



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:47 AM UTC

PDB ID : 3KDY / pdb_00003kdy
Title : X-ray crystal structure of tyrosine aminomutase mutant construct
Authors : Cooke, H.A.; Bruner, S.D.
Deposited on : 2009-10-23
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

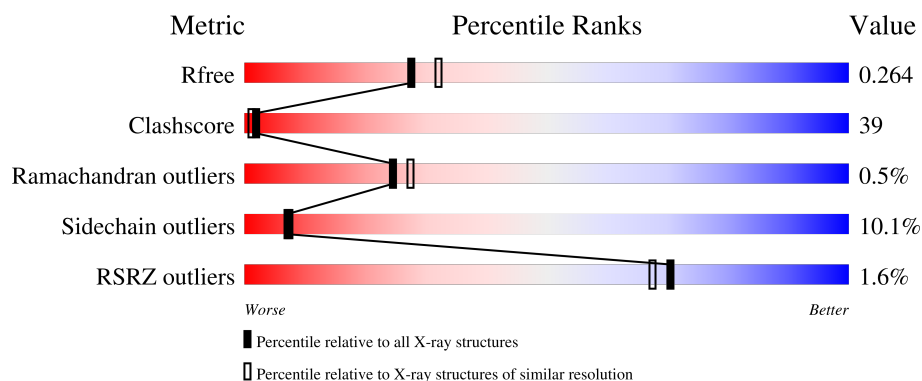
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	537	3% 47% 43% 9% .
1	B	537	% 53% 40% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8488 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4010	2506	728	768	8			
1	B	527	Total	C	N	O	S	0	0	0
			4010	2506	728	768	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	ALA	GLU	engineered mutation	UNP Q8GMG0
A	152	MDO	ALA	chromophore	UNP Q8GMG0
A	152	MDO	SER	chromophore	UNP Q8GMG0
A	152	MDO	GLY	chromophore	UNP Q8GMG0
B	71	ALA	GLU	engineered mutation	UNP Q8GMG0
B	152	MDO	ALA	chromophore	UNP Q8GMG0
B	152	MDO	SER	chromophore	UNP Q8GMG0
B	152	MDO	GLY	chromophore	UNP Q8GMG0

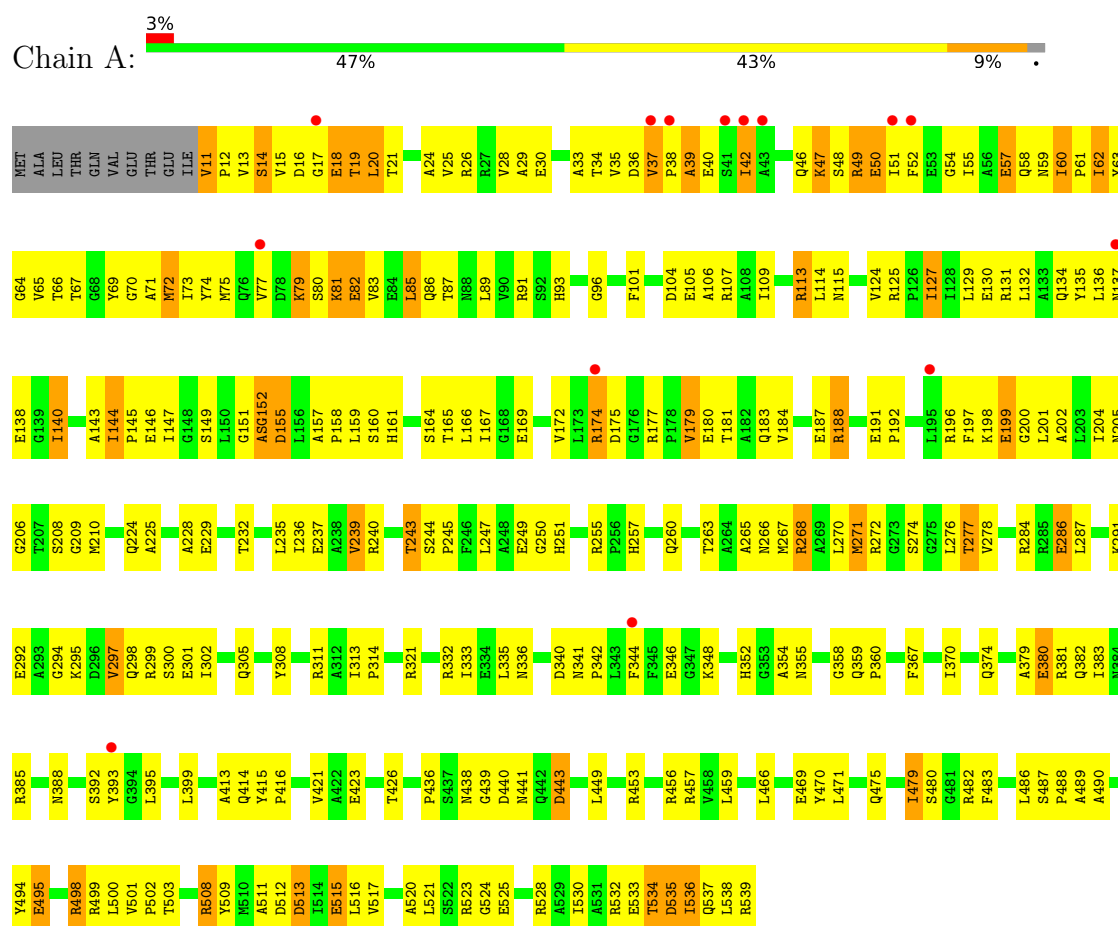
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	207	Total	O	0	0
			207	207		
2	B	261	Total	O	0	0
			261	261		

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: Histidine ammonia-lyase



• Molecule 1: Histidine ammonia-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.58Å 145.88Å 74.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.10 – 2.20 43.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (43.10-2.20) 91.2 (43.10-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.265 0.238 , 0.264	Depositor DCC
R_{free} test set	5017 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8488	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% 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 [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	0.38	3/4056 (0.1%)	0.78	6/5496 (0.1%)
1	B	0.37	1/4056 (0.0%)	0.75	4/5496 (0.1%)
All	All	0.38	4/8112 (0.0%)	0.77	10/10992 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	ASP	C-O	-7.43	1.17	1.24
1	A	151	GLY	CA-C	-7.37	1.38	1.52
1	A	14	SER	C-O	-7.31	1.15	1.24
1	A	14	SER	N-CA	-5.24	1.39	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	ASP	N-CA-C	12.15	128.96	108.67
1	B	295	LYS	N-CA-C	7.83	118.92	107.88
1	A	155	ASP	N-CA-CB	-7.64	97.52	110.50
1	B	295	LYS	CA-C-N	6.48	132.49	123.04
1	B	295	LYS	C-N-CA	6.48	132.49	123.04
1	A	81	LYS	CB-CA-C	-5.74	101.44	110.85
1	A	199	GLU	N-CA-C	5.70	117.57	111.36
1	A	144	ILE	N-CA-C	5.50	112.99	107.55
1	A	534	THR	CB-CA-C	-5.40	100.58	109.65
1	A	534	THR	N-CA-C	5.07	119.81	113.43

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	4010	0	4034	388	1
1	B	4010	0	4034	288	0
2	A	207	0	0	29	1
2	B	261	0	0	19	0
All	All	8488	0	8068	626	1

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 39.

