



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:17 PM UTC

PDB ID : 2WO0 / pdb_00002wo0
Title : EDTA treated E. coli copper amine oxidase
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Deposited on : 2009-07-21
Resolution : 2.60 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

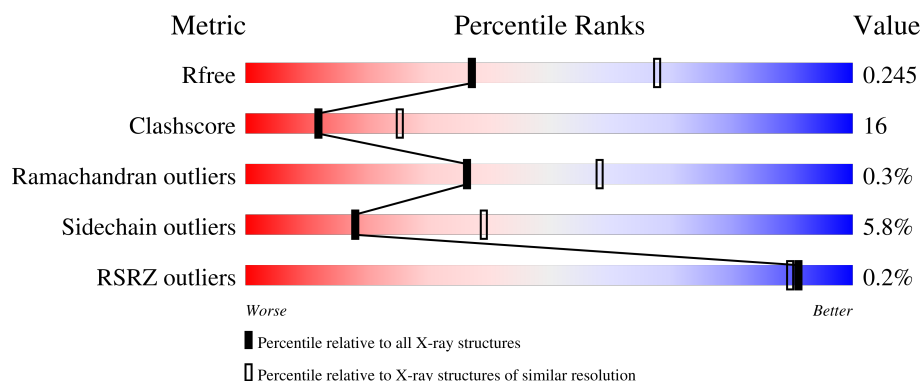
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	727	 70% 26% ..
1	B	727	 68% 27% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11792 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 PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	1	1
			5676	3610	965	1079	22			
1	B	721	Total	C	N	O	S	0	4	1
			5710	3634	970	1081	25			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		

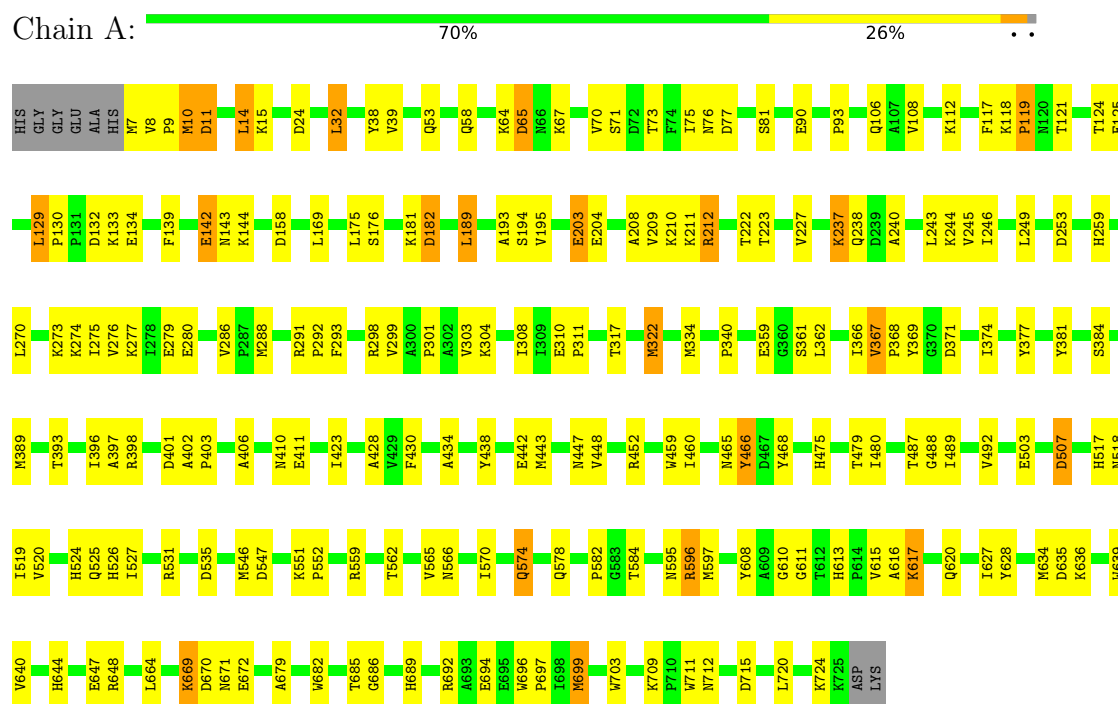
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	239	Total	O	0	0
			239	239		
4	B	161	Total	O	0	0
			161	161		

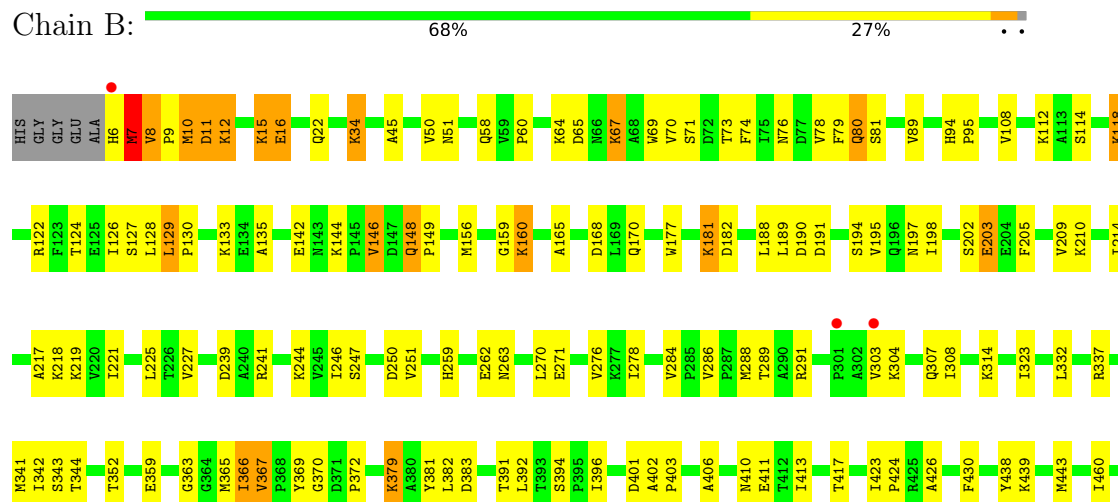
3 Residue-property plots [i](#)

