



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 AM GMT

PDB ID : 2OHY  
Title : X-ray Crystal Structure of Tyrosine Aminomutase from streptomyces globisporus  
Authors : Christianson, C.; Bruner, S.  
Deposited on : 2007-01-10  
Resolution : 2.50 Å(reported)

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

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

MolProbity : 4.02b-467  
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

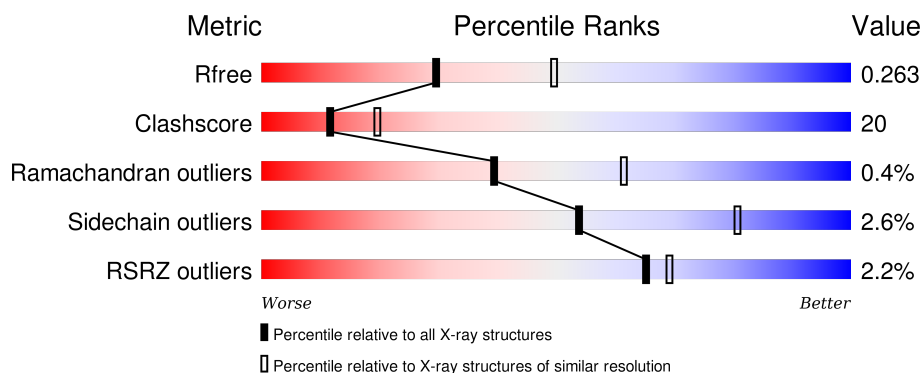
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	539	<div> <div>3%</div> <div>60%</div> <div>35%</div> <div>..</div> </div>
1	B	539	<div> <div>2%</div> <div>67%</div> <div>29%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8435 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
1	A	526	Total	C	N	O	S	0	0	0
			4007	2503	727	769	8			
1	B	527	Total	C	N	O	S	0	0	0
			4014	2508	728	770	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	MDO	ALA	MODIFIED RESIDUE	UNP Q8GMG0
A	152	MDO	SER	MODIFIED RESIDUE	UNP Q8GMG0
A	152	MDO	GLY	MODIFIED RESIDUE	UNP Q8GMG0
B	152	MDO	ALA	MODIFIED RESIDUE	UNP Q8GMG0
B	152	MDO	SER	MODIFIED RESIDUE	UNP Q8GMG0
B	152	MDO	GLY	MODIFIED RESIDUE	UNP Q8GMG0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	190	Total	O	0	0
			190	190		
2	B	224	Total	O	0	0
			224	224		

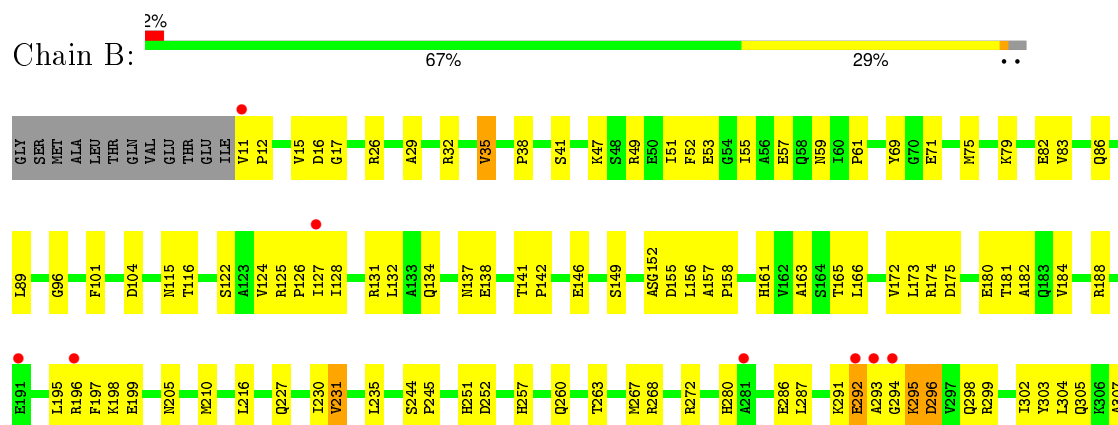
### 3 Residue-property plots [i](#)

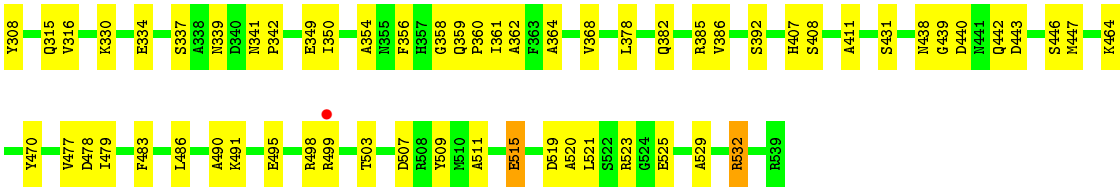
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Tyrosine aminomutase



#### • Molecule 1: Tyrosine aminomutase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.60 Å   146.18 Å   75.44 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.50 46.30 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.50) 96.3 (46.30-2.51)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.51 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.192   ,   0.263 0.192   ,   0.263	Depositor DCC
$R_{free}$ test set	3435 reflections (9.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 35743 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/4053	0.61	1/5490 (0.0%)
1	B	0.32	0/4060	0.59	0/5501
All	All	0.32	0/8113	0.60	1/10991 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	GLY	N-CA-C	-5.48	99.39	113.10

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4007	0	4035	195	0
1	B	4014	0	4043	158	0
2	A	190	0	0	9	0
2	B	224	0	0	6	0
All	All	8435	0	8078	327	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 20.

