



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:08 PM UTC

PDB ID : 2OHY / pdb_00002ohy
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

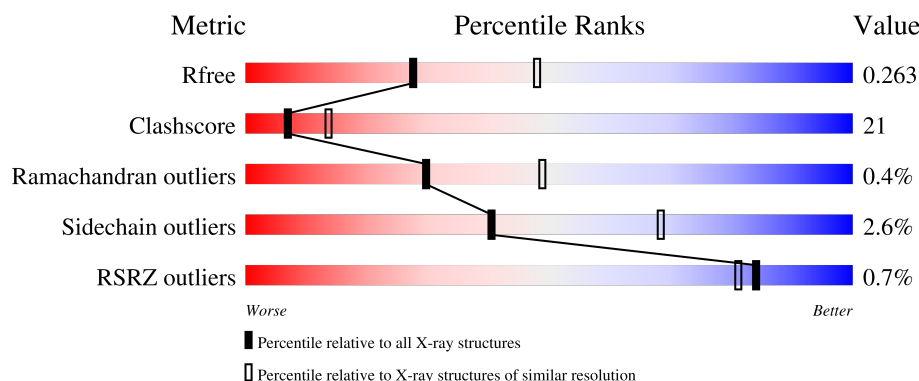
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. 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	58%36% . .
1	B	539	66%30% . .

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

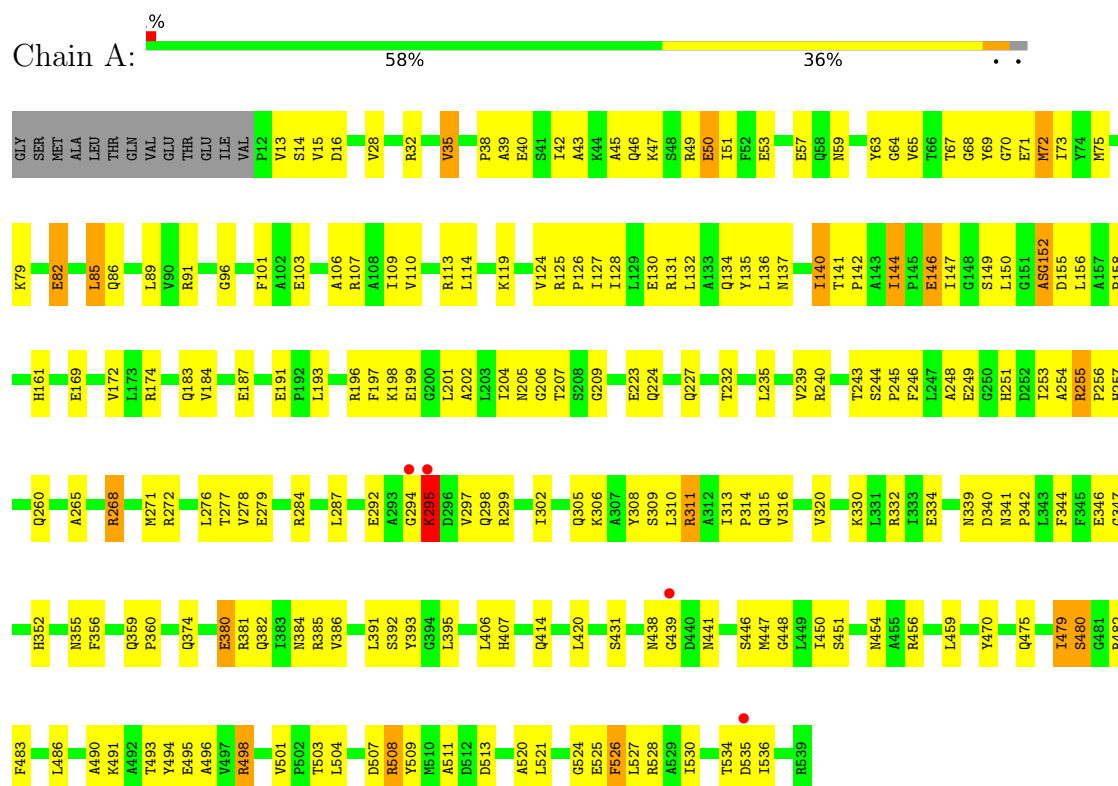
- Molecule 2 is water.