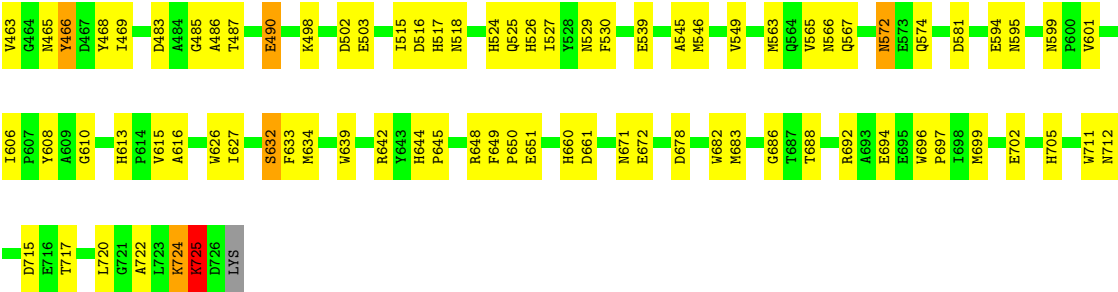
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PRIMARY AMINE OXIDASE



• Molecule 1: PRIMARY AMINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.68Å 166.62Å 79.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.52 – 2.60 39.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.52-2.60) 99.8 (39.52-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.182 , 0.248 0.185 , 0.245	Depositor DCC
R_{free} test set	1920 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11792	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: CU, TPQ, NA

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	0.85	1/5794 (0.0%)	1.09	17/7888 (0.2%)
1	B	0.80	1/5838 (0.0%)	1.07	15/7945 (0.2%)
All	All	0.82	2/11632 (0.0%)	1.08	32/15833 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	724	LYS	C-N	-6.50	1.24	1.33
1	B	725	LYS	C-N	-6.13	1.24	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLN	CA-C-N	8.04	128.04	119.76
1	A	53	GLN	C-N-CA	8.04	128.04	119.76
1	B	118	LYS	CA-C-N	7.82	127.54	119.56
1	B	118	LYS	C-N-CA	7.82	127.54	119.56
1	B	394	SER	CA-C-N	-7.30	112.24	119.76
1	B	394	SER	C-N-CA	-7.30	112.24	119.76
1	A	709	LYS	CA-C-N	-7.28	112.27	119.76
1	A	709	LYS	C-N-CA	-7.28	112.27	119.76
1	B	367	VAL	CA-C-N	6.88	128.44	119.84
1	B	367	VAL	C-N-CA	6.88	128.44	119.84
1	A	310	GLU	CA-C-N	6.77	126.40	119.56
1	A	310	GLU	C-N-CA	6.77	126.40	119.56
1	A	119	PRO	CA-C-N	-6.54	111.80	122.65
1	A	119	PRO	C-N-CA	-6.54	111.80	122.65
1	A	367	VAL	CA-C-N	6.36	127.79	119.84
1	A	367	VAL	C-N-CA	6.36	127.79	119.84
1	B	247	SER	N-CA-C	5.96	119.26	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	VAL	CA-C-N	-5.91	113.44	119.83
1	B	284	VAL	C-N-CA	-5.91	113.44	119.83
1	B	7	MET	N-CA-C	5.91	116.08	108.34
1	B	606	ILE	CA-C-N	5.86	125.48	119.56
1	B	606	ILE	C-N-CA	5.86	125.48	119.56
1	B	58	GLN	N-CA-C	-5.73	104.95	111.14
1	A	507	ASP	N-CA-C	-5.64	105.21	111.36
1	B	572	ASN	N-CA-C	5.18	116.68	108.96
1	A	182	ASP	N-CA-CB	-5.13	108.33	114.17
1	A	238	GLN	N-CA-C	5.13	116.95	111.36
1	A	699	MET	CA-C-N	5.11	125.40	119.93
1	A	699	MET	C-N-CA	5.11	125.40	119.93
1	A	291	ARG	CA-C-N	-5.11	115.31	120.31
1	A	291	ARG	C-N-CA	-5.11	115.31	120.31
1	B	417	THR	N-CA-C	-5.04	106.72	112.92

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	5676	0	5546	184	0
1	B	5710	0	5591	184	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	239	0	0	23	0
4	B	161	0	0	17	0
All	All	11792	0	11137	352	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 16.