All (327) 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:124:VAL:HG13	1:B:128:ILE:HD12	1.45	0.98
1:A:35:VAL:H	1:A:137:ASN:HD21	1.17	0.92
1:B:35:VAL:H	1:B:137:ASN:HD21	0.99	0.92
1:A:207:THR:H	1:A:339:ASN:HD22	1.22	0.86
1:B:184:VAL:O	1:B:188:ARG:HG3	1.76	0.86
1:A:292:GLU:H	1:A:298:GLN:HE22	1.23	0.84
1:A:268:ARG:HH11	1:A:268:ARG:HB2	1.42	0.83
1:B:149:SER:HB2	1:B:155:ASP:HA	1.57	0.83
1:B:163:ALA:HA	1:B:166:LEU:HD12	1.61	0.81
1:B:294:GLY:O	1:B:295:LYS:HB2	1.80	0.80
1:A:71:GLU:H	1:A:438:ASN:HD21	1.30	0.80
1:A:140:ILE:HD11	1:A:172:VAL:HG11	1.64	0.79
1:A:243:THR:HG23	1:A:277:THR:HG21	1.63	0.79
1:A:172:VAL:HG21	1:A:184:VAL:HG21	1.65	0.78
1:A:265:ALA:HA	1:A:268:ARG:HH12	1.49	0.78
1:B:52:PHE:O	1:B:55:ILE:HG22	1.84	0.78
1:A:526:PHE:O	1:A:527:LEU:HB3	1.82	0.77
1:B:330:LYS:HE2	1:B:330:LYS:HA	1.64	0.77
1:A:32:ARG:NH2	1:A:103:GLU:HG2	2.01	0.76
1:B:35:VAL:H	1:B:137:ASN:ND2	1.82	0.76
1:A:207:THR:H	1:A:339:ASN:ND2	1.84	0.75
1:A:69:TYR:HE1	1:A:85:LEU:HD22	1.52	0.75
1:A:113:ARG:HH12	1:A:206:GLY:HA3	1.53	0.73
1:B:235:LEU:HD11	1:B:386:VAL:CG1	2.19	0.73
1:A:251:HIS:HD2	1:A:260:GLN:HG2	1.51	0.73
1:A:64:GLY:HA3	1:A:201:LEU:HD22	1.70	0.73
1:A:305:GLN:HE22	1:B:341:ASN:HD21	1.34	0.72
1:A:152:MDO:HB21	1:B:308:TYR:OH	1.89	0.72
1:A:107:ARG:NH2	1:A:136:LEU:O	2.24	0.71
1:A:292:GLU:H	1:A:298:GLN:NE2	1.88	0.70
1:A:265:ALA:HA	1:A:268:ARG:NH1	2.07	0.69
1:B:35:VAL:N	1:B:137:ASN:HD21	1.82	0.69
1:A:243:THR:HG23	1:A:277:THR:CG2	2.23	0.69
1:A:268:ARG:HH11	1:A:268:ARG:CB	2.06	0.68
1:A:486:LEU:HD22	1:A:490:ALA:HB1	1.76	0.67
1:B:235:LEU:HD11	1:B:386:VAL:HG11	1.77	0.67
1:A:308:TYR:CZ	1:B:442:GLN:HG2	2.30	0.67
1:A:507:ASP:HB2	2:A:662:HOH:O	1.94	0.66
1:B:286:GLU:HG2	1:B:302:ILE:HD13	1.77	0.66
1:A:135:TYR:HA	1:A:140:ILE:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.78	0.66
1:A:268:ARG:HB2	1:A:268:ARG:NH1	2.10	0.66
1:A:198:LYS:HG2	1:A:198:LYS:O	1.96	0.66
1:A:135:TYR:HA	1:A:140:ILE:HG23	1.78	0.65
1:A:124:VAL:HG12	1:A:128:ILE:HG13	1.78	0.65
1:A:509:TYR:CE2	1:A:511:ALA:HB3	2.31	0.64
1:B:124:VAL:CG1	1:B:128:ILE:HB	2.26	0.64
1:A:480:SER:OG	1:A:482:ARG:HD2	1.97	0.64
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.79	0.64
1:B:286:GLU:HG2	1:B:302:ILE:CD1	2.28	0.64
1:A:113:ARG:NH1	1:A:206:GLY:HA3	2.13	0.64
1:B:71:GLU:H	1:B:438:ASN:HD21	1.43	0.64
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.63	0.63
1:A:355:ASN:ND2	1:B:315:GLN:HE21	1.97	0.63
1:A:534:THR:HG22	1:A:536:ILE:HG13	1.81	0.63