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

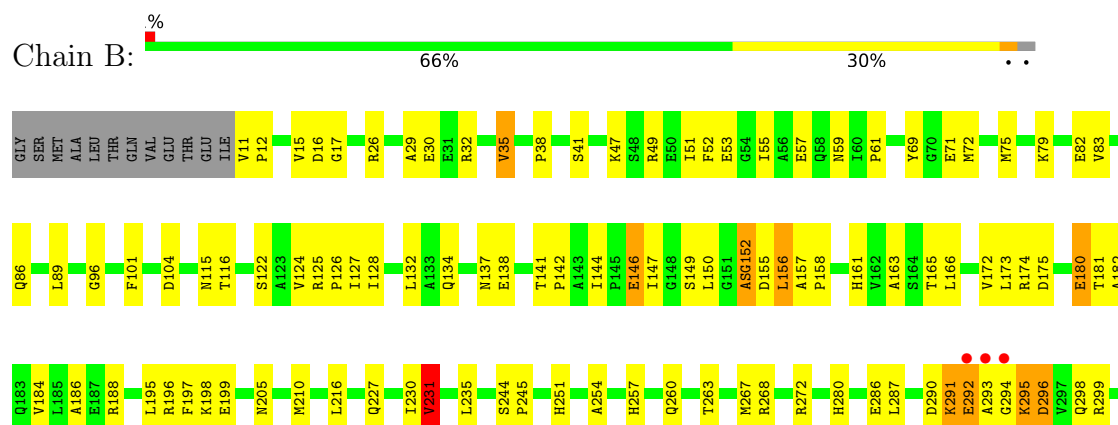
3 Residue-property plots

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



• Molecule 1: Tyrosine aminomutase



I302	Y303	L304	Q305	K306	A307	Y308		Q315	V316		K330		E334		S337	A338	N339	T340	N341	P342		E349	I350		A354	R355	F356	H357	G358	Q359	P360	I361	A362	F363	A364		V368		L378		Q382		R385	V386		S392		H407	S408		A411		S431		M438	G439	D440	N441	Q442
D443		S446	M447		L450		K464		Y470		V477	D478	I479		F483		L486		A490	K491		E495		R498	R499		T503		D507	R508	Y509	M510	A511	E515		D519	A520	L521	R522	R523	G524	E525		A529		R532		D535	I536		R539								

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.60Å 146.18Å 75.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.50) 96.3 (50.00-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.263 0.192 , 0.263	Depositor DCC
R_{free} test set	3565 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8435	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/4053	0.98	18/5490 (0.3%)
1	B	0.41	0/4060	0.95	13/5501 (0.2%)
All	All	0.41	0/8113	0.96	31/10991 (0.3%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ILE	N-CA-C	9.16	115.89	107.56
1	A	479	ILE	N-CA-C	-8.35	105.35	113.53
1	A	526	PHE	N-CA-C	-8.18	98.73	110.59
1	A	255	ARG	CA-C-N	8.04	129.90	119.84
1	A	255	ARG	C-N-CA	8.04	129.90	119.84
1	A	144	ILE	N-CA-C	7.69	115.16	107.55
1	B	291	LYS	N-CA-C	-6.83	105.73	112.97
1	A	146	GLU	N-CA-C	6.55	119.42	111.82
1	A	406	LEU	N-CA-C	-6.38	104.32	111.28
1	B	150	LEU	N-CA-C	-6.34	105.17	113.17
1	A	119	LYS	N-CA-C	-6.29	104.52	111.82
1	B	450	ILE	N-CA-C	-6.25	104.19	111.00
1	A	450	ILE	N-CA-C	-6.25	104.19	111.00
1	A	156	LEU	N-CA-C	6.20	118.58	111.02
1	B	254	ALA	N-CA-C	6.15	117.78	111.14
1	A	82	GLU	N-CA-C	6.05	118.38	111.11
1	B	146	GLU	N-CA-C	5.85	118.61	111.82
1	A	439	GLY	N-CA-C	-5.82	99.39	113.18
1	B	231	VAL	CB-CA-C	-5.79	104.32	112.14
1	B	156	LEU	N-CA-C	5.63	117.11	110.97
1	A	480	SER	N-CA-C	-5.58	106.64	113.50
1	A	204	ILE	N-CA-C	5.52	118.20	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ALA	N-CA-C	5.39	117.85	111.33
1	A	254	ALA	N-CA-C	5.26	118.86	112.23
1	A	147	ILE	N-CA-C	5.14	115.99	108.53
1	B	536	ILE	N-CA-C	5.13	115.72	109.30
1	B	30	GLU	N-CA-C	5.13	116.68	111.14
1	A	454	ASN	N-CA-C	-5.11	105.79	111.36
1	B	296	ASP	N-CA-C	-5.06	105.19	112.13
1	B	147	ILE	N-CA-C	5.05	115.85	108.53
1	B	535	ASP	N-CA-C	-5.01	106.42	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4027	204	0
1	B	4014	0	4035	162	0
2	A	190	0	0	9	0
2	B	224	0	0	7	0
All	All	8435	0	8062	340	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 21.