All (352) 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:490:GLU:HG2	1:B:699[B]:MET:CE	1.20	1.64
1:B:490:GLU:CG	1:B:699[B]:MET:HE3	1.33	1.52
1:B:443[B]:MET:HE2	4:B:2102:HOH:O	1.26	1.32
1:B:129:LEU:CD1	1:B:130:PRO:HD2	1.70	1.21
1:B:490:GLU:CG	1:B:699[B]:MET:CE	2.06	1.10
1:B:221:ILE:CD1	1:B:250:ASP:HB2	1.81	1.07
1:B:291:ARG:NH1	1:B:516:ASP:OD2	1.87	1.07
1:A:11:ASP:OD1	1:A:15:LYS:HE3	1.55	1.04
1:B:129:LEU:HD13	1:B:130:PRO:HD2	1.39	0.98
1:B:10:MET:HG3	1:B:70:VAL:HG13	1.45	0.98
1:B:129:LEU:HD12	1:B:130:PRO:CD	1.94	0.97
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.65	0.97
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.44	0.96
1:B:443[B]:MET:CE	4:B:2102:HOH:O	1.92	0.94
1:A:8:VAL:HG22	1:A:9:PRO:HD2	1.48	0.93
1:B:221:ILE:HD13	1:B:250:ASP:HB2	1.52	0.89
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.54	0.87
1:B:10:MET:HG3	1:B:70:VAL:CG1	2.05	0.87
1:B:129:LEU:CD1	1:B:130:PRO:CD	2.52	0.86
1:B:546:MET:HE1	4:B:2041:HOH:O	1.76	0.85
1:A:124:THR:HB	4:A:2041:HOH:O	1.77	0.85
1:A:552:PRO:HD2	4:A:2192:HOH:O	1.77	0.85
1:A:7:MET:HE2	1:A:7:MET:HA	1.60	0.84
1:B:129:LEU:HD12	1:B:130:PRO:N	1.94	0.83
1:A:574:GLN:HG3	1:A:671:ASN:CG	2.05	0.82
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.60	0.82
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.59	0.81
1:A:465:ASN:C	1:A:466[B]:TPQ:CA	2.53	0.81
1:B:304:LYS:O	4:B:2055:HOH:O	1.99	0.81
1:A:368:PRO:HG3	1:A:634:MET:HE1	1.62	0.79
1:A:616:ALA:HA	4:A:2228:HOH:O	1.81	0.79
1:B:76:ASN:O	1:B:80:GLN:HB2	1.82	0.78
1:A:7:MET:HE2	1:A:7:MET:CA	2.13	0.78
1:B:129:LEU:HD12	1:B:129:LEU:C	2.08	0.78
1:B:359:GLU:CD	1:B:648:ARG:HH22	1.92	0.77
1:A:237:LYS:HE3	1:A:240:ALA:HB2	1.67	0.76
1:B:149:PRO:HB3	1:B:170:GLN:OE1	1.86	0.75
1:A:189:LEU:HD13	4:A:2055:HOH:O	1.85	0.75
1:A:129:LEU:HD12	1:A:130:PRO:HD2	1.68	0.75
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.69	0.75
1:B:11:ASP:OD2	1:B:15:LYS:HE3	1.88	0.73
1:B:291:ARG:CD	4:B:2052:HOH:O	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ASP:HB3	4:A:2188:HOH:O	1.89	0.72
1:A:669:LYS:HD2	1:A:670:ASP:OD1	1.90	0.72
1:B:490:GLU:CG	1:B:699[B]:MET:HE2	2.15	0.72
1:B:546:MET:CE	4:B:2041:HOH:O	2.34	0.72
1:A:7:MET:HE2	1:A:7:MET:N	2.06	0.70
1:A:129:LEU:HD12	1:A:129:LEU:C	2.16	0.70
1:B:45:ALA:O	1:B:60:PRO:HB3	1.92	0.70
1:B:291:ARG:NH1	1:B:516:ASP:CG	2.50	0.69
1:B:225:LEU:HD12	1:B:246:ILE:HG12	1.75	0.69
1:A:134:GLU:CG	4:A:2045:HOH:O	2.39	0.69
1:A:527:ILE:CD1	1:A:634:MET:HE2	2.23	0.68
1:B:465:ASN:HD21	1:B:466[B]:TPQ:C3	2.06	0.68
1:B:574:GLN:HB2	1:B:671:ASN:OD1	1.94	0.67
1:A:322:MET:HE1	4:A:2024:HOH:O	1.94	0.67
1:A:584:THR:HG22	4:A:2188:HOH:O	1.94	0.67
1:A:8:VAL:CG2	1:A:9:PRO:HD2	2.22	0.67
1:A:527:ILE:HD12	1:A:634:MET:HE2	1.76	0.66
1:B:8:VAL:HG23	1:B:9:PRO:CD	2.25	0.66
1:A:77:ASP:O	1:A:81:SER:HB3	1.94	0.66
1:B:402:ALA:HB1	1:B:403:PRO:HD2	1.77	0.66
1:B:369:TYR:CD2	1:B:524:HIS:HB3	2.30	0.66
1:B:12:LYS:O	1:B:16:GLU:HG2	1.96	0.66
1:B:251:VAL:O	1:B:251:VAL:CG1	2.44	0.65
1:A:181:LYS:O	1:A:182:ASP:HB2	1.95	0.65
1:B:78:VAL:O	1:B:81:SER:HB3	1.96	0.65
1:B:382:LEU:N	1:B:382:LEU:HD12	2.11	0.65
1:B:466[B]:TPQ:H	1:B:466[B]:TPQ:C6	2.08	0.64
1:A:672:GLU:HB3	4:A:2226:HOH:O	1.97	0.64
1:B:644:HIS:ND1	1:B:645:PRO:HD2	2.13	0.64
1:A:366:ILE:HG21	1:A:634:MET:HE3	1.78	0.63
1:A:129:LEU:CD1	1:A:130:PRO:HD2	2.28	0.63
1:A:203:GLU:OE1	1:A:204:GLU:HB2	1.99	0.63
1:A:134:GLU:HG2	4:A:2045:HOH:O	1.95	0.63
1:B:549:VAL:HA	4:B:2124:HOH:O	1.98	0.63
1:A:203:GLU:CD	1:A:204:GLU:H	2.06	0.62
1:B:490:GLU:CD	1:B:699[B]:MET:CE	2.72	0.62
1:A:574:GLN:CG	1:A:671:ASN:CG	2.72	0.62
1:A:292:PRO:HD2	4:A:2101:HOH:O	1.99	0.62
1:B:6:HIS:C	1:B:7:MET:HG2	2.23	0.61
1:A:299:VAL:HG23	1:B:724:LYS:HD2	1.83	0.61
1:B:251:VAL:O	1:B:251:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASP:OD1	1:A:15:LYS:CE	2.42	0.61
1:A:129:LEU:HD12	1:A:130:PRO:CD	2.30	0.61
1:B:108:VAL:O	1:B:112:LYS:HG3	2.00	0.61
1:B:490:GLU:HG3	1:B:699[B]:MET:HE3	1.69	0.61
