1:A:128:ILE:N	2.25	0.51
1:A:125:ARG:HD2	1:A:196:ARG:HD3	1.91	0.51
1:A:284:ARG:HG3	1:B:61:PRO:HG2	1.92	0.51
1:A:330:LYS:NZ	1:B:257:HIS:HD2	2.09	0.51
1:B:524:GLY:O	1:B:528:ARG:HG3	2.11	0.50
1:A:93:HIS:NE2	2:A:1001:296:C6	2.75	0.50
1:A:129:LEU:HD12	1:A:129:LEU:N	2.26	0.50
1:A:55:ILE:CG2	1:A:60:ILE:HD11	2.41	0.50
1:B:113:ARG:HD2	1:B:208:SER:OG	2.12	0.50
1:A:124:VAL:HB	1:A:128:ILE:HD12	1.94	0.50
1:B:280:HIS:CE1	1:B:304:LEU:HD11	2.46	0.50
1:A:239:VAL:HG21	1:A:393:TYR:HD2	1.76	0.49
1:A:499:ARG:HG3	1:A:499:ARG:HH11	1.78	0.49
1:A:69:TYR:CE1	1:A:89:LEU:HD22	2.47	0.49
1:A:202:ALA:HA	1:A:340:ASP:OD1	2.13	0.49
1:A:489:ALA:HB2	1:A:536:ILE:CD1	2.43	0.49
1:A:129:LEU:HD12	1:A:129:LEU:H	1.78	0.49
1:B:230:ILE:CD1	1:B:530:ILE:HD12	2.43	0.49
1:A:227:GLN:HE21	1:A:526:PHE:HB2	1.77	0.49
1:B:11:VAL:HB	3:B:1085:HOH:O	2.12	0.49
1:A:131:ARG:NH1	3:A:1122:HOH:O	2.46	0.49
1:A:174:ARG:NH2	3:A:1053:HOH:O	2.40	0.49
1:A:315:GLN:HG2	1:B:354:ALA:O	2.12	0.49
1:A:449:LEU:O	1:A:453:ARG:HG3	2.13	0.49
1:A:526:PHE:O	1:A:527:LEU:CB	2.52	0.49
1:B:307:ALA:HB2	1:B:385:ARG:CZ	2.43	0.49
1:A:32:ARG:HH22	1:A:103:GLU:CG	2.24	0.48
1:A:288:GLN:OE1	1:A:291:LYS:HE2	2.12	0.48
1:A:127:ILE:HD13	1:A:193:LEU:HD22	1.94	0.48
1:A:534:THR:O	1:A:535:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:HE2	2:B:1001:296:C3	2.25	0.48
1:A:300:SER:O	1:B:74:TYR:HB2	2.13	0.48
1:B:97:VAL:O	1:B:147:ILE:HB	2.13	0.48
1:A:503:THR:HG22	1:A:504:LEU:N	2.29	0.48
2:A:1001:296:F2	1:B:308:TYR:OH	2.19	0.48
1:A:71:GLU:H	1:A:438:ASN:ND2	1.94	0.48
1:A:297:VAL:O	1:A:297:VAL:HG13	2.14	0.48
1:A:475:GLN:HE21	1:A:479:ILE:CD1	2.21	0.48
1:B:230:ILE:HD13	1:B:530:ILE:HD12	1.95	0.48
1:B:486:LEU:HB3	1:B:490:ALA:HB3	1.95	0.48
1:A:61:PRO:HB3	1:B:287:LEU:HD23	1.96	0.47
1:A:127:ILE:CD1	1:A:193:LEU:HD13	2.44	0.47
1:A:338:ALA:HB3	1:B:254:ALA:HB1	1.96	0.47
1:B:251:HIS:HD2	1:B:260:GLN:HG2	1.79	0.47
1:B:313:ILE:HB	1:B:314:PRO:HD3	1.96	0.47
1:A:524:GLY:O	1:A:528:ARG:HB2	2.14	0.47
1:B:128:ILE:CD1	1:B:199:GLU:HB3	2.43	0.47
1:A:295:LYS:HD2	1:A:298:GLN:HG2	1.96	0.47
1:B:424:ASN:ND2	3:B:1210:HOH:O	2.23	0.47
1:B:475:GLN:HE21	1:B:479:ILE:HD11	1.79	0.47
1:A:308:TYR:OH	2:B:1001:296:F2	2.20	0.47
1:A:128:ILE:HD11	1:A:199:GLU:HB3	1.97	0.47
1:A:359:GLN:HE22	1:B:374:GLN:NE2	2.12	0.47
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.96	0.46
1:A:32:ARG:NH2	1:A:103:GLU:OE2	2.44	0.46
1:B:231:VAL:HB	1:B:470:TYR:CZ	2.51	0.46
1:B:288:GLN:HA	1:B:291:LYS:HD3	1.96	0.46
1:B:310:LEU:HA	1:B:313:ILE:HD11	1.97	0.46
1:B:251:HIS:HD2	1:B:260:GLN:NE2	2.09	0.46
1:A:93:HIS:HE2	2:A:1001:296:C6	2.28	0.46
1:A:255:ARG:NE	1:B:334:GLU:OE2	2.46	0.45
1:B:198:LYS:HG2	1:B:198:LYS:O	2.16	0.45