All (340) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:330:LYS:HE2	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:A:243:THR:HG23	1:A:277:THR:CG2	2.23	0.69
1:B:35:VAL:N	1:B:137:ASN:HD21	1.82	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:A:308:TYR:CZ	1:B:442:GLN:HG2	2.30	0.67
1:B:235:LEU:HD11	1:B:386:VAL:HG11	1.77	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
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: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:198:LYS:O	1:A:198:LYS:HG2	1.96	0.64
1:A:509:TYR:CE2	1:A:511:ALA:HB3	2.31	0.64
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.79	0.64
1:A:480:SER:OG	1:A:482:ARG:HD2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:CG1	1:B:128:ILE:HB	2.26	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:HG12	1:B:11:VAL:O	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
1:B:359:GLN:N	1:B:360:PRO:HD2	2.18	0.58
1:B:96:GLY:H	1:B:161:HIS:HE1	1.49	0.58
1:B:287:LEU:HD21	1:B:302:ILE:HB	1.84	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:A:503:THR:HG22	1:A:504:LEU:N	2.19	0.58
1:B:334:GLU:HG3	1:B:361:ILE:CG1	2.34	0.58
1:A:251:HIS:CD2	1:A:260:GLN:HG2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:101:PHE:CE1	1:A:146:GLU:HA	2.40	0.57
1:B:251:HIS:CD2	1:B:260:GLN:HE21	2.21	0.57
1:A:82:GLU:HG3	1:A:197:PHE:CD1	2.40	0.57
1:A:243:THR:CG2	1:A:277:THR:HG21	2.31	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:246:PHE:CE2	1:A:271:MET:HE1	2.40	0.56
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:246:PHE:CD2	1:A:271:MET:HE1	2.41	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:15:VAL:HG23	1:B:15:VAL:O	2.06	0.55
1:B:83:VAL:HG13	1:B:195:LEU:O	2.07	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: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:O3	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:180:GLU:CD	1:B:180:GLU:H	2.14	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:125:ARG:HD3	1:A:199:GLU:OE2	2.08	0.53
1:A:475:GLN:HE21	1:A:479:ILE:HD12	1.74	0.53
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:HG3	1:B:32:ARG:HH11	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:526:PHE:C	1:A:528:ARG:H	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:150:LEU:HD22	1:A:447:MET:HE1	1.91	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:43:ALA:C	1:A:45:ALA:H	2.18	0.51
1:A:534:THR:CG2	1:A:536:ILE:HG13	2.40	0.51
1:A:82:GLU:OE2	1:A:196:ARG:HB3	2.10	0.51
1:B:149:SER:CB	1:B:155:ASP:HA	2.35	0.51
1:B:231:VAL:HG13	1:B:470:TYR:CD2	2.45	0.51
1:B:294:GLY:O	1:B:295:LYS:CB	2.55	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:308:TYR:CE2	1:B:442:GLN:HG2	2.46	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:A:150:LEU:CD2	1:A:447:MET:HE1	2.41	0.51
1:B:72:MET:HE3	2:B:618:HOH:O	2.10	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:470:TYR:CE1	1:B:521:LEU:HD21	2.46	0.51