1:B:486:ALA:O	1:B:699[A]:MET:HE3	2.02	0.60
1:A:517:HIS:O	1:A:518:ASN:HB2	2.00	0.60
1:A:142:GLU:O	1:A:143:ASN:HB2	2.02	0.60
1:B:365:MET:HE2	1:B:383:ASP:OD2	2.02	0.60
1:A:466[B]:TPQ:H6	1:A:487:THR:O	2.02	0.60
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.48	0.60
1:B:291:ARG:HH12	1:B:516:ASP:CG	2.09	0.60
1:A:574:GLN:HG3	1:A:671:ASN:ND2	2.16	0.60
1:B:262:GLU:O	1:B:263:ASN:HB2	2.01	0.59
1:B:366:ILE:HD12	1:B:382:LEU:CD1	2.32	0.59
1:A:7:MET:N	4:A:2001:HOH:O	2.33	0.59
1:B:209:VAL:HG13	1:B:214:ILE:HB	1.83	0.59
1:A:286:VAL:HB	1:A:288:MET:HE3	1.84	0.59
1:B:366:ILE:HD12	1:B:382:LEU:HD11	1.85	0.59
1:B:595:ASN:HB2	1:B:715:ASP:OD1	2.02	0.58
1:A:635:ASP:O	1:A:636:LYS:HD3	2.03	0.58
1:B:642:ARG:HD2	1:B:672:GLU:HB3	1.84	0.58
1:A:368:PRO:HG3	1:A:634:MET:CE	2.33	0.58
1:A:366:ILE:CG2	1:A:634:MET:HE3	2.34	0.58
1:A:367:VAL:HG21	1:A:468:TYR:OH	2.04	0.57
1:B:203:GLU:CD	1:B:203:GLU:H	2.12	0.57
1:B:483:ASP:CG	1:B:705:HIS:HD1	2.12	0.57
1:B:517:HIS:O	1:B:518:ASN:HB2	2.05	0.57
1:B:443[B]:MET:HE3	1:B:443[B]:MET:HA	1.87	0.57
1:B:168:ASP:OD1	1:B:168:ASP:C	2.47	0.57
1:B:632:SER:OG	1:B:661:ASP:OD2	2.23	0.57
1:B:396:ILE:HG23	1:B:401:ASP:HB2	1.87	0.57
1:A:194:SER:O	1:A:195:VAL:C	2.49	0.56
1:A:212:ARG:HH21	1:A:280:GLU:HB3	1.71	0.56
1:A:369:TYR:CD2	1:A:524:HIS:HB3	2.41	0.56
1:A:64:LYS:O	1:A:65:ASP:HB3	2.06	0.56
1:B:135:ALA:HB1	1:B:146:VAL:CG2	2.35	0.56
1:B:574:GLN:CB	1:B:671:ASN:OD1	2.54	0.56
1:A:546:MET:HE3	1:A:565:VAL:HG11	1.87	0.56
1:A:10:MET:HG2	1:A:14:LEU:CD2	2.36	0.56
1:A:492:VAL:HB	1:A:519:ILE:HG23	1.88	0.55
1:A:527:ILE:HD12	1:A:634:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:HG13	1:B:367:VAL:N	2.22	0.55
1:A:565:VAL:N	4:A:2197:HOH:O	2.28	0.54
1:A:249:LEU:CD2	1:A:288:MET:HE1	2.38	0.54
1:A:597:MET:SD	1:B:516:ASP:HA	2.48	0.54
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.43	0.54
1:B:539:GLU:O	1:B:678:ASP:HA	2.07	0.54
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.90	0.54
1:B:203:GLU:CD	1:B:203:GLU:N	2.66	0.54
1:A:596:ARG:NH2	1:B:516:ASP:OD1	2.41	0.54
1:A:299:VAL:CG2	1:B:724:LYS:HD2	2.38	0.54
1:A:610:GLY:HA3	1:B:610:GLY:HA3	1.90	0.53
1:B:221:ILE:CD1	1:B:250:ASP:CB	2.72	0.53
1:A:124:THR:CB	4:A:2041:HOH:O	2.45	0.53
1:A:466[A]:TPQ:HB3	1:A:468:TYR:CE2	2.43	0.53
1:A:223:THR:HG22	1:A:246:ILE:HB	1.91	0.53
1:B:194:SER:O	1:B:198:ILE:HG13	2.09	0.53
1:A:212:ARG:NH2	1:A:280:GLU:HB3	2.24	0.53
1:A:334:MET:HE1	1:A:393:THR:OG1	2.09	0.53
1:A:384:SER:HA	1:A:389:MET:HG3	1.91	0.52
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.90	0.52
1:A:286:VAL:HG12	1:A:288:MET:CE	2.39	0.52
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.45	0.52
1:A:286:VAL:CG1	1:A:288:MET:CE	2.88	0.52
1:B:381:TYR:CE1	1:B:466[B]:TPQ:O4	2.63	0.52
1:A:465:ASN:O	1:A:466[B]:TPQ:HA	2.10	0.52
1:B:332:LEU:HD13	1:B:342:ILE:CD1	2.40	0.52
1:B:225:LEU:CD1	1:B:246:ILE:HG12	2.39	0.52
1:B:202:SER:HB3	1:B:205:PHE:HB3	1.90	0.52
1:B:466[A]:TPQ:H6	1:B:487:THR:O	2.09	0.52
1:A:692:ARG:HG3	1:A:694:GLU:OE1	2.10	0.51
1:A:664:LEU:HD21	1:A:682:TRP:CD2	2.46	0.51
1:B:122:ARG:NH1	1:B:190:ASP:OD1	2.40	0.51
1:A:158:ASP:OD1	1:A:158:ASP:C	2.50	0.51
1:A:7:MET:HA	1:A:7:MET:CE	2.37	0.51
1:A:10:MET:HG3	1:A:70:VAL:CG1	2.40	0.51
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.92	0.51
1:A:273:LYS:O	1:A:274:LYS:HB3	2.10	0.51
1:B:7:MET:C	1:B:8:VAL:HG12	2.35	0.51
1:B:135:ALA:HB1	1:B:146:VAL:HG22	1.91	0.51
1:A:562:THR:HG21	1:B:372:PRO:HG3	1.93	0.51
1:B:724:LYS:O	1:B:725:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ILE:HG12	1:B:469:ILE:HG12	1.94	0.50
1:B:8:VAL:HG23	1:B:9:PRO:N	2.26	0.50
1:A:227:VAL:CG1	1:A:244:LYS:HG3	2.38	0.50
1:B:64:LYS:O	1:B:65:ASP:HB2	2.12	0.50
1:B:129:LEU:CD1	1:B:129:LEU:C	2.82	0.50
1:B:369:TYR:OH	1:B:466[B]:TPQ:H3	2.12	0.50
1:B:146:VAL:HG12	1:B:146:VAL:O	2.11	0.49
1:B:160:LYS:HE2	1:B:239:ASP:O	2.12	0.49
1:A:465:ASN:HB2	1:A:489:ILE:O	2.12	0.49
1:A:32:LEU:HB2	1:A:39:VAL:HB	1.92	0.49
1:A:7:MET:HE1	1:A:71:SER:HA	1.93	0.49