1:B:69:TYR:CZ	1:B:89:LEU:HD22	2.34	0.62
1:A:508:ARG:NH1	1:A:513:ASP:OD2	2.33	0.62
1:B:96:GLY:H	1:B:161:HIS:CE1	2.17	0.62
1:B:82:GLU:HG3	1:B:197:PHE:CD1	2.34	0.62
1:B:128:ILE:HD11	1:B:199:GLU:HB3	1.81	0.62
1:A:59:ASN:ND2	1:A:79:LYS:HG2	2.15	0.61
1:B:86:GLN:HG3	1:B:196:ARG:O	2.00	0.61
1:A:276:LEU:HD11	1:A:482:ARG:HB3	1.81	0.61
1:B:503:THR:HG22	2:B:691:HOH:O	2.01	0.61
1:A:257:HIS:HD2	1:B:330:LYS:NZ	1.99	0.61
1:A:330:LYS:NZ	1:B:257:HIS:HD2	1.99	0.60
1:A:71:GLU:N	1:A:438:ASN:HD21	1.98	0.60
1:A:287:LEU:HD13	1:A:302:ILE:HB	1.83	0.60
1:A:140:ILE:HD11	1:A:172:VAL:CG1	2.31	0.60
1:B:11:VAL:N	1:B:12:PRO:HA	2.17	0.60
1:A:172:VAL:CG2	1:A:184:VAL:HG21	2.32	0.60
1:A:59:ASN:HD21	1:A:79:LYS:HG2	1.66	0.60
1:B:11:VAL:O	1:B:11:VAL:HG12	2.02	0.60
1:A:16:ASP:HB3	1:A:38:PRO:HG3	1.82	0.60
1:A:284:ARG:HG3	1:B:61:PRO:HG2	1.84	0.59
1:B:172:VAL:HG21	1:B:184:VAL:HG21	1.84	0.59
1:B:364:ALA:O	1:B:368:VAL:HG23	2.03	0.59
1:A:63:TYR:HA	1:A:67:THR:OG1	2.02	0.59
1:A:244:SER:HB3	1:A:245:PRO:HD3	1.85	0.58
1:A:124:VAL:CG1	1:A:128:ILE:HG13	2.33	0.58
1:B:235:LEU:HD11	1:B:386:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:GLN:N	1:B:360:PRO:HD2	2.18	0.58
1:B:287:LEU:HD21	1:B:302:ILE:HB	1.84	0.58
1:B:96:GLY:H	1:B:161:HIS:HE1	1.49	0.58
1:A:71:GLU:H	1:A:438:ASN:ND2	2.01	0.58
1:A:438:ASN:HD22	1:A:441:ASN:HB3	1.68	0.58
1:B:334:GLU:HG3	1:B:361:ILE:CG1	2.34	0.58
1:A:503:THR:HG22	1:A:504:LEU:N	2.19	0.58
1:A:251:HIS:CD2	1:A:260:GLN:HG2	2.37	0.58
1:A:534:THR:O	1:A:535:ASP:HB3	2.02	0.57
1:B:251:HIS:HD2	1:B:260:GLN:HE21	1.51	0.57
1:A:359:GLN:N	1:A:360:PRO:HD2	2.20	0.57
1:A:360:PRO:HB3	2:B:722:HOH:O	2.03	0.57
1:A:65:VAL:HG22	1:A:198:LYS:HB2	1.85	0.57
1:B:251:HIS:CD2	1:B:260:GLN:HE21	2.21	0.57
1:A:101:PHE:CE1	1:A:146:GLU:HA	2.40	0.57
1:A:243:THR:CG2	1:A:277:THR:HG21	2.31	0.57
1:A:82:GLU:HG3	1:A:197:PHE:CD1	2.40	0.57
1:A:101:PHE:CE2	1:A:146:GLU:HG2	2.39	0.57
1:B:532:ARG:HG3	1:B:532:ARG:HH11	1.70	0.57
1:A:69:TYR:CE1	1:A:85:LEU:HD22	2.36	0.57
1:A:380:GLU:HG2	2:A:579:HOH:O	2.05	0.56
1:B:408:SER:HB3	1:B:411:ALA:HB3	1.87	0.56
1:B:529:ALA:HA	1:B:532:ARG:HD2	1.87	0.56
1:A:520:ALA:HB1	1:A:525:GLU:HG3	1.88	0.55
1:A:305:GLN:NE2	1:B:341:ASN:HD21	2.05	0.55
1:A:101:PHE:CZ	1:A:146:GLU:HG2	2.42	0.55
1:B:447:MET:HA	2:B:555:HOH:O	2.07	0.55
1:B:83:VAL:HG13	1:B:195:LEU:O	2.07	0.55
1:B:15:VAL:O	1:B:15:VAL:HG23	2.06	0.55
1:A:382:GLN:O	1:A:385:ARG:HB3	2.07	0.54
1:A:127:ILE:HA	1:A:130:GLU:HB2	1.89	0.54