1:A:277:THR:HG22	1:A:278:VAL:N	2.25	0.50
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: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
1:A:483:PHE:O	1:A:491:LYS:NZ	2.46	0.49
1:B:52:PHE:O	1:B:55:ILE:CG2	2.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLU:O	1:B:57:GLU:HB2	2.13	0.49
1:B:172:VAL:CG2	1:B:184:VAL:HG21	2.43	0.49
1:A:315:GLN:HG2	1:B:354:ALA:O	2.12	0.49
1:A:158:PRO:HG3	2:A:557:HOH:O	2.12	0.48
1:A:257:HIS:HE1	1:B:334:GLU:HG2	1.78	0.48
1:B:132:LEU:HD23	1:B:166:LEU:HD21	1.95	0.48
1:A:69:TYR:CE2	1:A:89:LEU:HD22	2.48	0.48
1:B:198:LYS:HG2	1:B:198:LYS:O	2.13	0.48
1:B:231:VAL:HG22	1:B:470:TYR:CZ	2.48	0.48
1:B:330:LYS:HA	1:B:330:LYS:CE	2.39	0.48
1:A:306:LYS:O	1:A:311:ARG:NH1	2.46	0.48
1:A:475:GLN:O	1:A:479:ILE:HB	2.14	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: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:73:ILE:HD11	1:B:304:LEU:HB3	1.96	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:A:438:ASN:HA	2:A:652:HOH:O	2.14	0.47
1:B:499:ARG:HG2	1:B:499:ARG:HH11	1.80	0.47
1:A:198:LYS:O	1:A:198:LYS:CG	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:272:ARG:C	1:B:272:ARG:HD2	2.40	0.47
1:A:223:GLU:O	1:A:227:GLN:HG3	2.15	0.46
1:B:235:LEU:CD1	1:B:386:VAL:HG11	2.43	0.46
1:B:128:ILE:HD11	1:B:199:GLU:CD	2.41	0.46
1:A:15:VAL:CG2	1:A:35:VAL:HG23	2.45	0.46
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.78	0.46
1:B:263:THR:O	1:B:267:MET:HG2	2.15	0.46
1:B:362:ALA:CB	1:B:446:SER:HB2	2.45	0.46
1:B:227:GLN:O	1:B:231:VAL:HG22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PHE:C	1:A:528:ARG:N	2.73	0.46
1:A:299:ARG:HG2	1:B:75:MET:SD	2.56	0.46
1:B:125:ARG:CZ	1:B:196:ARG:HD3	2.46	0.46
1:A:313:ILE:HB	1:A:314:PRO:HD3	1.98	0.46
1:A:32:ARG:HA	1:A:32:ARG:HD3	1.74	0.46
1:A:71:GLU:HB2	1:A:441:ASN:HB2	1.97	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:181:THR:O	1:B:182:ALA:C	2.59	0.45
1:B:116:THR:HG23	1:B:339:ASN:H	1.81	0.45
1:B:483:PHE:C	1:B:483:PHE:CD2	2.95	0.45
1:A:51:ILE:N	1:A:51:ILE:HD12	2.32	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:174:ARG:HG3	2:A:631:HOH:O	2.16	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: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:HA	1:A:525:GLU:OE2	2.16	0.44
1:B:165:THR:HA	1:B:181:THR:HG21	1.99	0.44
1:A:127:ILE:HD12	1:A:127:ILE:C	2.43	0.44
1:A:386:VAL:HG23	1:A:395:LEU:HD12	1.99	0.44
1:B:16:ASP:HB3	1:B:38:PRO:HG3	1.99	0.44
1:B:392:SER:HA	2:B:588:HOH:O	2.17	0.44
1:B:431:SER:HA	1:B:446:SER:O	2.17	0.44
1:B:439:GLY:O	1:B:440:ASP:HB2	2.17	0.44
1:A:43:ALA:O	1:A:46:GLN:HG2	2.17	0.44
1:A:257:HIS:CE1	1:B:334:GLU:HG2	2.52	0.44
1:A:524:GLY:O	1:A:526:PHE:O	2.35	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:346:GLU:O	1:A:347:GLY:C	2.60	0.43
1:A:374:GLN:OE1	1:A:374:GLN:HA	2.18	0.43
1:A:255:ARG:HG3	1:B:337:SER:HB2	2.00	0.43
1:A:279:GLU:HB3	2:A:642:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PHE:O	1:A:528:ARG:N	2.47	0.43