1:A:368:PRO:CG	1:A:634:MET:HE1	2.39	0.49
1:B:410:ASN:OD1	1:B:424:PRO:HA	2.13	0.49
1:A:10:MET:HG2	1:A:14:LEU:HD23	1.93	0.49
1:B:337:ARG:HD3	1:B:649:PHE:CE1	2.47	0.49
1:A:531:ARG:HD2	1:A:682:TRP:CH2	2.48	0.49
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.94	0.49
1:A:582:PRO:HB2	1:B:615:VAL:HG12	1.94	0.49
1:B:490:GLU:CD	1:B:699[B]:MET:HE2	2.37	0.49
1:B:127:SER:O	1:B:128:LEU:C	2.56	0.49
1:B:717:THR:HB	1:B:720:LEU:HG	1.95	0.49
1:A:301:PRO:HA	4:A:2103:HOH:O	2.13	0.48
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.38	0.48
1:B:10:MET:HG3	1:B:70:VAL:HG11	1.93	0.48
1:A:208:ALA:O	1:A:211:LYS:HB2	2.13	0.48
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.14	0.48
1:B:529:ASN:HA	1:B:683:MET:O	2.13	0.48
1:A:410:ASN:C	1:A:411:GLU:HG2	2.37	0.48
1:B:221:ILE:HD11	1:B:250:ASP:CB	2.34	0.48
1:B:711:TRP:O	1:B:712:ASN:HB2	2.13	0.48
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.44	0.48
1:B:410:ASN:C	1:B:411:GLU:HG2	2.39	0.48
1:A:134:GLU:HG3	4:A:2045:HOH:O	2.07	0.47
1:A:203:GLU:CG	1:A:204:GLU:N	2.77	0.47
1:A:359:GLU:CD	1:A:648:ARG:HH22	2.22	0.47
1:B:94:HIS:CG	1:B:95:PRO:HD2	2.49	0.47
1:A:117:PHE:CZ	1:A:121:THR:HB	2.49	0.47
1:B:546:MET:HB3	1:B:565:VAL:HG11	1.95	0.47
1:A:507:ASP:HB2	4:A:2181:HOH:O	2.14	0.47
1:B:7:MET:HE3	1:B:70:VAL:C	2.40	0.47
1:A:10:MET:HG3	1:A:70:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASN:O	1:A:466[B]:TPQ:CA	2.63	0.47
1:A:617:LYS:HD3	4:B:2134:HOH:O	2.14	0.47
1:B:67:LYS:HE2	1:B:67:LYS:HB3	1.75	0.47
1:B:286:VAL:O	1:B:288:MET:HG2	2.13	0.47
1:B:660:HIS:ND1	1:B:660:HIS:N	2.62	0.47
1:A:397:ALA:O	1:A:398:ARG:C	2.58	0.47
1:B:566:ASN:HB3	4:B:2129:HOH:O	2.14	0.46
1:A:487:THR:OG1	1:A:488:GLY:N	2.48	0.46
1:A:223:THR:CG2	1:A:246:ILE:HB	2.45	0.46
1:B:644:HIS:ND1	1:B:645:PRO:CD	2.77	0.46
1:B:545:ALA:O	1:B:567:GLN:HA	2.15	0.46
1:A:129:LEU:HD12	1:A:130:PRO:N	2.30	0.46
1:B:7:MET:HE3	1:B:7:MET:HB3	1.63	0.46
1:B:159:GLY:C	1:B:271:GLU:OE2	2.59	0.46
1:B:574:GLN:N	1:B:671:ASN:OD1	2.39	0.46
1:A:443:MET:CE	1:B:392:LEU:CD2	2.94	0.46
1:B:156:MET:HE1	1:B:177:TRP:CZ3	2.50	0.46
1:A:24:ASP:OD1	1:A:24:ASP:C	2.59	0.46
1:A:90:GLU:CD	1:A:93:PRO:HA	2.40	0.46
1:B:259:HIS:HE1	1:B:289:THR:O	1.99	0.46
1:B:696:TRP:CD2	1:B:697:PRO:HA	2.50	0.46
1:A:381:TYR:CG	1:A:466[A]:TPQ:O5	2.69	0.45
1:A:396:ILE:HD13	1:A:428:ALA:HB2	1.98	0.45
1:B:438:TYR:CD1	1:B:438:TYR:C	2.95	0.45
1:A:393:THR:HB	1:A:423:ILE:HD13	1.97	0.45
1:B:181:LYS:O	1:B:182:ASP:HB2	2.15	0.45
1:A:562:THR:CG2	1:B:372:PRO:HG3	2.46	0.45
1:B:239:ASP:OD1	1:B:239:ASP:C	2.58	0.45
1:B:406:ALA:HA	1:B:430:PHE:HB3	1.98	0.45
1:A:611:GLY:HA2	1:A:703:TRP:O	2.17	0.45
1:B:50:VAL:O	1:B:51:ASN:C	2.59	0.45
1:B:382:LEU:HD23	1:B:651:GLU:HG3	1.98	0.45
1:A:65:ASP:CG	1:A:65:ASP:O	2.60	0.45
1:A:670:ASP:O	1:A:671:ASN:C	2.60	0.45
1:B:307:GLN:HG2	4:B:2056:HOH:O	2.16	0.45
1:A:361:SER:O	1:A:362:LEU:C	2.60	0.45
1:B:67:LYS:HE2	1:B:69:TRP:HE1	1.82	0.45
1:B:615:VAL:HG22	1:B:616:ALA:N	2.31	0.45
1:A:38:TYR:CG	1:A:311:PRO:HA	2.52	0.45
1:A:125:GLU:HA	4:A:2118:HOH:O	2.16	0.45
1:B:79:PHE:C	1:B:81:SER:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HB	4:B:2024:HOH:O	2.17	0.44
1:B:391:THR:HA	1:B:413:ILE:HD11	2.00	0.44
1:B:549:VAL:CA	4:B:2124:HOH:O	2.61	0.44
1:A:276:VAL:O	1:A:277:LYS:HB2	2.16	0.44
1:B:217:ALA:C	1:B:219:LYS:N	2.75	0.44
1:A:371:ASP:OD1	1:A:371:ASP:C	2.61	0.44
1:B:363:GLY:O	1:B:650:PRO:HD2	2.17	0.44
1:A:525:GLN:HE21	1:A:616:ALA:HB2	1.82	0.44
1:B:490:GLU:HG2	1:B:699[B]:MET:HE3	0.47	0.44
1:A:7:MET:CA	1:A:7:MET:CE	2.89	0.44
1:A:117:PHE:CD1	1:A:117:PHE:C	2.96	0.44
1:A:298:ARG:HA	1:B:722:ALA:O	2.18	0.44
1:A:398:ARG:HD3	4:A:2137:HOH:O	2.18	0.44
1:B:94:HIS:ND1	1:B:95:PRO:HD2	2.33	0.44
1:B:465:ASN:ND2	1:B:466[B]:TPQ:C3	2.78	0.44
1:B:498:LYS:N	1:B:502:ASP:OD2	2.47	0.44
1:A:210:LYS:O	1:A:211:LYS:C	2.61	0.44
1:A:76:ASN:O	1:A:77:ASP:C	2.60	0.44
1:A:106:GLN:NE2	1:A:169:LEU:O	2.38	0.43
1:A:442:GLU:HG3	4:A:2162:HOH:O	2.18	0.43
1:A:286:VAL:HG12	1:A:288:MET:HE2	2.00	0.43