1:A:232:THR:HG21	1:A:313:ILE:HG12	1.88	0.54
1:A:267:MET:O	1:A:271:MET:HE2	2.07	0.54
1:A:49:ARG:NE	1:A:125:ARG:HG3	2.22	0.54
1:B:491:LYS:O	1:B:495:GLU:HG3	2.07	0.54
1:B:152:MDO:O	1:B:156:LEU:N	2.40	0.54
1:A:255:ARG:NE	1:B:334:GLU:OE2	2.41	0.54
1:B:26:ARG:HG2	1:B:216:LEU:HD23	1.90	0.54
1:A:287:LEU:HA	1:A:302:ILE:HD12	1.90	0.53
1:A:475:GLN:HE21	1:A:479:ILE:HD12	1.74	0.53
1:A:125:ARG:HD3	1:A:199:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ALA:HA	1:A:340:ASP:OD1	2.09	0.53
1:A:308:TYR:OH	1:B:152:MDO:HB21	2.08	0.53
1:B:32:ARG:HH11	1:B:32:ARG:HG3	1.73	0.53
1:A:491:LYS:O	1:A:495:GLU:HG2	2.09	0.52
1:B:407:HIS:CD2	1:B:507:ASP:H	2.27	0.52
1:A:240:ARG:HD2	1:A:276:LEU:O	2.09	0.52
1:A:135:TYR:CA	1:A:140:ILE:HG23	2.40	0.52
1:A:294:GLY:O	1:A:295:LYS:HD2	2.09	0.52
1:B:86:GLN:NE2	1:B:198:LYS:H	2.07	0.52
1:B:158:PRO:HG3	2:B:716:HOH:O	2.09	0.52
1:B:251:HIS:HD2	1:B:260:GLN:HG2	1.75	0.52
1:A:46:GLN:HB3	1:A:126:PRO:HG2	1.92	0.52
1:A:534:THR:CG2	1:A:536:ILE:HG13	2.40	0.51
1:A:277:THR:HG22	1:A:278:VAL:N	2.25	0.51
1:B:149:SER:CB	1:B:155:ASP:HA	2.35	0.51
1:B:294:GLY:O	1:B:295:LYS:CB	2.55	0.51
1:A:82:GLU:OE2	1:A:196:ARG:HB3	2.10	0.51
1:B:231:VAL:HG13	1:B:470:TYR:CD2	2.45	0.51
1:A:308:TYR:CE2	1:B:442:GLN:HG2	2.46	0.51
1:A:125:ARG:HD2	1:A:196:ARG:HD3	1.91	0.51
1:A:205:ASN:O	1:A:340:ASP:HA	2.11	0.51
1:A:392:SER:O	1:A:393:TYR:HB2	2.11	0.51
1:A:39:ALA:HA	1:A:42:ILE:HG22	1.93	0.51
1:B:470:TYR:CE1	1:B:521:LEU:HD21	2.46	0.51
1:A:96:GLY:H	1:A:161:HIS:HE1	1.57	0.51
1:B:244:SER:HB3	1:B:245:PRO:HD3	1.92	0.51
1:B:128:ILE:CD1	1:B:199:GLU:HB3	2.40	0.50
1:B:478:ASP:OD2	1:B:498:ARG:NH1	2.44	0.50
1:A:149:SER:OG	1:A:155:ASP:HA	2.11	0.50
1:A:239:VAL:HG21	1:A:393:TYR:HD2	1.75	0.50
1:B:509:TYR:CE2	1:B:511:ALA:HB3	2.46	0.50
1:A:53:GLU:O	1:A:57:GLU:HG2	2.11	0.50
1:B:334:GLU:HG3	1:B:361:ILE:HG12	1.92	0.50
1:B:124:VAL:HG13	1:B:128:ILE:CD1	2.30	0.50
1:B:17:GLY:H	1:B:115:ASN:ND2	2.11	0.49
1:A:69:TYR:HE1	1:A:85:LEU:CD2	2.23	0.49
1:A:316:VAL:O	1:A:320:VAL:HG23	2.13	0.49
1:A:431:SER:HA	1:A:446:SER:O	2.13	0.49
1:B:180:GLU:CD	1:B:180:GLU:H	2.14	0.49
1:A:91:ARG:HD3	1:A:169:GLU:OE1	2.11	0.49
1:A:39:ALA:O	1:A:42:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:VAL:CG2	1:B:184:VAL:HG21	2.43	0.49
1:B:52:PHE:O	1:B:55:ILE:CG2	2.59	0.49
1:A:483:PHE:O	1:A:491:LYS:NZ	2.46	0.49
1:B:53:GLU:O	1:B:57:GLU:HB2	2.13	0.49
1:A:315:GLN:HG2	1:B:354:ALA:O	2.12	0.49
1:B:132:LEU:HD23	1:B:166:LEU:HD21	1.95	0.48