1:B:303:TYR:HB3	1:B:305:GLN:O	2.18	0.43
1:B:378:LEU:O	1:B:382:GLN:HG3	2.17	0.43
1:A:40:GLU:H	1:A:40:GLU:CD	2.26	0.43
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:H	1:B:292:GLU:HG3	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:70:GLY:HA3	1:A:438:ASN:HD21	1.84	0.42
1:A:292:GLU:HB2	1:A:298:GLN:NE2	2.33	0.42
1:A:131:ARG:HD3	1:A:134:GLN:NE2	2.34	0.42
1:A:309:SER:O	1:A:313:ILE:HD11	2.19	0.42
1:A:494:TYR:CE2	1:A:498:ARG:HG3	2.55	0.42
1:B:125:ARG:CB	1:B:127:ILE:HG22	2.49	0.42
1:B:268:ARG:HH11	1:B:268:ARG:HB2	1.84	0.42
1:A:297:VAL:HG23	1:A:297:VAL:O	2.18	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: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:106:ALA:HA	1:A:144:ILE:HD12	2.02	0.42
1:A:110:VAL:HG13	1:A:132:LEU:HD22	2.01	0.42
1:A:352:HIS:CE1	1:B:280:HIS:NE2	2.87	0.42
1:B:38:PRO:HG2	1:B:41:SER:OG	2.20	0.42
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.84	0.42
1:A:470:TYR:CE1	1:A:521:LEU:HD21	2.54	0.42
1:B:47:LYS:O	1:B:51:ILE:HG13	2.20	0.42
1:B:134:GLN:O	1:B:138:GLU:HB2	2.20	0.42
1:B:251:HIS:CD2	1:B:260:GLN:HG2	2.53	0.42
1:A:356:PHE:CD1	1:A:356:PHE:C	2.98	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: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:210:MET:HE1	1:B:358:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:ASP:O	1:B:523:ARG:HG2	2.20	0.41
1:A:207:THR:N	1:A:339:ASN:HD22	2.03	0.41
1:B:49:ARG:HG2	1:B:125:ARG:HG2	2.02	0.41
1:B:101:PHE:CE2	1:B:146:GLU:HG2	2.55	0.41
1:B:227:GLN:HA	1:B:230:ILE:HD12	2.02	0.41
1:B:362:ALA:HB2	1:B:446:SER:HB2	2.03	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:191:GLU:H	1:A:191:GLU:CD	2.29	0.41
1:A:498:ARG:HA	1:A:501:VAL:O	2.21	0.41
1:B:122:SER:HB2	2:B:648:HOH:O	2.20	0.41
1:B:290:ASP:C	1:B:292:GLU:H	2.27	0.41
1:B:515:GLU:OE1	1:B:515:GLU:HA	2.20	0.41
1:B:205:ASN:HD21	1:B:356:PHE:HD2	1.68	0.41
1:B:268:ARG:HB2	1:B:268:ARG:NH1	2.35	0.41
1:B:295:LYS:HB3	1:B:296:ASP:H	1.42	0.41
1:A:109:ILE:HG12	1:A:209:GLY:HA2	2.03	0.41
1:B:69:TYR:CE2	1:B:89:LEU:HD22	2.56	0.41
1:A:127:ILE:HD12	1:A:128:ILE:N	2.35	0.41
1:A:249:GLU:O	1:A:253:ILE:HB	2.21	0.41
1:A:380:GLU:CG	2:A:579:HOH:O	2.67	0.41
1:A:524:GLY:O	1:A:528:ARG:HB2	2.21	0.41
1:B:116:THR:OG1	1:B:339:ASN:ND2	2.54	0.41
1:B:124:VAL:HG12	1:B:125:ARG:O	2.21	0.41
1:B:291:LYS:HB3	1:B:298:GLN:NE2	2.36	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:141:THR:HA	1:B:142:PRO:HD3	1.89	0.41
1:B:186:ALA:C	1:B:188:ARG:H	2.29	0.41
1:B:523:ARG:HG3	1:B:525:GLU:HG2	2.03	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:HG2	1:A:191:GLU:O	2.21	0.40
1:A:448:GLY:O	1:A:451:SER:HB2	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:CD	1:A:456:ARG:HH12	2.29	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	521/539 (97%)	477 (92%)	42 (8%)	2 (0%)	30	49
1	B	522/539 (97%)	488 (94%)	32 (6%)	2 (0%)	30	49
All	All	1043/1078 (97%)	965 (92%)	74 (7%)	4 (0%)	30	49