1:B:124:VAL:HG12	1:B:125:ARG:O	2.16	0.45
1:A:13:VAL:HG21	1:A:28:VAL:HG23	1.99	0.45
1:A:223:GLU:O	1:A:227:GLN:HG3	2.17	0.45
1:A:93:HIS:HE2	2:A:1001:296:C1	2.29	0.45
1:A:486:LEU:HD22	1:A:490:ALA:HB1	1.99	0.45
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.81	0.45
1:B:383:ILE:O	1:B:387:LEU:HG	2.17	0.45
1:A:308:TYR:CD2	1:B:442:GLN:HA	2.52	0.45
1:B:84:GLU:HB2	3:B:1158:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:H	1:A:191:GLU:CD	2.21	0.45
1:A:274:SER:HB2	1:A:487:SER:HB3	1.99	0.45
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.32	0.44
1:B:93:HIS:HE2	2:B:1001:296:C1	2.28	0.44
1:A:39:ALA:O	1:A:42:ILE:HG22	2.16	0.44
1:A:251:HIS:CD2	1:A:260:GLN:HE21	2.35	0.44
1:A:239:VAL:CG2	1:A:393:TYR:HD2	2.31	0.44
1:A:470:TYR:CE1	1:A:521:LEU:HD21	2.53	0.44
1:A:286:GLU:HG2	1:A:302:ILE:HD13	1.99	0.44
1:A:291:LYS:HD2	1:B:76:GLN:HB3	2.00	0.44
1:A:299:ARG:HG2	1:B:75:MET:SD	2.58	0.44
1:A:354:ALA:O	1:B:315:GLN:HG2	2.18	0.44
1:B:52:PHE:O	1:B:55:ILE:CG2	2.66	0.44
1:B:235:LEU:HD11	1:B:386:VAL:HG13	2.00	0.44
1:B:52:PHE:O	1:B:55:ILE:HG23	2.18	0.44
1:B:231:VAL:CG2	1:B:469:GLU:HG2	2.47	0.44
1:B:478:ASP:OD1	1:B:478:ASP:N	2.47	0.44
1:A:352:HIS:CE1	1:B:280:HIS:CE1	3.06	0.43
1:A:374:GLN:OE1	1:A:374:GLN:HA	2.18	0.43
1:B:342:PRO:HB2	1:B:350:ILE:HG22	2.00	0.43
1:B:407:HIS:CD2	1:B:507:ASP:H	2.35	0.43
1:A:534:THR:HG21	1:A:536:ILE:CD1	2.48	0.43
1:B:287:LEU:O	1:B:291:LYS:HG3	2.18	0.43
1:A:26:ARG:HD2	1:A:219:GLY:HA3	2.00	0.43
1:A:226:GLN:O	1:A:230:ILE:HG13	2.18	0.43
1:A:431:SER:HA	1:A:446:SER:O	2.19	0.43
1:A:363:PHE:CD2	1:B:319:ALA:HB1	2.52	0.43
3:A:1015:HOH:O	1:B:326:HIS:HE1	2.01	0.43
1:B:380:GLU:HG2	3:B:1076:HOH:O	2.18	0.43
1:A:237:GLU:OE2	1:A:490:ALA:HB2	2.18	0.43
1:B:38:PRO:HG2	1:B:41:SER:HB2	2.01	0.42
1:A:113:ARG:HD2	1:A:113:ARG:HA	1.70	0.42
1:A:334:GLU:OE1	1:B:257:HIS:HE1	2.02	0.42
1:A:370:ILE:HG23	1:B:432:THR:HG23	2.01	0.42
1:B:439:GLY:O	1:B:440:ASP:HB2	2.18	0.42
1:A:475:GLN:O	1:A:479:ILE:HB	2.20	0.42
1:B:101:PHE:CE2	1:B:146:GLU:HG2	2.54	0.42
1:B:165:THR:HA	1:B:181:THR:HG21	2.01	0.42
1:B:431:SER:HA	1:B:446:SER:O	2.19	0.42
1:A:313:ILE:HB	1:A:314:PRO:HD3	2.01	0.42
1:A:407:HIS:HD2	1:A:507:ASP:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:TYR:CD1	1:B:73:ILE:HD12	2.55	0.42
1:A:43:ALA:O	1:A:46:GLN:HG2	2.19	0.42
1:A:159:LEU:HB3	1:A:204:ILE:HA	2.01	0.42
1:A:227:GLN:NE2	1:A:526:PHE:HB2	2.33	0.42
1:B:93:HIS:NE2	2:B:1001:296:C6	2.81	0.42
1:B:494:TYR:CE2	1:B:498:ARG:HG3	2.55	0.42
1:A:297:VAL:HA	1:B:76:GLN:O	2.19	0.42
1:A:526:PHE:C	1:A:528:ARG:N	2.73	0.42
1:B:21:THR:O	1:B:25:VAL:HG23	2.20	0.42
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.34	0.42
1:B:509:TYR:CE2	1:B:511:ALA:HB3	2.55	0.42