1:A:257:HIS:HE1	1:B:334:GLU:HG2	1.78	0.48
1:A:158:PRO:HG3	2:A:557:HOH:O	2.12	0.48
1:B:198:LYS:HG2	1:B:198:LYS:O	2.13	0.48
1:B:330:LYS:CE	1:B:330:LYS:HA	2.39	0.48
1:A:69:TYR:CE2	1:A:89:LEU:HD22	2.48	0.48
1:B:231:VAL:HG22	1:B:470:TYR:CZ	2.48	0.48
1:A:475:GLN:O	1:A:479:ILE:HB	2.14	0.48
1:A:306:LYS:O	1:A:311:ARG:NH1	2.46	0.48
1:A:131:ARG:NH1	1:A:193:LEU:HG	2.27	0.48
1:A:257:HIS:HD2	1:B:330:LYS:HZ1	1.61	0.48
1:A:520:ALA:O	1:A:525:GLU:HG2	2.14	0.48
1:B:231:VAL:HG13	1:B:470:TYR:CE2	2.48	0.48
1:B:71:GLU:H	1:B:438:ASN:ND2	2.12	0.48
1:A:526:PHE:C	1:A:528:ARG:H	2.17	0.47
1:A:15:VAL:HG23	1:A:35:VAL:HG23	1.94	0.47
1:A:276:LEU:CD1	1:A:482:ARG:HB3	2.44	0.47
1:A:355:ASN:HD22	1:B:315:GLN:HE21	1.61	0.47
1:B:477:VAL:HG11	1:B:486:LEU:HD11	1.96	0.47
1:A:224:GLN:NE2	1:A:459:LEU:HD12	2.29	0.47
1:A:305:GLN:HE22	1:B:341:ASN:ND2	2.08	0.47
1:B:287:LEU:CD2	1:B:302:ILE:HB	2.44	0.47
1:A:438:ASN:HA	2:A:652:HOH:O	2.14	0.47
1:A:113:ARG:HD2	1:A:113:ARG:HA	1.68	0.47
1:A:284:ARG:NH1	1:B:349:GLU:OE2	2.47	0.47
1:B:499:ARG:HH11	1:B:499:ARG:HG2	1.80	0.47
1:A:73:ILE:HD11	1:B:304:LEU:HB3	1.96	0.47
1:A:198:LYS:CG	1:A:198:LYS:O	2.63	0.47
1:A:498:ARG:HE	1:A:498:ARG:HA	1.78	0.47
1:B:197:PHE:O	1:B:198:LYS:HB3	2.15	0.47
1:B:235:LEU:CD1	1:B:386:VAL:HG11	2.43	0.46
1:A:223:GLU:O	1:A:227:GLN:HG3	2.15	0.46
1:A:15:VAL:CG2	1:A:35:VAL:HG23	2.45	0.46
1:B:362:ALA:CB	1:B:446:SER:HB2	2.45	0.46
1:A:420:LEU:HA	1:A:420:LEU:HD23	1.78	0.46
1:B:263:THR:O	1:B:267:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:C	1:A:45:ALA:H	2.18	0.46
1:B:227:GLN:O	1:B:231:VAL:HG22	2.15	0.46
1:B:125:ARG:CZ	1:B:196:ARG:HD3	2.46	0.46
1:A:299:ARG:HG2	1:B:75:MET:SD	2.56	0.46
1:A:313:ILE:HB	1:A:314:PRO:HD3	1.98	0.46
1:A:71:GLU:HB2	1:A:441:ASN:HB2	1.97	0.46
1:A:32:ARG:HD3	1:A:32:ARG:HA	1.74	0.46
1:A:114:LEU:HD13	1:A:132:LEU:HB2	1.96	0.46
1:A:124:VAL:HG11	1:A:128:ILE:HG21	1.97	0.45
1:A:183:GLN:O	1:A:187:GLU:HB2	2.16	0.45
1:A:13:VAL:HG21	1:A:28:VAL:HG23	1.97	0.45
1:A:475:GLN:OE1	1:A:504:LEU:HB3	2.16	0.45
1:B:116:THR:HG23	1:B:339:ASN:H	1.81	0.45
1:A:359:GLN:HG2	1:B:316:VAL:HA	1.99	0.45
1:B:464:LYS:HE3	1:B:515:GLU:OE1	2.16	0.45
1:A:51:ILE:HD12	1:A:51:ILE:N	2.32	0.45
1:B:125:ARG:HB2	1:B:127:ILE:HG22	1.99	0.45
1:B:498:ARG:CZ	1:B:503:THR:HA	2.46	0.45
1:A:174:ARG:HG3	2:A:631:HOH:O	2.16	0.45
1:A:96:GLY:H	1:A:161:HIS:CE1	2.34	0.45
1:A:334:GLU:OE1	1:B:257:HIS:HE1	1.99	0.44
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.30	0.44