All (626) 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:287:LEU:HG	1:B:302:ILE:CD1	1.18	1.60
1:B:287:LEU:CG	1:B:302:ILE:HD11	1.13	1.60
1:A:82:GLU:HB2	1:A:197:PHE:CE1	1.52	1.42
1:A:257:HIS:HD2	1:B:330:LYS:NZ	1.30	1.29
1:A:125:ARG:NH1	1:A:196:ARG:HG2	1.50	1.26
1:A:392:SER:OG	1:A:395:LEU:HB2	1.38	1.22
1:A:534:THR:HG21	1:A:536:ILE:CD1	1.70	1.19
1:A:534:THR:CG2	1:A:536:ILE:HD12	1.74	1.18
1:A:125:ARG:NH1	1:A:196:ARG:CG	2.08	1.15
1:A:257:HIS:CD2	1:B:330:LYS:HZ2	1.65	1.13
1:B:149:SER:HB2	1:B:155:ASP:HA	1.30	1.10
1:B:279:GLU:HG3	2:B:763:HOH:O	1.49	1.10
1:B:447:MET:HG3	1:B:450:ILE:HD12	1.32	1.10
1:A:82:GLU:HB2	1:A:197:PHE:CZ	1.88	1.08
1:A:257:HIS:CD2	1:B:330:LYS:NZ	2.23	1.04
1:A:86:GLN:NE2	1:A:200:GLY:H	1.57	1.01
1:B:287:LEU:CB	1:B:302:ILE:HD11	1.90	1.00
1:A:77:VAL:HG21	1:A:85:LEU:CD1	1.91	1.00
1:A:82:GLU:CB	1:A:197:PHE:CE1	2.45	1.00
1:A:486:LEU:HD22	1:A:490:ALA:HB1	1.40	0.99
1:B:287:LEU:HG	1:B:302:ILE:CG1	1.92	0.99
1:A:135:TYR:HA	1:A:140:ILE:CG2	1.92	0.99
1:A:299:ARG:HG2	1:B:75:MET:SD	2.05	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:N	1:A:12:PRO:HD2	1.80	0.96
1:B:82:GLU:HG3	1:B:197:PHE:CD1	2.01	0.95
1:A:11:VAL:N	1:A:12:PRO:CD	2.30	0.95
1:A:486:LEU:HD22	1:A:490:ALA:CB	1.97	0.95
1:A:58:GLN:HB3	2:A:680:HOH:O	1.67	0.94
1:A:188:ARG:HG2	1:A:188:ARG:HH11	1.32	0.94
1:B:227:GLN:HE22	1:B:524:GLY:HA2	1.32	0.94
1:A:175:ASP:HA	2:A:697:HOH:O	1.66	0.94
1:B:287:LEU:HD12	1:B:304:LEU:HD13	1.49	0.94
1:A:125:ARG:HH11	1:A:196:ARG:HG3	1.33	0.94
1:A:13:VAL:HG11	1:A:24:ALA:HB1	1.47	0.93
1:A:86:GLN:HE21	1:A:200:GLY:H	1.14	0.93
1:A:276:LEU:HD11	1:A:482:ARG:HB3	1.50	0.92
1:B:96:GLY:H	1:B:161:HIS:HE1	1.09	0.92
1:B:295:LYS:HA	2:B:794:HOH:O	1.71	0.91
1:A:125:ARG:HH11	1:A:196:ARG:CG	1.81	0.91
1:A:152:MDO:CB2	2:B:758:HOH:O	2.17	0.91
1:B:299:ARG:HH11	1:B:299:ARG:HB3	1.35	0.91
1:B:11:VAL:N	1:B:12:PRO:CD	2.33	0.91
1:A:532:ARG:HG2	1:A:533:GLU:N	1.84	0.90
1:A:438:ASN:HD22	1:A:441:ASN:HB3	1.37	0.90
1:A:251:HIS:HD2	1:A:260:GLN:HG2	1.38	0.89
1:A:267:MET:HE3	1:A:271:MET:HE2	1.53	0.88
1:A:15:VAL:CG1	1:A:115:ASN:HA	2.05	0.86
1:A:77:VAL:HG21	1:A:85:LEU:HD11	1.55	0.86
1:B:11:VAL:N	1:B:12:PRO:HD2	1.90	0.86
1:A:292:GLU:HB2	1:A:298:GLN:NE2	1.90	0.86
1:A:69:TYR:CE2	1:A:89:LEU:HD22	2.11	0.85
1:A:15:VAL:HG12	1:A:115:ASN:HA	1.58	0.85
1:B:65:VAL:HG22	1:B:198:LYS:HB2	1.59	0.85
1:B:494:TYR:CE2	1:B:498:ARG:HG3	2.11	0.85
1:B:152:MDO:HB22	2:B:732:HOH:O	1.75	0.84
1:A:305:GLN:HE22	1:B:341:ASN:HD21	1.22	0.84
1:A:20:LEU:HD12	1:A:21:THR:N	1.92	0.84
1:A:292:GLU:HB2	1:A:298:GLN:HE22	1.41	0.84
1:A:297:VAL:CG2	1:B:75:MET:HE3	2.07	0.84
1:A:71:ALA:O	1:A:74:TYR:CE1	2.30	0.84
1:A:392:SER:HG	1:A:395:LEU:HB2	1.42	0.83
1:A:308:TYR:OH	1:B:152:MDO:HB21	1.79	0.83
1:A:530:ILE:O	1:A:534:THR:HB	1.77	0.83
1:A:152:MDO:HB21	1:B:308:TYR:OH	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:HB2	1:A:197:PHE:CD1	2.12	0.82
1:B:15:VAL:HG23	1:B:15:VAL:O	1.78	0.82
1:B:287:LEU:CD2	1:B:302:ILE:HD11	2.08	0.82
1:A:35:VAL:H	1:A:137:ASN:HD21	1.27	0.82
1:A:257:HIS:HD2	1:B:330:LYS:HZ2	0.86	0.82
1:A:60:ILE:O	1:A:62:ILE:HG13	1.80	0.81
1:A:125:ARG:HH12	1:A:196:ARG:HG2	1.45	0.81
1:A:355:ASN:HD21	1:B:260:GLN:HE22	1.28	0.81
1:A:443:ASP:OD2	1:B:309:SER:OG	1.98	0.81
1:A:355:ASN:ND2	1:B:260:GLN:HE22	1.77	0.81
1:B:64:GLY:HA3	1:B:201:LEU:HD22	1.63	0.81
1:B:57:GLU:OE2	1:B:57:GLU:HA	1.80	0.80
1:A:508:ARG:HG3	2:A:676:HOH:O	1.80	0.80
1:A:524:GLY:O	1:A:528:ARG:HG2	1.80	0.80
1:B:71:ALA:H	1:B:438:ASN:HD21	1.30	0.80
1:A:257:HIS:HD2	1:B:330:LYS:HZ3	1.29	0.80
1:A:305:GLN:HE22	1:B:341:ASN:ND2	1.80	0.80
1:A:305:GLN:NE2	1:B:341:ASN:HD21	1.79	0.80
1:A:86:GLN:NE2	1:A:200:GLY:N	2.30	0.79
1:A:131:ARG:HG3	1:A:166:LEU:HD22	1.65	0.79
1:B:227:GLN:NE2	1:B:524:GLY:HA2	1.97	0.79
1:A:487:SER:HB2	1:A:488:PRO:HD2	1.65	0.78
1:B:96:GLY:H	1:B:161:HIS:CE1	1.99	0.78
1:B:299:ARG:HB3	1:B:299:ARG:NH1	1.98	0.78
1:A:115:ASN:ND2	1:A:335:LEU:O	2.17	0.78