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%)	403 (97%)	12 (3%)	37	65
1	B	416/426 (98%)	406 (98%)	10 (2%)	43	70
All	All	831/852 (98%)	809 (97%)	22 (3%)	40	68

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

Mol	Chain	Res	Type
1	A	35	VAL
1	A	50	GLU
1	A	72	MET
1	A	85	LEU
1	A	140	ILE
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	A	530	ILE
1	B	35	VAL
1	B	126	PRO
1	B	173	LEU
1	B	180	GLU
1	B	231	VAL
1	B	292	GLU
1	B	443	ASP
1	B	479	ILE
1	B	515	GLU
1	B	532	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) 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	205	ASN
1	A	224	GLN
1	A	251	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	384	ASN
1	A	414	GLN
1	A	438	ASN
1	A	442	GLN
1	A	462	ASN
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	288	GLN
1	B	326	HIS
1	B	329	HIS
1	B	382	GLN
1	B	384	ASN
1	B	407	HIS
1	B	414	GLN
1	B	438	ASN
1	B	442	GLN

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	B	152	1	11,13,14	2.59	4 (36%)	15,18,20	2.16	2 (13%)
1	MDO	A	152	1	11,13,14	2.60	4 (36%)	15,18,20	2.21	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	1	-	2/4/23/24	0/1/1/1
1	MDO	A	152	1	-	1/4/23/24	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	MDO	O2-C2	6.58	1.36	1.23
1	B	152	MDO	O2-C2	6.55	1.36	1.23
1	B	152	MDO	CA2-N2	-3.25	1.33	1.39
1	A	152	MDO	CA2-N2	-3.18	1.33	1.39
1	B	152	MDO	C2-N3	-2.91	1.33	1.40
1	A	152	MDO	C2-N3	-2.90	1.33	1.40
1	A	152	MDO	C1-N3	-2.28	1.33	1.37
1	B	152	MDO	C1-N3	-2.24	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	MDO	O2-C2-CA2	-6.95	126.58	131.02
1	B	152	MDO	O2-C2-CA2	-6.64	126.78	131.02
1	A	152	MDO	CA2-C2-N3	3.74	106.64	103.50
1	B	152	MDO	CA2-C2-N3	3.64	106.55	103.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	152	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	B	152	MDO	2	0
1	A	152	MDO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	525/539 (97%)	-0.11	4 (0%) 82 80	12, 28, 46, 56	0
1	B	526/539 (97%)	-0.31	3 (0%) 85 83	10, 24, 41, 61	0
All	All	1051/1078 (97%)	-0.21	7 (0%) 84 81	10, 25, 44, 61	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	ASP	3.1
1	B	294	GLY	3.0
1	A	294	GLY	2.6
1	A	439	GLY	2.5
1	B	293	ALA	2.5
1	A	295	LYS	2.1
1	B	292	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. 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	A	152	13/14	0.83	0.11	21,25,28,28	0
1	MDO	B	152	13/14	0.85	0.10	18,21,22,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.