1:A:503:THR:CG2	1:A:504:LEU:N	2.80	0.44
1:A:525:GLU:OE2	1:A:525:GLU:HA	2.16	0.44
1:B:165:THR:HA	1:B:181:THR:HG21	1.99	0.44
1:B:16:ASP:HB3	1:B:38:PRO:HG3	1.99	0.44
1:A:386:VAL:HG23	1:A:395:LEU:HD12	1.99	0.44
1:B:431:SER:HA	1:B:446:SER:O	2.17	0.44
1:B:392:SER:HA	2:B:588:HOH:O	2.17	0.44
1:B:439:GLY:O	1:B:440:ASP:HB2	2.17	0.44
1:A:524:GLY:O	1:A:526:PHE:O	2.35	0.44
1:A:257:HIS:CE1	1:B:334:GLU:HG2	2.52	0.44
1:A:43:ALA:O	1:A:46:GLN:HG2	2.17	0.44
1:A:14:SER:HB3	2:A:617:HOH:O	2.18	0.44
1:A:47:LYS:O	1:A:50:GLU:HB2	2.18	0.44
1:A:374:GLN:OE1	1:A:374:GLN:HA	2.18	0.43
1:A:526:PHE:O	1:A:528:ARG:N	2.47	0.43
1:A:255:ARG:HG3	1:B:337:SER:HB2	2.00	0.43
1:B:378:LEU:O	1:B:382:GLN:HG3	2.17	0.43
1:B:303:TYR:HB3	1:B:305:GLN:O	2.18	0.43
1:A:279:GLU:HB3	2:A:642:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:N	1:A:314:PRO:CD	2.81	0.43
1:B:291:LYS:HB3	1:B:298:GLN:HE22	1.83	0.43
1:B:292:GLU:HG3	1:B:292:GLU:H	1.61	0.43
1:B:342:PRO:HB2	1:B:350:ILE:HG22	1.99	0.43
1:B:174:ARG:O	1:B:175:ASP:HB2	2.19	0.43
1:B:124:VAL:HG11	1:B:128:ILE:HB	1.99	0.43
1:A:75:MET:SD	1:B:299:ARG:HB3	2.59	0.43
1:A:493:THR:O	1:A:496:ALA:HB3	2.19	0.43
1:A:384:ASN:HA	1:A:414:GLN:NE2	2.34	0.43
1:A:292:GLU:HB2	1:A:298:GLN:NE2	2.33	0.42
1:A:70:GLY:HA3	1:A:438:ASN:HD21	1.84	0.42
1:B:125:ARG:CB	1:B:127:ILE:HG22	2.49	0.42
1:A:309:SER:O	1:A:313:ILE:HD11	2.19	0.42
1:A:131:ARG:HD3	1:A:134:GLN:NE2	2.34	0.42
1:A:494:TYR:CE2	1:A:498:ARG:HG3	2.55	0.42
1:B:268:ARG:HH11	1:B:268:ARG:HB2	1.84	0.42
1:B:15:VAL:HB	1:B:115:ASN:HD22	1.85	0.42
1:B:227:GLN:O	1:B:231:VAL:CG2	2.67	0.42
1:A:297:VAL:HG23	1:A:297:VAL:O	2.18	0.42
1:A:68:GLY:HA3	1:A:72:MET:O	2.20	0.42
1:B:520:ALA:O	1:B:525:GLU:HG2	2.20	0.42
1:A:110:VAL:HG13	1:A:132:LEU:HD22	2.01	0.42
1:B:38:PRO:HG2	1:B:41:SER:OG	2.20	0.42
1:A:106:ALA:HA	1:A:144:ILE:HD12	2.02	0.42
1:A:352:HIS:CE1	1:B:280:HIS:NE2	2.87	0.42
1:B:251:HIS:CD2	1:B:260:GLN:HG2	2.53	0.42
1:B:47:LYS:O	1:B:51:ILE:HG13	2.20	0.42
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.84	0.42
1:B:272:ARG:C	1:B:272:ARG:HD2	2.40	0.42
1:B:134:GLN:O	1:B:138:GLU:HB2	2.20	0.42
1:A:470:TYR:CE1	1:A:521:LEU:HD21	2.54	0.42
1:B:11:VAL:N	1:B:12:PRO:CA	2.82	0.42
1:B:17:GLY:H	1:B:115:ASN:HD21	1.68	0.42
1:B:210:MET:CE	1:B:358:GLY:HA3	2.50	0.42
1:B:128:ILE:HD11	1:B:199:GLU:CD	2.41	0.41
1:B:519:ASP:O	1:B:523:ARG:HG2	2.20	0.41
1:A:235:LEU:HD22	1:A:310:LEU:HD21	2.00	0.41
1:B:29:ALA:HB1	1:B:104:ASP:O	2.20	0.41