1:A:480:SER:OG	1:A:482:ARG:HD2	1.84	0.78
1:B:359:GLN:N	1:B:360:PRO:HD2	1.99	0.78
1:A:272:ARG:HD2	2:A:579:HOH:O	1.83	0.78
1:A:292:GLU:H	1:A:298:GLN:HE22	1.30	0.78
1:A:61:PRO:O	1:A:62:ILE:HG12	1.84	0.77
1:B:113:ARG:HH12	1:B:339:ASN:ND2	1.82	0.77
1:B:159:LEU:HD12	1:B:204:ILE:O	1.84	0.76
1:A:64:GLY:HA3	1:A:201:LEU:HD22	1.67	0.76
1:B:65:VAL:CG2	1:B:198:LYS:HB2	2.16	0.76
1:A:297:VAL:CG2	1:B:75:MET:CE	2.64	0.76
1:A:172:VAL:HG21	1:A:184:VAL:HG21	1.66	0.75
1:A:77:VAL:HG11	1:A:85:LEU:HD13	1.67	0.75
1:A:355:ASN:ND2	1:B:255:ARG:HD2	2.01	0.75
1:A:57:GLU:HA	1:A:57:GLU:OE1	1.86	0.75
1:A:188:ARG:HG2	1:A:188:ARG:NH1	2.02	0.75
1:B:287:LEU:CG	1:B:302:ILE:CD1	2.05	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:OD1	1:B:79:LYS:HG2	1.86	0.75
1:B:31:GLU:O	1:B:32:ARG:HB2	1.85	0.74
1:B:486:LEU:HD22	1:B:490:ALA:HB1	1.68	0.74
1:A:313:ILE:HB	1:A:314:PRO:HD3	1.70	0.74
1:A:475:GLN:HE21	1:A:479:ILE:HD12	1.52	0.74
1:A:86:GLN:HE21	1:A:200:GLY:N	1.86	0.74
1:A:225:ALA:O	1:A:229:GLU:HG3	1.89	0.73
1:A:475:GLN:HG3	1:A:479:ILE:HD12	1.70	0.73
1:B:113:ARG:HH12	1:B:339:ASN:HD22	1.35	0.73
1:B:244:SER:O	1:B:247:LEU:HG	1.88	0.73
1:A:127:ILE:HD13	1:A:130:GLU:OE1	1.89	0.73
1:A:135:TYR:CA	1:A:140:ILE:CG2	2.67	0.73
1:B:69:TYR:CZ	1:B:89:LEU:HD22	2.24	0.72
1:B:287:LEU:CD2	1:B:302:ILE:CD1	2.67	0.72
1:A:21:THR:O	1:A:25:VAL:HG23	1.90	0.72
1:A:87:THR:HG22	1:A:91:ARG:HE	1.54	0.72
1:A:535:ASP:OD1	1:A:535:ASP:C	2.30	0.72
1:B:480:SER:HB2	1:B:482:ARG:HD2	1.71	0.72
1:A:49:ARG:HG2	1:A:125:ARG:HA	1.69	0.72
1:B:529:ALA:O	1:B:533:GLU:HB2	1.89	0.72
1:A:15:VAL:CG1	1:A:115:ASN:CA	2.68	0.71
1:B:196:ARG:HB2	1:B:199:GLU:OE1	1.91	0.71
1:A:265:ALA:HA	1:A:268:ARG:NH2	2.06	0.71
1:A:276:LEU:CD1	1:A:482:ARG:HB3	2.20	0.71
1:A:267:MET:HB3	1:A:271:MET:CE	2.20	0.71
1:B:237:GLU:OE1	1:B:274:SER:OG	2.08	0.71
1:A:392:SER:OG	1:A:395:LEU:CB	2.30	0.71
1:B:86:GLN:HG3	1:B:196:ARG:O	1.91	0.71
1:B:299:ARG:HH11	1:B:299:ARG:CB	2.04	0.70
1:A:196:ARG:HG3	1:A:196:ARG:HH11	1.57	0.70
1:A:297:VAL:HG22	1:B:75:MET:CE	2.21	0.70
1:B:447:MET:CG	1:B:450:ILE:HD12	2.17	0.70
1:A:16:ASP:OD2	1:A:19:THR:OG1	2.08	0.70
1:A:71:ALA:O	1:A:74:TYR:HE1	1.74	0.70
1:A:20:LEU:HD23	1:A:115:ASN:HB2	1.74	0.69
1:A:149:SER:HB2	1:A:158:PRO:HG3	1.73	0.69
1:A:292:GLU:CB	1:A:298:GLN:HE22	2.04	0.69
1:A:183:GLN:O	1:A:187:GLU:HB2	1.92	0.69
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.56	0.69
1:B:470:TYR:CE1	1:B:521:LEU:HD21	2.28	0.69
1:B:515:GLU:OE1	1:B:515:GLU:HA	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:HD22	1:B:255:ARG:HD2	1.57	0.69
1:B:205:ASN:HD21	1:B:356:PHE:HD2	1.38	0.69
1:A:71:ALA:O	1:A:74:TYR:CD1	2.46	0.69
1:A:96:GLY:H	1:A:161:HIS:HE1	1.41	0.69
1:B:198:LYS:HG2	1:B:198:LYS:O	1.91	0.68
1:B:305:GLN:O	1:B:306:LYS:HD3	1.92	0.68
1:A:65:VAL:HG13	1:A:197:PHE:HB3	1.75	0.68
1:B:235:LEU:HD11	1:B:386:VAL:CG1	2.23	0.68
1:A:284:ARG:NH2	1:B:349:GLU:OE2	2.26	0.68
1:A:523:ARG:HD3	2:A:716:HOH:O	1.93	0.68
1:A:475:GLN:O	1:A:479:ILE:HB	1.94	0.68
1:A:237:GLU:OE1	1:A:274:SER:OG	2.11	0.68
1:A:107:ARG:NH1	1:A:136:LEU:O	2.24	0.67
1:B:26:ARG:HG2	1:B:216:LEU:HD23	1.75	0.67
1:B:101:PHE:CE2	1:B:213:LEU:HD22	2.28	0.67
1:B:21:THR:O	1:B:25:VAL:HG23	1.93	0.67
1:A:308:TYR:CE2	1:B:442:GLN:HG2	2.30	0.67
1:A:172:VAL:CG2	1:A:184:VAL:HG21	2.24	0.67
1:B:149:SER:CB	1:B:155:ASP:HA	2.17	0.67
1:A:51:ILE:HB	1:A:344:PHE:CZ	2.30	0.66
1:A:470:TYR:CE1	1:A:521:LEU:HD21	2.30	0.66
1:A:82:GLU:CB	1:A:197:PHE:CZ	2.72	0.66
1:B:59:ASN:CG	1:B:79:LYS:HG2	2.20	0.66
1:B:69:TYR:CE2	1:B:89:LEU:HD22	2.30	0.66
1:B:82:GLU:HB2	1:B:197:PHE:CE1	2.30	0.66
1:A:135:TYR:CA	1:A:140:ILE:HG23	2.26	0.66
1:A:355:ASN:HD21	1:B:260:GLN:NE2	1.93	0.66
1:A:152:MDO:HB21	2:B:758:HOH:O	1.91	0.66
1:A:109:ILE:HD13	1:A:209:GLY:HA2	1.78	0.66
1:B:532:ARG:HB2	1:B:532:ARG:NH1	2.10	0.66
1:A:86:GLN:HE22	1:A:201:LEU:H	1.42	0.66
1:B:96:GLY:N	1:B:161:HIS:HE1	1.89	0.66
1:B:231:VAL:HB	1:B:470:TYR:CZ	2.30	0.66