1:B:148:GLN:HE21	1:B:148:GLN:HB3	1.56	0.43
1:A:689:HIS:HE1	1:A:699:MET:SD	2.40	0.43
1:A:696:TRP:CD2	1:A:697:PRO:HA	2.53	0.43
1:A:193:ALA:O	1:A:194:SER:C	2.61	0.43
1:A:222:THR:HG22	1:A:245:VAL:HG11	2.00	0.43
1:A:479:THR:HG22	1:A:480:ILE:N	2.33	0.43
1:A:559:ARG:HH22	1:B:370:GLY:HA2	1.83	0.43
1:A:570:ILE:HD13	1:A:578:GLN:HE22	1.84	0.43
1:A:628:TYR:CD1	1:A:628:TYR:C	2.97	0.43
1:B:124:THR:CB	4:B:2024:HOH:O	2.67	0.43
1:B:291:ARG:HD3	4:B:2052:HOH:O	2.10	0.43
1:B:367:VAL:HG21	1:B:468:TYR:OH	2.18	0.43
1:B:210:LYS:HA	1:B:214:ILE:O	2.19	0.43
1:B:423:ILE:HG22	1:B:426:ALA:HB2	2.01	0.43
1:B:642:ARG:CD	1:B:672:GLU:HB3	2.47	0.43
1:A:447:ASN:HB3	4:A:2165:HOH:O	2.18	0.42
1:B:382:LEU:N	1:B:382:LEU:CD1	2.81	0.42
1:B:633:PHE:HA	1:B:639:TRP:CZ2	2.55	0.42
1:A:620:GLN:HB2	1:B:563:MET:HE2	2.02	0.42
1:A:118:LYS:HA	1:A:119:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:HIS:O	1:B:686:GLY:HA2	2.19	0.42
1:A:644:HIS:HB3	1:A:647:GLU:HG3	2.02	0.42
1:A:133:LYS:CE	1:A:535:ASP:OD2	2.68	0.42
1:A:133:LYS:HE2	1:A:535:ASP:OD2	2.20	0.42
1:A:139:PHE:O	1:A:143:ASN:HA	2.20	0.42
1:A:303:VAL:HG12	1:A:304:LYS:O	2.19	0.42
1:A:243:LEU:HD12	1:A:270:LEU:HD11	2.01	0.42
1:A:253:ASP:OD2	1:A:259:HIS:NE2	2.38	0.42
1:A:402:ALA:HB1	1:A:403:PRO:HD2	2.02	0.42
1:A:525:GLN:NE2	1:A:616:ALA:CB	2.83	0.42
1:B:73:THR:O	1:B:74:PHE:C	2.60	0.42
1:B:214:ILE:HD11	1:B:286:VAL:HG21	2.02	0.42
1:B:341:MET:HE2	1:B:341:MET:HB3	1.88	0.42
1:B:485:GLY:HA2	1:B:702:GLU:O	2.20	0.42
1:B:530:PHE:O	1:B:682:TRP:HA	2.19	0.42
1:B:594:GLU:HA	1:B:599:ASN:O	2.19	0.42
1:A:377:TYR:CD1	1:A:377:TYR:C	2.97	0.42
1:A:293:PHE:CD1	1:A:293:PHE:C	2.98	0.42
1:A:434:ALA:HB3	1:A:452:ARG:HG2	2.00	0.42
1:B:246:ILE:HA	1:B:246:ILE:HD13	1.76	0.41
1:A:664:LEU:HD21	1:A:682:TRP:CG	2.56	0.41
1:B:724:LYS:C	1:B:725:LYS:HG2	2.45	0.41
1:A:460:ILE:HG21	1:B:439:LYS:HE2	2.02	0.41
1:A:475:HIS:CD2	1:A:475:HIS:N	2.88	0.41
1:B:8:VAL:CG2	1:B:9:PRO:N	2.81	0.41
1:B:725:LYS:N	4:B:2161:HOH:O	2.52	0.41
1:A:438:TYR:OH	1:A:720:LEU:HD23	2.19	0.41
1:A:466[B]:TPQ:O5	1:A:699:MET:SD	2.79	0.41
1:A:546:MET:HE2	1:A:546:MET:HB3	1.78	0.41
1:A:403:PRO:HG3	1:A:430:PHE:CE2	2.55	0.41
1:B:241:ARG:HG2	1:B:270:LEU:HD12	2.03	0.41
1:B:343:SER:O	1:B:344:THR:C	2.64	0.41
1:A:689:HIS:CE1	1:A:699:MET:SD	3.14	0.41
1:B:367:VAL:HG13	1:B:525:GLN:O	2.21	0.41
1:B:626:TRP:O	1:B:627:ILE:C	2.63	0.41
1:A:448:VAL:HA	4:A:2167:HOH:O	2.21	0.41
1:A:466[A]:TPQ:C6	1:A:466[A]:TPQ:H	2.33	0.41
1:A:640:VAL:CG1	1:A:679:ALA:HB1	2.51	0.41
1:A:212:ARG:HD3	4:A:2094:HOH:O	2.19	0.41
1:B:34:LYS:HA	4:B:2006:HOH:O	2.21	0.41
1:A:108:VAL:O	1:A:112:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:LEU:HD23	1:A:720:LEU:HA	1.82	0.41
1:B:156:MET:HE2	1:B:165:ALA:CB	2.51	0.41
1:B:188:LEU:O	1:B:191:ASP:HB2	2.20	0.41
1:B:527:ILE:HD12	1:B:634:MET:CG	2.51	0.41
1:A:308:ILE:HG12	1:B:308:ILE:HG12	2.02	0.41
1:B:581:ASP:C	1:B:581:ASP:OD1	2.63	0.41
1:A:367:VAL:HG13	1:A:525:GLN:O	2.20	0.40
1:A:406:ALA:HA	1:A:430:PHE:HB3	2.02	0.40
1:A:526:HIS:O	1:A:686:GLY:HA2	2.20	0.40
1:A:203:GLU:CG	1:A:204:GLU:H	2.32	0.40
1:A:466[A]:TPQ:CB	1:A:468:TYR:CZ	3.04	0.40
1:A:711:TRP:O	1:A:712:ASN:HB2	2.22	0.40
1:B:692:ARG:HG3	1:B:694:GLU:OE1	2.21	0.40
1:A:139:PHE:CD1	1:A:139:PHE:C	2.99	0.40
1:A:340:PRO:HD3	1:A:459:TRP:CD2	2.55	0.40
1:B:601:VAL:O	1:B:601:VAL:HG23	2.21	0.40
1:A:175:LEU:O	1:A:176:SER:HB3	2.21	0.40
1:A:527:ILE:HD13	1:A:634:MET:HE2	2.01	0.40
1:A:132:ASP:C	1:A:132:ASP:OD1	2.64	0.40
1:A:374:ILE:HD12	1:A:374:ILE:HA	1.83	0.40
1:A:401:ASP:OD2	1:B:439:LYS:NZ	2.48	0.40
1:B:314:LYS:HE2	4:B:2058:HOH:O	2.21	0.40
1:B:383:ASP:HB3	1:B:463:VAL:HG21	2.03	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	716/727 (98%)	674 (94%)	39 (5%)	3 (0%)	30 51
1	B	721/727 (99%)	690 (96%)	29 (4%)	2 (0%)	36 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1437/1454 (99%)	1364 (95%)	68 (5%)	5 (0%)	36 58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	596	ARG
1	A	212	ARG
1	B	133	LYS
1	B	379	LYS