1:B:49:ARG:HG2	1:B:125:ARG:HG2	2.02	0.41
1:A:207:THR:N	1:A:339:ASN:HD22	2.03	0.41
1:B:227:GLN:HA	1:B:230:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ALA:HB2	1:B:446:SER:HB2	2.03	0.41
1:B:101:PHE:CE2	1:B:146:GLU:HG2	2.55	0.41
1:A:526:PHE:C	1:A:528:ARG:N	2.73	0.41
1:A:40:GLU:O	1:A:43:ALA:HB3	2.20	0.41
1:B:59:ASN:OD1	1:B:79:LYS:HB3	2.20	0.41
1:A:284:ARG:CG	1:B:61:PRO:HG2	2.49	0.41
1:B:101:PHE:CE1	1:B:146:GLU:HA	2.54	0.41
1:B:268:ARG:HH11	1:B:268:ARG:CB	2.33	0.41
1:A:498:ARG:HA	1:A:501:VAL:O	2.21	0.41
1:B:515:GLU:OE1	1:B:515:GLU:HA	2.20	0.41
1:B:122:SER:HB2	2:B:648:HOH:O	2.20	0.41
1:B:295:LYS:HB3	1:B:296:ASP:H	1.42	0.41
1:B:268:ARG:HB2	1:B:268:ARG:NH1	2.35	0.41
1:B:205:ASN:HD21	1:B:356:PHE:HD2	1.68	0.41
1:B:69:TYR:CE2	1:B:89:LEU:HD22	2.56	0.41
1:A:109:ILE:HG12	1:A:209:GLY:HA2	2.03	0.41
1:B:124:VAL:HG12	1:B:125:ARG:O	2.21	0.41
1:A:524:GLY:O	1:A:528:ARG:HB2	2.21	0.41
1:A:127:ILE:HD12	1:A:128:ILE:N	2.35	0.41
1:A:380:GLU:CG	2:A:579:HOH:O	2.67	0.41
1:B:116:THR:OG1	1:B:339:ASN:ND2	2.54	0.41
1:B:181:THR:O	1:B:182:ALA:C	2.59	0.41
1:B:291:LYS:HB3	1:B:298:GLN:NE2	2.36	0.41
1:A:249:GLU:O	1:A:253:ILE:HB	2.21	0.41
1:A:251:HIS:CD2	1:A:260:GLN:HE21	2.39	0.41
1:A:407:HIS:HD2	1:A:507:ASP:H	1.69	0.41
1:B:523:ARG:HG3	1:B:525:GLU:HG2	2.03	0.41
1:B:141:THR:HA	1:B:142:PRO:HD3	1.89	0.41
1:A:243:THR:HG22	2:A:646:HOH:O	2.21	0.40
1:B:307:ALA:HB2	1:B:385:ARG:CZ	2.51	0.40
1:A:51:ILE:CG2	1:A:344:PHE:HZ	2.35	0.40
1:A:191:GLU:O	1:A:191:GLU:HG2	2.21	0.40
1:A:448:GLY:O	1:A:451:SER:HB2	2.22	0.40
1:B:483:PHE:CD2	1:B:483:PHE:C	2.95	0.40
1:A:141:THR:HA	1:A:142:PRO:HD3	1.94	0.40
1:A:341:ASN:OD1	1:A:342:PRO:HA	2.21	0.40
1:A:49:ARG:O	1:A:53:GLU:HB2	2.21	0.40
1:A:385:ARG:CZ	1:A:391:LEU:HB3	2.51	0.40
1:B:486:LEU:HB3	1:B:490:ALA:HB3	2.03	0.40
1:A:86:GLN:HG3	1:A:196:ARG:O	2.21	0.40
1:A:380:GLU:HG3	1:A:381:ARG:N	2.37	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	523/539 (97%)	478 (91%)	43 (8%)	2 (0%)	39	61
1	B	524/539 (97%)	489 (93%)	33 (6%)	2 (0%)	39	61
All	All	1047/1078 (97%)	967 (92%)	76 (7%)	4 (0%)	39	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	LYS
1	B	293	ALA
1	B	295	LYS
1	A	256	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	415/426 (97%)	405 (98%)	10 (2%)	57	82
1	B	416/426 (98%)	404 (97%)	12 (3%)	50	77
All	All	831/852 (98%)	809 (97%)	22 (3%)	54	81

All (22) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	35	VAL
1	A	85	LEU
1	A	140	ILE