1:B:235:LEU:HD11	1:B:386:VAL:HG13	1.78	0.66
1:B:194:GLU:OE1	1:B:196:ARG:NH2	2.29	0.66
1:B:415:TYR:N	1:B:416:PRO:HD2	2.11	0.66
1:A:157:ALA:HB2	2:A:684:HOH:O	1.95	0.65
1:A:255:ARG:NH2	1:B:334:GLU:OE2	2.30	0.65
1:A:131:ARG:CG	1:A:166:LEU:HD22	2.27	0.65
1:B:332:ARG:HG2	1:B:332:ARG:HH11	1.60	0.65
1:A:33:ALA:O	2:A:744:HOH:O	2.15	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HG21	1:A:313:ILE:HG12	1.78	0.64
1:A:359:GLN:N	1:A:360:PRO:CD	2.61	0.64
1:B:155:ASP:O	1:B:159:LEU:HG	1.97	0.64
1:A:509:TYR:CE2	1:A:511:ALA:HB3	2.32	0.64
1:B:35:VAL:H	1:B:137:ASN:HD21	1.43	0.64
1:B:287:LEU:HD21	1:B:302:ILE:HG12	1.79	0.64
1:A:134:GLN:NE2	1:A:138:GLU:OE2	2.30	0.64
1:A:237:GLU:OE1	1:A:274:SER:CB	2.45	0.64
1:A:532:ARG:HG2	1:A:533:GLU:H	1.62	0.64
1:A:71:ALA:H	1:A:438:ASN:HD21	1.44	0.64
1:A:28:VAL:HA	1:A:33:ALA:HB3	1.79	0.64
1:B:113:ARG:HD2	1:B:208:SER:OG	1.98	0.64
1:A:308:TYR:CZ	1:B:442:GLN:HG2	2.33	0.64
1:B:198:LYS:O	1:B:198:LYS:CG	2.46	0.64
1:A:268:ARG:NH2	2:A:742:HOH:O	2.31	0.63
1:A:355:ASN:HD22	1:B:255:ARG:CD	2.12	0.63
1:A:438:ASN:ND2	1:A:441:ASN:HB3	2.13	0.63
1:A:523:ARG:NH2	1:A:525:GLU:HG3	2.13	0.63
1:B:152:MDO:CB2	2:B:732:HOH:O	2.40	0.63
1:A:276:LEU:HD21	1:A:482:ARG:HG2	1.79	0.63
1:A:532:ARG:CG	1:A:533:GLU:N	2.57	0.63
1:A:14:SER:HA	1:A:36:ASP:O	1.99	0.63
1:A:149:SER:OG	1:A:155:ASP:OD1	2.15	0.63
1:A:101:PHE:CE1	1:A:146:GLU:HA	2.33	0.62
1:A:276:LEU:CD2	1:A:482:ARG:HG2	2.29	0.62
1:A:523:ARG:CD	2:A:716:HOH:O	2.45	0.62
1:B:307:ALA:HB2	1:B:385:ARG:CZ	2.29	0.62
1:A:392:SER:O	1:A:393:TYR:HB2	1.99	0.62
1:A:104:ASP:OD1	1:A:105:GLU:N	2.31	0.62
1:A:286:GLU:HG2	1:A:302:ILE:HD13	1.80	0.62
1:A:87:THR:HG21	1:A:91:ARG:HH21	1.65	0.62
1:A:534:THR:O	1:A:535:ASP:CB	2.48	0.62
1:A:125:ARG:NH1	1:A:196:ARG:HG3	1.96	0.62
1:A:51:ILE:HB	1:A:344:PHE:HZ	1.63	0.61
1:A:237:GLU:OE1	1:A:274:SER:HB2	1.99	0.61
1:A:423:GLU:O	1:A:426:THR:OG1	2.17	0.61
1:A:135:TYR:HA	1:A:140:ILE:HG21	1.78	0.61
1:A:292:GLU:H	1:A:298:GLN:NE2	1.98	0.61
2:A:558:HOH:O	1:B:326:HIS:HE1	1.83	0.61
1:B:195:LEU:HD13	1:B:200:GLY:CA	2.31	0.61
1:A:413:ALA:O	1:A:416:PRO:HD2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLN:OE1	1:A:459:LEU:HD12	2.01	0.61
1:A:277:THR:CG2	1:A:278:VAL:N	2.64	0.61
1:A:159:LEU:HD21	1:A:208:SER:HB2	1.83	0.61
1:A:113:ARG:HD3	1:A:208:SER:OG	2.00	0.60
1:B:128:ILE:HD11	1:B:199:GLU:HG2	1.81	0.60
1:B:71:ALA:H	1:B:438:ASN:ND2	1.97	0.60
1:B:439:GLY:O	1:B:440:ASP:HB2	2.02	0.60
1:B:124:VAL:HG12	1:B:125:ARG:O	2.02	0.60
1:A:495:GLU:O	1:A:499:ARG:HG3	2.02	0.60
1:B:251:HIS:HD2	1:B:260:GLN:HG2	1.67	0.59
1:B:287:LEU:CD2	1:B:302:ILE:HG12	2.31	0.59
1:B:396:PRO:HD2	1:B:479:ILE:HG21	1.84	0.59
1:A:15:VAL:HG21	1:A:114:LEU:HD23	1.83	0.59
1:A:77:VAL:HG21	1:A:85:LEU:HD13	1.80	0.59
1:A:292:GLU:N	1:A:298:GLN:HE22	1.99	0.59
1:B:227:GLN:HE22	1:B:524:GLY:CA	2.12	0.59
1:A:415:TYR:N	1:A:416:PRO:HD2	2.17	0.59
1:A:423:GLU:OE2	1:A:457:ARG:NH2	2.26	0.59
1:A:129:LEU:H	1:A:129:LEU:HD12	1.67	0.59
1:A:28:VAL:O	1:A:107:ARG:NH2	2.24	0.59
1:A:348:LYS:HD2	1:B:249:GLU:HG2	1.84	0.59
1:A:131:ARG:HG3	1:A:166:LEU:CD2	2.31	0.59
1:B:134:GLN:NE2	1:B:190:ILE:HD11	2.17	0.59
1:B:287:LEU:CD1	1:B:304:LEU:HD13	2.28	0.59
1:A:15:VAL:HG13	1:A:115:ASN:HB2	1.84	0.59
1:A:64:GLY:O	1:A:85:LEU:CD2	2.50	0.59
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.67	0.59
1:B:424:ASN:HA	1:B:427:ILE:HD12	1.83	0.59
1:A:75:MET:SD	1:B:299:ARG:HG2	2.43	0.59
1:B:494:TYR:CZ	1:B:498:ARG:HG3	2.38	0.58
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.17	0.58
1:A:534:THR:HG21	1:A:536:ILE:HD12	0.79	0.58
1:A:135:TYR:CB	1:A:140:ILE:HG23	2.33	0.58
1:B:65:VAL:HG22	1:B:198:LYS:CB	2.33	0.58
1:A:157:ALA:N	1:A:158:PRO:HD2	2.18	0.58
1:A:243:THR:C	1:A:245:PRO:HD2	2.29	0.58
1:A:63:TYR:HA	1:A:67:THR:OG1	2.04	0.58
1:A:201:LEU:O	1:A:205:ASN:HB2	2.04	0.58
1:A:257:HIS:CD2	1:B:330:LYS:HZ3	2.10	0.57
1:A:475:GLN:HE21	1:A:479:ILE:CD1	2.16	0.57
1:B:231:VAL:HB	1:B:470:TYR:CE1	2.39	0.57