1:A:255:ARG:HD3	1:A:260:GLN:OE1	2.19	0.42
1:B:167:ILE:HG21	1:B:195:LEU:HG	2.02	0.42
1:B:508:ARG:HD3	3:B:1021:HOH:O	2.20	0.41
1:A:371:ALA:HA	1:B:363:PHE:CZ	2.55	0.41
1:B:183:GLN:O	1:B:187:GLU:HG3	2.20	0.41
1:B:341:ASN:OD1	1:B:342:PRO:HA	2.21	0.41
1:B:519:ASP:O	1:B:523:ARG:HG2	2.21	0.41
1:A:534:THR:CG2	1:A:536:ILE:N	2.75	0.41
1:B:512:ASP:HB2	3:B:1218:HOH:O	2.21	0.41
1:A:251:HIS:CD2	1:A:260:GLN:HG2	2.50	0.41
1:A:527:LEU:O	1:A:527:LEU:HG	2.20	0.41
1:B:303:TYR:HB3	1:B:305:GLN:O	2.21	0.41
1:A:498:ARG:HA	1:A:501:VAL:O	2.20	0.41
1:A:395:LEU:HB3	1:A:396:PRO:HD2	2.03	0.41
1:A:59:ASN:ND2	1:A:79:LYS:HB3	2.36	0.41
1:A:313:ILE:HD12	1:A:313:ILE:H	1.86	0.41
1:A:534:THR:HG21	1:A:536:ILE:CG1	2.51	0.41
1:B:62:ILE:HB	1:B:65:VAL:HB	2.03	0.41
1:A:157:ALA:HB3	1:A:158:PRO:HD3	2.03	0.41
1:A:309:SER:O	1:A:313:ILE:HD11	2.19	0.41
1:A:310:LEU:HA	1:A:313:ILE:HD11	2.02	0.41
1:A:364:ALA:O	1:A:368:VAL:HG23	2.21	0.41
1:A:475:GLN:OE1	1:A:504:LEU:HB3	2.21	0.41
1:B:226:GLN:O	1:B:230:ILE:HG13	2.21	0.41
1:A:235:LEU:CD2	1:A:310:LEU:HD21	2.49	0.40
1:A:288:GLN:OE1	1:B:61:PRO:HD3	2.20	0.40
1:A:308:TYR:HH	1:B:152:MDO:HB21	1.86	0.40
1:A:155:ASP:O	1:A:158:PRO:HD2	2.21	0.40
1:A:385:ARG:NH1	1:A:391:LEU:HB3	2.36	0.40
1:B:15:VAL:O	1:B:15:VAL:CG2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:HG23	1:B:128:ILE:N	2.36	0.40
1:A:104:ASP:OD1	1:A:105:GLU:N	2.54	0.40
1:A:146:GLU:OE1	1:A:453:ARG:HD2	2.21	0.40
1:B:82:GLU:OE2	1:B:196:ARG:HB3	2.20	0.40
1:B:313:ILE:H	1:B:313:ILE:CD1	2.34	0.40
1:B:286:GLU:HG2	1:B:302:ILE:CD1	2.51	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	521/537 (97%)	492 (94%)	29 (6%)	0	100	100
1	B	522/537 (97%)	500 (96%)	21 (4%)	1 (0%)	47	62
All	All	1043/1074 (97%)	992 (95%)	50 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ALA

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	415/425 (98%)	410 (99%)	5 (1%)	71 85
1	B	416/425 (98%)	414 (100%)	2 (0%)	88 95
All	All	831/850 (98%)	824 (99%)	7 (1%)	81 91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	239	VAL
1	A	479	ILE
1	A	535	ASP
1	A	536	ILE
1	B	296	ASP
1	B	478	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	115	ASN
1	A	161	HIS
1	A	224	GLN
1	A	227	GLN
1	A	251	HIS
1	A	280	HIS
1	A	298	GLN
1	A	305	GLN
1	A	326	HIS
1	A	329	HIS
1	A	339	ASN
1	A	359	GLN
1	A	407	HIS
1	A	438	ASN
1	B	134	GLN
1	B	161	HIS
1	B	251	HIS
1	B	257	HIS
1	B	326	HIS
1	B	339	ASN
1	B	407	HIS
1	B	438	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)

2 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	B	152	2,1	12,13,14	2.44	4 (33%)	15,18,20	2.63	2 (13%)
1	MDO	A	152	2,1	12,13,14	2.43	4 (33%)	15,18,20	2.63	2 (13%)