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	609/615 (99%)	582 (96%)	27 (4%)	25 50
1	B	614/615 (100%)	570 (93%)	44 (7%)	13 30
All	All	1223/1230 (99%)	1152 (94%)	71 (6%)	18 39

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	11	ASP
1	A	14	LEU
1	A	32	LEU
1	A	58	GLN
1	A	67	LYS
1	A	73	THR
1	A	75	ILE
1	A	129	LEU
1	A	142	GLU
1	A	144	LYS
1	A	189	LEU
1	A	203	GLU

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Mol	Chain	Res	Type
1	A	209	VAL
1	A	237	LYS
1	A	275	ILE
1	A	317	THR
1	A	322	MET
1	A	503	GLU
1	A	520	VAL
1	A	551	LYS
1	A	566	ASN
1	A	574	GLN
1	A	613	HIS
1	A	617	LYS
1	A	669	LYS
1	A	685	THR
1	B	7	MET
1	B	8	VAL
1	B	10	MET
1	B	11	ASP
1	B	12	LYS
1	B	15	LYS
1	B	16	GLU
1	B	22	GLN
1	B	34	LYS
1	B	67	LYS
1	B	71	SER
1	B	80	GLN
1	B	89	VAL
1	B	114	SER
1	B	118	LYS
1	B	126	ILE
1	B	129	LEU
1	B	142	GLU
1	B	144	LYS
1	B	146	VAL
1	B	148	GLN
1	B	160	LYS
1	B	181	LYS
1	B	189	LEU
1	B	195	VAL
1	B	197	ASN
1	B	203	GLU
1	B	218	LYS