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	2.03	0.57
1:B:82:GLU:HG3	1:B:197:PHE:CE1	2.40	0.57
1:B:533:GLU:HA	1:B:533:GLU:OE1	2.04	0.57
1:A:62:ILE:HB	1:A:65:VAL:HB	1.87	0.57
1:B:285:ARG:O	1:B:289:LYS:HG3	2.04	0.57
1:B:332:ARG:HG2	1:B:332:ARG:NH1	2.20	0.57
1:A:380:GLU:HG3	1:A:381:ARG:N	2.19	0.57
1:A:536:ILE:HG22	1:A:538:LEU:HG	1.85	0.57
1:B:15:VAL:HG13	1:B:35:VAL:CG2	2.34	0.57
1:B:267:MET:O	1:B:271:MET:HG3	2.05	0.57
1:B:274:SER:HB2	1:B:487:SER:HB3	1.86	0.57
1:B:407:HIS:CD2	1:B:507:ASP:H	2.22	0.57
1:B:497:VAL:HG23	1:B:526:PHE:CE1	2.39	0.57
1:A:525:GLU:HG3	2:A:688:HOH:O	2.05	0.57
1:A:147:ILE:HG12	1:A:453:ARG:NH2	2.20	0.56
1:B:17:GLY:C	1:B:18:GLU:HG2	2.29	0.56
1:B:101:PHE:HE2	1:B:213:LEU:HD22	1.68	0.56
1:B:359:GLN:N	1:B:360:PRO:CD	2.68	0.56
1:A:87:THR:O	1:A:91:ARG:HG3	2.05	0.56
1:B:59:ASN:OD1	1:B:79:LYS:CG	2.54	0.56
1:B:181:THR:O	1:B:185:LEU:HG	2.05	0.56
1:A:263:THR:CG2	1:A:314:PRO:HA	2.36	0.56
1:A:512:ASP:HB2	2:A:681:HOH:O	2.05	0.56
1:B:290:ASP:C	1:B:292:GLU:H	2.14	0.56
1:A:114:LEU:HD13	1:A:132:LEU:HB2	1.86	0.56
1:A:15:VAL:O	1:A:37:VAL:HG12	2.05	0.56
1:A:59:ASN:CG	1:A:79:LYS:HG2	2.30	0.56
1:A:152:MDO:HB21	1:B:308:TYR:HH	1.69	0.56
1:B:23:GLU:OE2	1:B:27:ARG:NH1	2.38	0.56
1:B:313:ILE:N	1:B:314:PRO:CD	2.69	0.56
1:A:20:LEU:HD12	1:A:21:THR:H	1.66	0.55
1:A:86:GLN:HG3	1:A:196:ARG:O	2.06	0.55
1:A:355:ASN:ND2	1:B:255:ARG:CD	2.67	0.55
1:B:11:VAL:HG12	1:B:11:VAL:O	2.06	0.55
1:B:287:LEU:CA	1:B:302:ILE:HD11	2.36	0.55
1:B:399:LEU:O	1:B:479:ILE:HD11	2.05	0.55
1:A:15:VAL:HG13	1:A:115:ASN:CB	2.36	0.55
1:B:54:GLY:HA3	2:B:756:HOH:O	2.05	0.55
1:A:35:VAL:N	1:A:137:ASN:HD21	2.01	0.55
1:A:46:GLN:O	1:A:47:LYS:C	2.49	0.55
1:B:68:GLY:HA3	1:B:72:MET:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:CD2	1:B:302:ILE:CG1	2.85	0.55
1:A:332:ARG:HD2	2:A:668:HOH:O	2.06	0.55
1:A:20:LEU:HD12	1:A:20:LEU:C	2.31	0.54
1:A:232:THR:O	1:A:236:ILE:HD12	2.07	0.54
1:A:71:ALA:N	1:A:438:ASN:HD21	2.05	0.54
1:B:480:SER:CB	1:B:482:ARG:HD2	2.36	0.54
1:A:82:GLU:OE2	1:A:197:PHE:CD2	2.61	0.54
1:B:131:ARG:HB2	1:B:193:LEU:HD11	1.90	0.54
1:B:174:ARG:O	1:B:175:ASP:HB2	2.06	0.54
1:B:407:HIS:HD2	1:B:507:ASP:H	1.56	0.54
1:B:359:GLN:NE2	1:B:363:PHE:CE1	2.75	0.54
1:B:423:GLU:OE2	1:B:457:ARG:NH2	2.36	0.54
1:B:508:ARG:HD3	2:B:556:HOH:O	2.06	0.54
1:B:244:SER:N	1:B:245:PRO:CD	2.71	0.54
1:A:13:VAL:O	1:A:35:VAL:HA	2.08	0.53
1:A:61:PRO:C	1:A:62:ILE:CG1	2.81	0.53
1:A:87:THR:CG2	1:A:91:ARG:HE	2.20	0.53
1:A:266:ASN:OD1	1:A:539:ARG:HG3	2.08	0.53
1:B:124:VAL:HG11	1:B:128:ILE:HG21	1.89	0.53
1:B:157:ALA:N	1:B:158:PRO:HD2	2.23	0.53
1:B:15:VAL:O	1:B:15:VAL:CG2	2.51	0.53
1:A:244:SER:HB3	1:A:245:PRO:HD3	1.90	0.53
1:A:287:LEU:HD23	1:B:61:PRO:HB3	1.89	0.53
1:A:487:SER:HB2	1:A:488:PRO:CD	2.35	0.53
1:A:113:ARG:NH1	1:A:206:GLY:HA3	2.23	0.53
1:B:272:ARG:O	1:B:488:PRO:HD2	2.09	0.53
1:A:109:ILE:CD1	1:A:209:GLY:HA2	2.38	0.53
1:B:390:HIS:HD2	2:B:696:HOH:O	1.91	0.53
1:A:251:HIS:CD2	1:A:260:GLN:HG2	2.30	0.53
1:B:436:PRO:HD3	2:B:543:HOH:O	2.08	0.53
1:A:352:HIS:HB3	1:B:305:GLN:OE1	2.09	0.52
1:B:287:LEU:CG	1:B:302:ILE:CG1	2.67	0.52
1:A:534:THR:CG2	1:A:536:ILE:CD1	2.57	0.52
1:B:380:GLU:HG2	2:B:606:HOH:O	2.08	0.52
1:A:196:ARG:C	1:A:199:GLU:HG3	2.35	0.52
1:B:15:VAL:HG13	1:B:35:VAL:HG22	1.91	0.52
1:B:174:ARG:HD2	2:B:672:HOH:O	2.08	0.52
1:A:79:LYS:C	1:A:81:LYS:H	2.17	0.52
1:A:113:ARG:NH2	1:A:202:ALA:O	2.39	0.52
1:B:287:LEU:CA	1:B:302:ILE:CD1	2.87	0.52
1:B:523:ARG:HB2	1:B:525:GLU:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HA	1:A:137:ASN:ND2	2.24	0.52
1:B:509:TYR:CE2	1:B:511:ALA:HB3	2.45	0.52
1:A:137:ASN:ND2	2:A:744:HOH:O	2.43	0.52
1:A:508:ARG:HD3	2:A:573:HOH:O	2.10	0.52
1:A:51:ILE:CG2	1:A:344:PHE:HZ	2.22	0.52
1:A:383:ILE:HG13	1:A:469:GLU:HG3	1.91	0.52
1:B:213:LEU:HD12	1:B:213:LEU:O	2.09	0.52
1:B:532:ARG:HB2	1:B:532:ARG:HH11	1.75	0.52
1:A:291:LYS:HD3	1:B:76:GLN:HB3	1.92	0.51
1:B:287:LEU:HA	1:B:302:ILE:HD13	1.92	0.51
1:A:498:ARG:HA	1:A:501:VAL:O	2.10	0.51
1:B:101:PHE:CE1	1:B:146:GLU:HA	2.45	0.51
1:A:15:VAL:HG13	1:A:115:ASN:CA	2.41	0.51
1:A:149:SER:HB2	1:A:158:PRO:CG	2.39	0.51
1:A:13:VAL:CG1	1:A:24:ALA:HB1	2.30	0.51
1:A:101:PHE:CZ	1:A:146:GLU:HG2	2.45	0.51
1:B:159:LEU:HB3	1:B:204:ILE:HA	1.93	0.51
1:B:287:LEU:HA	1:B:302:ILE:CD1	2.40	0.51
1:A:196:ARG:HG3	1:A:196:ARG:NH1	2.23	0.51
1:B:497:VAL:HG23	1:B:526:PHE:HE1	1.75	0.51
1:A:65:VAL:HG22	1:A:198:LYS:HB2	1.92	0.51
1:A:239:VAL:O	1:A:239:VAL:HG13	2.10	0.51
1:A:374:GLN:HB3	1:B:363:PHE:HZ	1.75	0.51
1:A:443:ASP:OD1	1:A:443:ASP:N	2.38	0.51
1:A:20:LEU:HD23	1:A:115:ASN:CB	2.41	0.51
1:A:244:SER:N	1:A:245:PRO:CD	2.73	0.51
1:A:263:THR:HG21	1:A:314:PRO:HA	1.93	0.51
1:A:294:GLY:CA	2:A:708:HOH:O	2.59	0.51
1:A:174:ARG:NH1	2:A:727:HOH:O	2.44	0.50
1:B:90:VAL:HG21	1:B:195:LEU:HD11	1.93	0.50
1:B:313:ILE:HB	1:B:314:PRO:HD3	1.93	0.50
1:A:51:ILE:CB	1:A:344:PHE:HZ	2.25	0.50
1:A:367:PHE:CD1	1:B:367:PHE:CD1	2.99	0.50
1:A:77:VAL:CG1	1:A:85:LEU:HD13	2.39	0.50
1:A:297:VAL:HG23	1:B:75:MET:HE3	1.89	0.50
1:A:16:ASP:HB3	1:A:38:PRO:HG3	1.93	0.50
1:A:179:VAL:O	1:A:180:GLU:C	2.54	0.50
1:B:124:VAL:CG1	1:B:128:ILE:HB	2.41	0.50