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	B	152	2,1	-	2/4/23/24	0/1/1/1
1	MDO	A	152	2,1	-	2/4/23/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	MDO	O2-C2	6.34	1.36	1.23
1	A	152	MDO	O2-C2	6.31	1.36	1.23
1	B	152	MDO	CA2-N2	-3.04	1.33	1.39
1	A	152	MDO	CA2-N2	-2.97	1.33	1.39
1	B	152	MDO	C2-N3	-2.85	1.33	1.39
1	A	152	MDO	C2-N3	-2.84	1.33	1.39
1	A	152	MDO	C1-N3	-2.08	1.33	1.37
1	B	152	MDO	C1-N3	-2.01	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	152	MDO	O2-C2-CA2	-7.30	126.86	130.96
1	A	152	MDO	O2-C2-CA2	-6.95	127.06	130.96
1	A	152	MDO	CA2-C2-N3	6.86	106.61	103.37
1	B	152	MDO	CA2-C2-N3	6.45	106.42	103.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152	MDO	N2-C1-CA1-CB
1	B	152	MDO	N2-C1-CA1-CB
1	A	152	MDO	N3-C1-CA1-CB
1	B	152	MDO	N3-C1-CA1-CB

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	152	MDO	13	0
1	A	152	MDO	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	296	A	1001	1	14,16,16	0.67	0	20,23,23	1.14	1 (5%)
2	296	B	1001	1	14,16,16	0.67	0	20,23,23	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	296	A	1001	1	-	6/16/18/18	0/1/1/1
2	296	B	1001	1	-	6/16/18/18	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	296	C1-O2-C3	-3.67	109.54	117.51
2	A	1001	296	C1-O2-C3	-3.29	110.38	117.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	296	C5-C8-C9-C11
2	A	1001	296	C7-C8-C9-C11
2	A	1001	296	C9-C11-C12-O13
2	B	1001	296	C5-C8-C9-C11
2	B	1001	296	C7-C8-C9-C11
2	B	1001	296	C9-C11-C12-O13
2	A	1001	296	C4-C3-O2-C1
2	B	1001	296	C4-C3-O2-C1
2	B	1001	296	C6-C3-O2-C1
2	A	1001	296	C6-C3-O2-C1
2	A	1001	296	F1-C11-C12-O14
2	B	1001	296	F1-C11-C12-O14

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	296	8	0
2	B	1001	296	17	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	525/537 (97%)	-0.08	13 (2%)	57	55	22, 37, 58, 68	0
1	B	526/537 (97%)	-0.16	9 (1%)	70	68	19, 33, 53, 77	0
All	All	1051/1074 (97%)	-0.12	22 (2%)	63	61	19, 35, 56, 77	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	VAL	5.0
1	A	175	ASP	4.1
1	A	174	ARG	3.8
1	B	528	ARG	3.8
1	B	175	ASP	3.0
1	A	535	ASP	2.9
1	B	186	ALA	2.8
1	A	506	VAL	2.8
1	A	177	ARG	2.8
1	B	296	ASP	2.8
1	B	176	GLY	2.7
1	A	484	ASP	2.7
1	A	191	GLU	2.6
1	A	528	ARG	2.5
1	B	177	ARG	2.4
1	A	294	GLY	2.4
1	B	57	GLU	2.4
1	B	231	VAL	2.3
1	A	394	GLY	2.2
1	A	293	ALA	2.1
1	A	534	THR	2.1
1	A	393	TYR	2.1

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	152	13/14	0.86	0.18	29,35,38,40	0
1	MDO	A	152	13/14	0.90	0.14	36,38,40,43	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	296	A	1001	16/16	0.29	0.71	0,23,25,27	0
2	296	B	1001	16/16	0.45	0.61	0,23,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.