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Mol	Chain	Res	Type
1	B	276	VAL
1	B	278	ILE
1	B	303	VAL
1	B	323	ILE
1	B	352	THR
1	B	366	ILE
1	B	379	LYS
1	B	490	GLU
1	B	503	GLU
1	B	515	ILE
1	B	572	ASN
1	B	613	HIS
1	B	632	SER
1	B	688	THR
1	B	724	LYS
1	B	725	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	143	ASN
1	A	161	HIS
1	A	197	ASN
1	A	307	GLN
1	A	574	GLN
1	B	53	GLN
1	B	171	ASN
1	B	272	GLN
1	B	501	HIS
1	B	529	ASN
1	B	567	GLN
1	B	604	GLN
1	B	666	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TPQ	B	466[A]	2	13,14,15	2.16	3 (23%)	13,19,21	0.92	0
1	TPQ	B	466[B]	-	13,14,15	2.14	4 (30%)	13,19,21	1.71	3 (23%)
1	TPQ	A	466[A]	-	13,14,15	2.23	4 (30%)	13,19,21	1.89	3 (23%)
1	TPQ	A	466[B]	-	13,14,15	2.51	5 (38%)	13,19,21	1.16	1 (7%)

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	TPQ	B	466[A]	2	-	4/5/22/24	0/1/1/1
1	TPQ	B	466[B]	-	-	2/5/22/24	0/1/1/1
1	TPQ	A	466[A]	-	-	2/5/22/24	0/1/1/1
1	TPQ	A	466[B]	-	-	4/5/22/24	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466[B]	TPQ	O5-C5	5.18	1.38	1.24
1	A	466[A]	TPQ	O2-C2	5.06	1.38	1.24
1	A	466[B]	TPQ	O2-C2	4.83	1.37	1.24
1	B	466[A]	TPQ	O5-C5	4.76	1.37	1.24
1	B	466[B]	TPQ	O2-C2	4.73	1.37	1.24
1	B	466[A]	TPQ	O2-C2	4.31	1.36	1.24
1	A	466[A]	TPQ	O5-C5	4.29	1.35	1.24
1	B	466[B]	TPQ	O5-C5	4.15	1.35	1.24
1	A	466[B]	TPQ	CB-C1	2.81	1.55	1.50
1	A	466[B]	TPQ	C6-C1	2.81	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466[A]	TPQ	C6-C5	-2.61	1.37	1.44
1	B	466[B]	TPQ	C6-C5	-2.51	1.38	1.44
1	B	466[B]	TPQ	C3-C2	-2.21	1.39	1.44
1	A	466[B]	TPQ	C3-C4	2.19	1.40	1.36
1	B	466[A]	TPQ	C6-C1	2.08	1.39	1.34
1	A	466[A]	TPQ	C3-C2	-2.05	1.39	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466[A]	TPQ	C6-C1-C2	4.84	122.11	118.66
1	B	466[B]	TPQ	C6-C1-C2	3.43	121.10	118.66
1	B	466[B]	TPQ	C6-C5-C4	2.56	121.28	116.80
1	A	466[A]	TPQ	C1-C6-C5	-2.56	118.28	122.59
1	B	466[B]	TPQ	C1-C6-C5	-2.39	118.56	122.59
1	A	466[B]	TPQ	C6-C1-C2	-2.29	117.02	118.66
1	A	466[A]	TPQ	C6-C5-C4	2.12	120.51	116.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	466[A]	TPQ	N-CA-CB-C1
1	A	466[A]	TPQ	C-CA-CB-C1
1	B	466[A]	TPQ	C-CA-CB-C1
1	B	466[A]	TPQ	C2-C1-CB-CA
1	B	466[B]	TPQ	N-CA-CB-C1
1	B	466[B]	TPQ	C-CA-CB-C1
1	A	466[B]	TPQ	N-CA-CB-C1
1	B	466[A]	TPQ	N-CA-CB-C1
1	A	466[B]	TPQ	C2-C1-CB-CA
1	B	466[A]	TPQ	C6-C1-CB-CA
1	A	466[B]	TPQ	C6-C1-CB-CA
1	A	466[B]	TPQ	C-CA-CB-C1

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466[A]	TPQ	1	0
1	B	466[B]	TPQ	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466[A]	TPQ	4	0
1	A	466[B]	TPQ	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	465:ASN	C	466:TPQ	N	1.71
1	B	466:TPQ	C	467:ASP	N	1.11

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	718/727 (98%)	-0.63	0	100 100	13, 27, 45, 57	0
1	B	720/727 (99%)	-0.50	3 (0%)	88 86	14, 30, 50, 69	3 (0%)
All	All	1438/1454 (98%)	-0.57	3 (0%)	91 90	13, 28, 49, 69	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	PRO	2.7
1	B	6	HIS	2.5
1	B	303	VAL	2.2

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	TPQ	A	466[A]	14/15	0.92	0.12	19,22,23,25	11
1	TPQ	A	466[B]	14/15	0.92	0.12	22,25,27,27	11
1	TPQ	B	466[A]	14/15	0.94	0.11	33,34,34,36	11
1	TPQ	B	466[B]	14/15	0.94	0.11	33,35,38,39	11

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	1727	1/1	0.76	0.21	35,35,35,35	0
3	NA	B	1728	1/1	0.81	0.15	40,40,40,40	0
3	NA	B	1727	1/1	0.97	0.04	25,25,25,25	0
3	NA	A	1726	1/1	0.97	0.03	26,26,26,26	0
2	CU	A	1725	1/1	0.99	0.02	36,36,36,36	0
2	CU	B	1726	1/1	0.99	0.03	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.