1:B:128:ILE:CD1	1:B:199:GLU:HG2	2.42	0.50
1:B:350:ILE:HA	2:B:559:HOH:O	2.12	0.50
1:B:22:VAL:HG21	1:B:328:ARG:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:O	1:B:276:LEU:HD13	2.12	0.50
1:B:340:ASP:CG	1:B:341:ASN:N	2.70	0.50
1:A:17:GLY:C	1:A:18:GLU:HG2	2.37	0.50
1:B:172:VAL:HG21	1:B:184:VAL:HG21	1.93	0.50
1:A:29:ALA:HB1	1:A:104:ASP:O	2.12	0.49
1:A:49:ARG:HD3	1:A:125:ARG:N	2.27	0.49
1:A:244:SER:O	1:A:247:LEU:HG	2.11	0.49
1:A:383:ILE:CG1	1:A:469:GLU:HG3	2.42	0.49
1:A:414:GLN:HG2	1:A:414:GLN:O	2.12	0.49
1:B:235:LEU:HD11	1:B:386:VAL:HG11	1.93	0.49
1:B:237:GLU:HG2	1:B:277:THR:HG23	1.93	0.49
1:B:263:THR:CG2	1:B:314:PRO:HA	2.42	0.49
1:A:52:PHE:O	1:A:55:ILE:N	2.46	0.49
1:B:340:ASP:OD1	1:B:341:ASN:N	2.40	0.49
1:B:466:LEU:O	1:B:470:TYR:HD1	1.95	0.49
1:A:300:SER:O	1:B:74:TYR:HB2	2.12	0.49
1:A:513:ASP:OD1	1:A:513:ASP:N	2.45	0.49
1:B:235:LEU:CD1	1:B:386:VAL:HG11	2.43	0.49
1:B:487:SER:HB2	1:B:488:PRO:HD2	1.95	0.49
1:B:157:ALA:HB3	1:B:158:PRO:CD	2.42	0.49
1:B:288:GLN:O	1:B:288:GLN:HG3	2.12	0.49
1:A:224:GLN:CD	1:A:459:LEU:HD12	2.37	0.49
1:A:267:MET:O	1:A:271:MET:HG3	2.13	0.49
1:A:388:ASN:O	1:A:392:SER:N	2.44	0.49
1:A:466:LEU:O	1:A:470:TYR:HD1	1.95	0.49
1:A:537:GLN:N	2:A:737:HOH:O	2.41	0.49
1:A:354:ALA:CB	1:B:312:ALA:HB2	2.43	0.48
1:A:26:ARG:O	1:A:30:GLU:HB2	2.14	0.48
1:A:520:ALA:HA	1:A:523:ARG:NH1	2.27	0.48
1:A:523:ARG:NH2	1:A:525:GLU:CG	2.76	0.48
1:B:127:ILE:HG23	1:B:128:ILE:HD12	1.96	0.48
1:B:244:SER:HB3	1:B:245:PRO:HD3	1.94	0.48
1:B:131:ARG:HG3	1:B:166:LEU:HD22	1.95	0.48
1:B:291:LYS:HB3	1:B:298:GLN:HE22	1.79	0.48
1:B:15:VAL:CG1	1:B:35:VAL:CG2	2.91	0.48
1:A:73:ILE:CG2	1:B:303:TYR:CD1	2.97	0.48
1:A:244:SER:HA	1:A:247:LEU:HG	1.95	0.48
1:B:263:THR:HG21	1:B:314:PRO:HA	1.95	0.48
1:A:39:ALA:HA	1:A:42:ILE:HG13	1.95	0.48
1:A:49:ARG:HD3	1:A:124:VAL:C	2.38	0.48
1:A:72:MET:HA	1:A:74:TYR:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:HB3	1:A:449:LEU:HD23	1.96	0.48
1:B:11:VAL:O	1:B:11:VAL:CG1	2.62	0.48
1:B:340:ASP:CG	1:B:341:ASN:H	2.21	0.48
1:B:420:LEU:HD22	1:B:461:ASN:HB3	1.94	0.48
1:A:313:ILE:HD12	1:A:313:ILE:N	2.29	0.48
1:A:471:LEU:HD21	1:A:517:VAL:HG21	1.96	0.48
1:A:157:ALA:HB3	1:A:158:PRO:CD	2.44	0.48
1:A:421:VAL:HA	2:A:582:HOH:O	2.13	0.47
1:A:38:PRO:HG2	2:A:542:HOH:O	2.15	0.47
1:A:305:GLN:HB2	1:B:73:ILE:HD13	1.96	0.47
1:B:124:VAL:CG1	1:B:125:ARG:N	2.77	0.47
1:A:374:GLN:OE1	1:A:374:GLN:HA	2.13	0.47
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.95	0.47
1:A:276:LEU:HD11	1:A:482:ARG:O	2.14	0.47
1:A:333:ILE:HG23	1:B:256:PRO:HG2	1.97	0.47
1:B:16:ASP:HB3	1:B:38:PRO:HG3	1.96	0.47
1:A:439:GLY:O	1:A:440:ASP:HB2	2.15	0.47
1:B:113:ARG:NH1	1:B:339:ASN:ND2	2.57	0.47
1:A:70:GLY:HA3	1:A:438:ASN:HD21	1.80	0.47
1:A:101:PHE:CE2	1:A:146:GLU:HG2	2.50	0.47
1:A:105:GLU:CD	2:A:674:HOH:O	2.58	0.47
1:B:195:LEU:HD13	1:B:200:GLY:HA3	1.97	0.47
1:A:294:GLY:HA2	2:A:708:HOH:O	2.14	0.47
1:B:57:GLU:OE2	1:B:57:GLU:CA	2.53	0.47
1:A:250:GLY:HA3	1:B:351:PHE:CZ	2.50	0.46
1:B:113:ARG:NH1	1:B:206:GLY:HA3	2.30	0.46
1:A:152:MDO:HB22	2:B:758:HOH:O	2.02	0.46
1:B:138:GLU:O	1:B:188:ARG:NH2	2.47	0.46
1:A:537:GLN:CA	2:A:737:HOH:O	2.62	0.46
1:A:165:THR:HA	1:A:169:GLU:O	2.16	0.46
1:B:213:LEU:O	1:B:217:VAL:HG23	2.15	0.46
1:A:73:ILE:CG2	1:B:303:TYR:HD1	2.29	0.46
1:A:107:ARG:HG2	1:A:136:LEU:HD23	1.96	0.46
1:A:267:MET:HB3	1:A:271:MET:HE3	1.94	0.46
1:A:277:THR:HG22	1:A:278:VAL:N	2.30	0.46
1:A:224:GLN:O	1:A:228:ALA:N	2.47	0.46
1:A:243:THR:O	1:A:244:SER:C	2.59	0.46
1:B:32:ARG:O	1:B:33:ALA:C	2.59	0.46
1:A:167:ILE:HD12	1:A:169:GLU:OE2	2.16	0.46
1:B:517:VAL:HG12	1:B:521:LEU:HD12	1.98	0.46
1:A:66:THR:C	1:A:67:THR:HG23	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ALA:O	1:A:515:GLU:OE2	2.35	0.45
1:B:332:ARG:HD2	2:B:698:HOH:O	2.16	0.45
1:B:498:ARG:HA	1:B:498:ARG:NE	2.30	0.45
1:A:274:SER:HB2	1:A:487:SER:HB3	1.97	0.45
1:B:13:VAL:HG21	1:B:28:VAL:HG23	1.98	0.45
1:A:14:SER:CA	1:A:36:ASP:O	2.63	0.45
1:A:38:PRO:O	1:A:40:GLU:N	2.50	0.45
1:A:174:ARG:HG2	2:A:613:HOH:O	2.16	0.45
1:A:494:TYR:CZ	1:A:498:ARG:HD2	2.51	0.45
1:B:124:VAL:HG11	1:B:128:ILE:CG2	2.46	0.45
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.81	0.45
1:A:436:PRO:HD3	2:A:575:HOH:O	2.16	0.45
1:A:79:LYS:C	1:A:81:LYS:N	2.75	0.45
1:A:508:ARG:O	1:A:509:TYR:C	2.60	0.45
1:B:218:VAL:HG21	1:B:331:LEU:CD1	2.46	0.45
1:B:380:GLU:HG3	1:B:381:ARG:N	2.32	0.45
1:A:172:VAL:CG1	1:A:181:THR:HG23	2.47	0.45
1:B:40:GLU:H	1:B:40:GLU:HG2	1.41	0.44
1:A:18:GLU:HA	1:A:336:ASN:HB3	1.98	0.44
1:B:149:SER:HB3	1:B:158:PRO:CD	2.48	0.44
1:B:415:TYR:N	1:B:416:PRO:CD	2.80	0.44
1:A:113:ARG:HA	1:A:113:ARG:HD2	1.59	0.44
1:A:537:GLN:HB2	2:A:737:HOH:O	2.17	0.44
1:A:210:MET:SD	1:A:358:GLY:HA3	2.58	0.44
1:A:286:GLU:CG	1:A:302:ILE:HD13	2.47	0.44
1:A:537:GLN:CB	2:A:737:HOH:O	2.65	0.44
1:A:77:VAL:HG11	1:A:85:LEU:CD1	2.43	0.44
1:A:483:PHE:O	1:A:486:LEU:HB2	2.18	0.44
1:B:131:ARG:HD2	1:B:135:TYR:CE1	2.53	0.44
1:B:358:GLY:C	1:B:360:PRO:HD2	2.42	0.44
1:A:60:ILE:O	1:A:62:ILE:CG1	2.60	0.44
1:A:75:MET:HA	1:A:75:MET:HE3	1.99	0.44
1:A:71:ALA:H	1:A:438:ASN:ND2	2.15	0.43
1:A:89:LEU:O	1:A:93:HIS:HB2	2.17	0.43