1	A	252	ASP
1	A	268	ARG
1	A	295	LYS
1	A	311	ARG
1	A	380	GLU
1	A	498	ARG
1	A	508	ARG
1	B	35	VAL
1	B	126	PRO
1	B	131	ARG
1	B	173	LEU
1	B	231	VAL
1	B	252	ASP
1	B	292	GLU
1	B	296	ASP
1	B	443	ASP
1	B	479	ILE
1	B	515	GLU
1	B	532	ARG

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	86	GLN
1	A	134	GLN
1	A	137	ASN
1	A	161	HIS
1	A	227	GLN
1	A	251	HIS
1	A	257	HIS
1	A	298	GLN
1	A	305	GLN
1	A	326	HIS
1	A	339	ASN
1	A	355	ASN
1	A	414	GLN
1	A	438	ASN
1	A	442	GLN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	115	ASN
1	B	134	GLN
1	B	137	ASN
1	B	161	HIS
1	B	183	GLN
1	B	205	ASN
1	B	251	HIS
1	B	257	HIS
1	B	326	HIS
1	B	384	ASN
1	B	407	HIS
1	B	414	GLN
1	B	438	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	152	1	11,13,14	2.44	4 (36%)	13,18,20	2.94	2 (15%)
1	MDO	B	152	1	11,13,14	2.44	4 (36%)	13,18,20	2.87	2 (15%)

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	152	1	-	0/4/23/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MDO	B	152	1	-	0/4/23/24	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	C2-N3	-3.04	1.33	1.39
1	A	152	MDO	C2-N3	-3.03	1.33	1.39
1	B	152	MDO	CA2-N2	-2.48	1.33	1.39
1	A	152	MDO	CA2-N2	-2.42	1.33	1.39
1	A	152	MDO	C1-N3	-2.15	1.33	1.37
1	B	152	MDO	C1-N3	-2.11	1.33	1.37
1	B	152	MDO	O2-C2	6.30	1.36	1.23
1	A	152	MDO	O2-C2	6.33	1.36	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	MDO	O2-C2-CA2	-8.08	126.58	130.95
1	B	152	MDO	O2-C2-CA2	-7.71	126.78	130.95
1	B	152	MDO	CA2-C2-N3	6.06	106.55	103.39
1	A	152	MDO	CA2-C2-N3	6.23	106.64	103.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	152	MDO	1	0
1	B	152	MDO	2	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	525/539 (97%)	0.08	14 (2%) 58 62	12, 28, 46, 56	0
1	B	526/539 (97%)	-0.07	9 (1%) 73 76	10, 24, 41, 61	0
All	All	1051/1078 (97%)	0.00	23 (2%) 65 69	10, 25, 44, 61	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	ASP	5.3
1	B	293	ALA	4.1
1	A	295	LYS	3.6
1	A	294	GLY	3.2
1	B	294	GLY	3.1
1	A	46	GLN	2.7
1	B	196	ARG	2.7
1	A	344	PHE	2.7
1	B	127	ILE	2.6
1	A	182	ALA	2.6
1	A	47	LYS	2.4
1	B	281	ALA	2.4
1	B	292	GLU	2.4
1	B	11	VAL	2.4
1	A	127	ILE	2.3
1	A	345	PHE	2.2
1	A	195	LEU	2.1
1	B	499	ARG	2.1
1	A	54	GLY	2.1
1	A	57	GLU	2.1
1	A	52	PHE	2.0
1	A	400	VAL	2.0
1	B	191	GLU	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MDO	A	152	13/14	0.89	0.16	-	21,25,28,28	0
1	MDO	B	152	13/14	0.91	0.18	-	18,21,22,25	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.