1:B:44:LYS:HG2	1:B:120:GLY:HA3	2.00	0.43
1:B:127:ILE:HG23	1:B:128:ILE:N	2.33	0.43
1:B:149:SER:HB3	1:B:158:PRO:HG3	2.00	0.43
1:B:378:LEU:HD21	2:B:764:HOH:O	2.18	0.43
1:A:38:PRO:C	1:A:40:GLU:N	2.76	0.43
1:B:142:PRO:HB3	1:B:165:THR:HG21	1.99	0.43
1:A:69:TYR:CZ	1:A:89:LEU:HD22	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:VAL:HA	1:A:502:PRO:HD3	1.87	0.43
1:A:54:GLY:O	1:A:57:GLU:HB2	2.19	0.43
1:A:75:MET:HE1	1:B:299:ARG:HG2	1.99	0.43
1:A:341:ASN:HA	1:A:342:PRO:C	2.44	0.43
1:A:255:ARG:HH21	1:B:334:GLU:CD	2.26	0.43
1:B:227:GLN:HA	1:B:230:ILE:HD12	2.01	0.43
1:B:321:ARG:HG2	1:B:321:ARG:NH1	2.31	0.43
1:A:134:GLN:O	1:A:135:TYR:C	2.61	0.43
1:A:265:ALA:HA	1:A:268:ARG:HH21	1.82	0.43
1:B:159:LEU:CB	1:B:204:ILE:HA	2.49	0.43
1:A:380:GLU:HG2	2:A:576:HOH:O	2.17	0.43
1:A:47:LYS:HZ2	1:A:346:GLU:HG2	1.83	0.43
1:A:77:VAL:CG2	1:A:85:LEU:HD13	2.48	0.43
1:A:198:LYS:NZ	1:A:340:ASP:OD2	2.51	0.43
1:A:321:ARG:NH2	1:A:539:ARG:OXT	2.52	0.43
1:B:156:LEU:CD2	1:B:204:ILE:HG13	2.49	0.43
1:A:51:ILE:CG2	1:A:344:PHE:CZ	3.01	0.43
1:A:174:ARG:HB2	1:A:179:VAL:HG22	2.01	0.43
1:A:251:HIS:O	1:A:255:ARG:C	2.62	0.43
1:A:399:LEU:HB3	1:A:479:ILE:HD13	2.01	0.43
1:B:64:GLY:HA2	1:B:69:TYR:CE2	2.53	0.43
1:B:131:ARG:HD3	1:B:131:ARG:HA	1.63	0.43
1:B:312:ALA:HA	1:B:315:GLN:OE1	2.18	0.43
1:B:345:PHE:O	1:B:348:LYS:HB2	2.19	0.43
1:B:378:LEU:CD2	2:B:764:HOH:O	2.67	0.43
1:B:179:VAL:O	1:B:180:GLU:C	2.62	0.42
1:B:307:ALA:CB	1:B:385:ARG:CZ	2.95	0.42
1:B:310:LEU:HA	1:B:313:ILE:HD11	2.01	0.42
1:A:48:SER:C	1:A:50:GLU:N	2.77	0.42
1:B:22:VAL:HG23	2:B:540:HOH:O	2.19	0.42
1:A:82:GLU:HG2	1:A:83:VAL:N	2.35	0.42
1:A:143:ALA:O	1:A:145:PRO:HD3	2.19	0.42
1:A:249:GLU:HG3	1:B:345:PHE:CD2	2.54	0.42
1:A:340:ASP:CG	1:A:341:ASN:H	2.27	0.42
1:A:525:GLU:O	1:A:528:ARG:HG3	2.19	0.42
1:A:530:ILE:CG2	1:A:536:ILE:HB	2.49	0.42
1:B:195:LEU:HD13	1:B:200:GLY:HA2	2.00	0.42
1:A:16:ASP:OD1	1:A:16:ASP:N	2.49	0.42
1:A:81:LYS:HA	2:A:673:HOH:O	2.20	0.42
1:A:532:ARG:C	1:A:534:THR:H	2.28	0.42
1:A:77:VAL:CB	1:A:85:LEU:HD13	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HE	1:A:240:ARG:HB3	1.66	0.42
1:A:370:ILE:HG23	1:B:432:THR:CG2	2.49	0.42
1:A:513:ASP:O	1:A:517:VAL:HG23	2.20	0.42
1:B:191:GLU:HG3	1:B:192:PRO:HD2	2.00	0.42
1:B:308:TYR:N	1:B:308:TYR:CD1	2.87	0.42
1:A:47:LYS:NZ	1:A:346:GLU:HG2	2.34	0.42
1:A:48:SER:O	1:A:50:GLU:N	2.53	0.42
1:A:131:ARG:HD2	1:A:135:TYR:CE1	2.55	0.42
1:B:51:ILE:HG21	1:B:344:PHE:HZ	1.85	0.42
1:B:431:SER:HA	1:B:446:SER:O	2.20	0.42
1:A:79:LYS:O	1:A:81:LYS:N	2.53	0.42
1:B:326:HIS:HD2	2:B:681:HOH:O	2.03	0.42
1:B:342:PRO:HB2	1:B:350:ILE:CG2	2.50	0.42
1:B:508:ARG:O	1:B:510:MET:HG2	2.20	0.42
1:A:276:LEU:HD22	1:A:482:ARG:HG2	2.03	0.41
1:A:297:VAL:HG22	1:B:75:MET:HE1	2.01	0.41
1:B:74:TYR:CE2	1:B:75:MET:HG2	2.54	0.41
1:A:127:ILE:HD13	1:A:127:ILE:HA	1.89	0.41
1:A:129:LEU:HD12	1:A:129:LEU:N	2.33	0.41
1:B:134:GLN:O	1:B:138:GLU:HG3	2.19	0.41
1:A:146:GLU:CD	1:A:456:ARG:HH12	2.25	0.41
1:A:313:ILE:CB	1:A:314:PRO:HD3	2.45	0.41
1:B:168:GLY:HA2	1:B:181:THR:HG22	2.02	0.41
1:A:174:ARG:O	1:A:175:ASP:C	2.64	0.41
1:B:63:TYR:CD1	1:B:73:ILE:HD12	2.55	0.41
1:B:71:ALA:N	1:B:438:ASN:HD21	2.08	0.41
1:B:72:MET:HE3	1:B:72:MET:HB2	1.80	0.41
1:B:177:ARG:HG2	1:B:177:ARG:HH11	1.85	0.41
1:B:291:LYS:C	1:B:293:ALA:N	2.77	0.41
1:B:498:ARG:HA	1:B:498:ARG:HE	1.84	0.41
1:A:81:LYS:O	1:A:82:GLU:C	2.63	0.41
1:A:69:TYR:CG	1:A:89:LEU:HD13	2.55	0.41
1:A:413:ALA:O	1:A:416:PRO:HG2	2.21	0.41
1:B:251:HIS:CD2	1:B:260:GLN:HG2	2.52	0.41
1:A:196:ARG:CA	1:A:199:GLU:HG3	2.51	0.41
1:A:270:LEU:O	1:A:489:ALA:HB3	2.21	0.41
1:B:205:ASN:ND2	1:B:356:PHE:HD2	2.13	0.41
1:B:239:VAL:O	1:B:240:ARG:HB2	2.20	0.41
1:B:274:SER:CB	1:B:487:SER:HB3	2.50	0.41
1:B:400:VAL:HG22	1:B:409:GLY:HA3	2.01	0.41
1:A:38:PRO:O	1:A:39:ALA:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ALA:CB	1:A:144:ILE:HD12	2.51	0.41
1:A:125:ARG:HH12	1:A:196:ARG:CG	2.12	0.41
1:A:157:ALA:HB3	1:A:158:PRO:HD3	2.03	0.41
1:A:201:LEU:O	1:A:205:ASN:CB	2.68	0.41
1:A:311:ARG:HD2	1:B:353:GLY:O	2.21	0.41
1:A:379:ALA:O	1:A:382:GLN:HB2	2.21	0.41
1:B:124:VAL:HG12	1:B:125:ARG:N	2.35	0.41
1:B:400:VAL:HG22	1:B:409:GLY:CA	2.51	0.41
1:A:55:ILE:CG2	1:A:60:ILE:HD11	2.51	0.41
1:A:359:GLN:N	1:A:360:PRO:HD2	2.33	0.41
1:B:252:ASP:OD1	1:B:261:ILE:HG23	2.20	0.41
1:B:528:ARG:C	1:B:530:ILE:N	2.78	0.41
1:A:34:THR:HA	1:A:137:ASN:HD21	1.86	0.40
1:A:35:VAL:O	1:A:35:VAL:HG23	2.19	0.40
1:A:131:ARG:HA	1:A:131:ARG:HD3	1.84	0.40
1:A:344:PHE:CD2	1:A:344:PHE:C	2.98	0.40
1:A:370:ILE:HG23	1:B:432:THR:HG23	2.01	0.40
1:B:134:GLN:HE22	1:B:190:ILE:HD11	1.86	0.40
1:A:29:ALA:HA	1:A:107:ARG:HE	1.86	0.40
1:A:530:ILE:O	1:A:534:THR:CB	2.61	0.40
1:A:534:THR:O	1:A:535:ASP:CG	2.64	0.40
1:B:82:GLU:OE1	1:B:83:VAL:HG23	2.22	0.40
1:A:48:SER:C	1:A:50:GLU:H	2.29	0.40
1:A:155:ASP:O	1:A:158:PRO:HG2	2.21	0.40
1:A:66:THR:C	1:A:67:THR:CG2	2.93	0.40
1:A:501:VAL:HG23	1:A:516:LEU:HD23	2.03	0.40
1:B:140:ILE:O	1:B:140:ILE:HG22	2.21	0.40
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.94	0.40
1:B:379:ALA:HA	1:B:382:GLN:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:TYR:OH	2:A:710:HOH:O[2_555]	1.93	0.27

5.3 Torsion angles

5.3.1 Protein backbone

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	522/537 (97%)	474 (91%)	43 (8%)	5 (1%)	12	11
1	B	522/537 (97%)	484 (93%)	38 (7%)	0	100	100
All	All	1044/1074 (97%)	958 (92%)	81 (8%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	A	49	ARG
1	A	80	SER
1	A	192	PRO
1	A	62	ILE

5.3.2 Protein sidechains

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	415/424 (98%)	368 (89%)	47 (11%)	5	5
1	B	415/424 (98%)	378 (91%)	37 (9%)	9	10
All	All	830/848 (98%)	746 (90%)	84 (10%)	7	7

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	18	GLU
1	A	19	THR
1	A	20	LEU
1	A	37	VAL
1	A	42	ILE
1	A	47	LYS
1	A	50	GLU
1	A	57	GLU
1	A	60	ILE
1	A	72	MET
1	A	79	LYS
1	A	82	GLU
1	A	85	LEU
1	A	113	ARG
1	A	127	ILE
1	A	140	ILE
1	A	160	SER
1	A	164	SER
1	A	174	ARG
1	A	179	VAL
1	A	188	ARG
1	A	191	GLU
1	A	204	ILE
1	A	235	LEU
1	A	239	VAL
1	A	243	THR
1	A	268	ARG
1	A	271	MET
1	A	277	THR
1	A	286	GLU
1	A	295	LYS
1	A	297	VAL
1	A	301	GLU
1	A	380	GLU
1	A	385	ARG
1	A	443	ASP
1	A	479	ILE
1	A	495	GLU
1	A	498	ARG
1	A	500	LEU
1	A	503	THR
1	A	508	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	513	ASP
1	A	515	GLU
1	A	535	ASP
1	A	536	ILE
1	B	23	GLU
1	B	35	VAL
1	B	40	GLU
1	B	57	GLU
1	B	60	ILE
1	B	72	MET
1	B	79	LYS
1	B	82	GLU
1	B	127	ILE
1	B	128	ILE
1	B	131	ARG
1	B	134	GLN
1	B	160	SER
1	B	164	SER
1	B	166	LEU
1	B	172	VAL
1	B	174	ARG
1	B	198	LYS
1	B	199	GLU
1	B	204	ILE
1	B	286	GLU
1	B	292	GLU
1	B	295	LYS
1	B	297	VAL
1	B	302	ILE
1	B	309	SER
1	B	321	ARG
1	B	339	ASN
1	B	380	GLU
1	B	386	VAL
1	B	443	ASP
1	B	444	VAL
1	B	464	LYS
1	B	479	ILE
1	B	497	VAL
1	B	515	GLU
1	B	534	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	137	ASN
1	A	161	HIS
1	A	227	GLN
1	A	257	HIS
1	A	298	GLN
1	A	305	GLN
1	A	326	HIS
1	A	329	HIS
1	A	355	ASN
1	A	438	ASN
1	A	441	ASN
1	A	442	GLN
1	B	46	GLN
1	B	134	GLN
1	B	137	ASN
1	B	161	HIS
1	B	183	GLN
1	B	227	GLN
1	B	251	HIS
1	B	326	HIS
1	B	339	ASN
1	B	407	HIS
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	A	152	1	11,13,14	2.87	6 (54%)	15,18,20	2.35	4 (26%)
1	MDO	B	152	1	11,13,14	2.66	5 (45%)	15,18,20	2.31	3 (20%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	MDO	O2-C2	6.56	1.36	1.23
1	A	152	MDO	O2-C2	6.52	1.36	1.23
1	B	152	MDO	CA2-N2	-3.28	1.33	1.39
1	A	152	MDO	CA1-N1	-3.27	1.37	1.48
1	A	152	MDO	CA2-N2	-3.20	1.33	1.39
1	A	152	MDO	C2-N3	-3.03	1.33	1.40
1	B	152	MDO	C2-N3	-2.93	1.33	1.40
1	A	152	MDO	O3-C3	2.42	1.33	1.20
1	A	152	MDO	C1-N3	-2.37	1.33	1.37
1	B	152	MDO	C1-N3	-2.20	1.33	1.37
1	B	152	MDO	O3-C3	2.12	1.32	1.20

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MDO	O2-C2-CA2	-7.18	126.44	131.02
1	A	152	MDO	O2-C2-CA2	-6.44	126.91	131.02
1	B	152	MDO	CA2-C2-N3	3.52	106.46	103.50
1	A	152	MDO	CA2-C2-N3	3.46	106.41	103.50
1	A	152	MDO	C1-CA1-N1	-3.11	99.98	109.13
1	A	152	MDO	CB-CA1-N1	3.00	120.07	109.98
1	B	152	MDO	O3-C3-CA3	2.39	136.25	125.47

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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	152	MDO	5	0
1	B	152	MDO	3	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 ⓘ

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, 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	526/537 (97%)	0.47	14 (2%) 56 53	18, 41, 62, 73	0
1	B	526/537 (97%)	0.21	3 (0%) 85 83	18, 35, 55, 84	0
All	All	1052/1074 (97%)	0.34	17 (1%) 70 67	18, 38, 61, 84	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	ALA	4.6
1	A	38	PRO	3.2
1	A	344	PHE	3.2
1	A	42	ILE	3.1
1	A	77	VAL	3.1
1	A	43	ALA	2.8
1	A	17	GLY	2.7
1	B	297	VAL	2.7
1	A	195	LEU	2.6
1	A	52	PHE	2.5
1	A	137	ASN	2.5
1	A	393	TYR	2.4
1	A	37	VAL	2.4
1	A	174	ARG	2.2
1	A	41	SER	2.1
1	B	294	GLY	2.0
1	A	51	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
1	MDO	B	152	13/14	0.89	0.09	27,31,34,34	0
1	MDO	A	152	13/14	0.91	0.09	28,30,36,38	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.