



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2024 – 08:36 AM JST

PDB ID : 5ZE3  
Title : Crystal structure of human lysyl oxidase-like 2 (hLOXL2) in a precursor state  
Authors : Zhang, X.; Liu, M.  
Deposited on : 2018-02-25  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

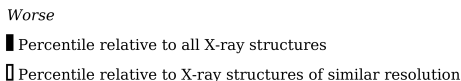
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

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## X-RAY DIFFRACTION

A.

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 <sub>free</sub>	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	457	<div> <div>7%</div> <div>61%</div> <div>29%</div> <div>6%</div> <div>• •</div> </div>
1	B	457	<div> <div>14%</div> <div>53%</div> <div>34%</div> <div>10%</div> <div>•</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7153 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 Lysyl oxidase homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3451	2134	618	665	34			
1	B	443	Total	C	N	O	S	0	0	0
			3463	2145	617	667	34			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLN	ASN	engineered mutation	UNP Q9Y4K0
A	570	LEU	MET	engineered mutation	UNP Q9Y4K0
B	455	GLN	ASN	engineered mutation	UNP Q9Y4K0
B	570	LEU	MET	engineered mutation	UNP Q9Y4K0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

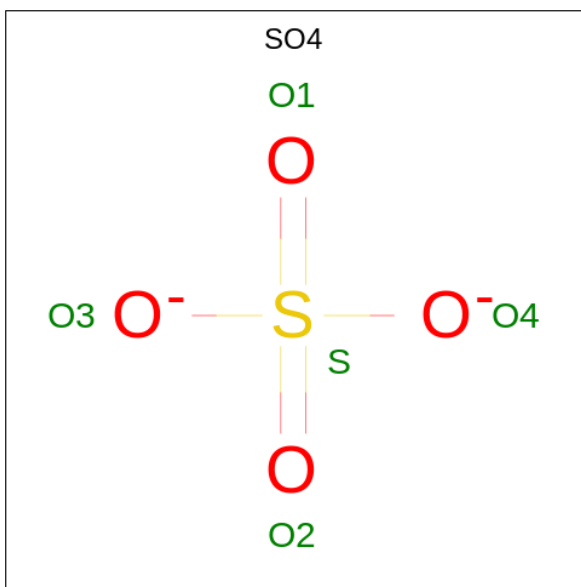


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

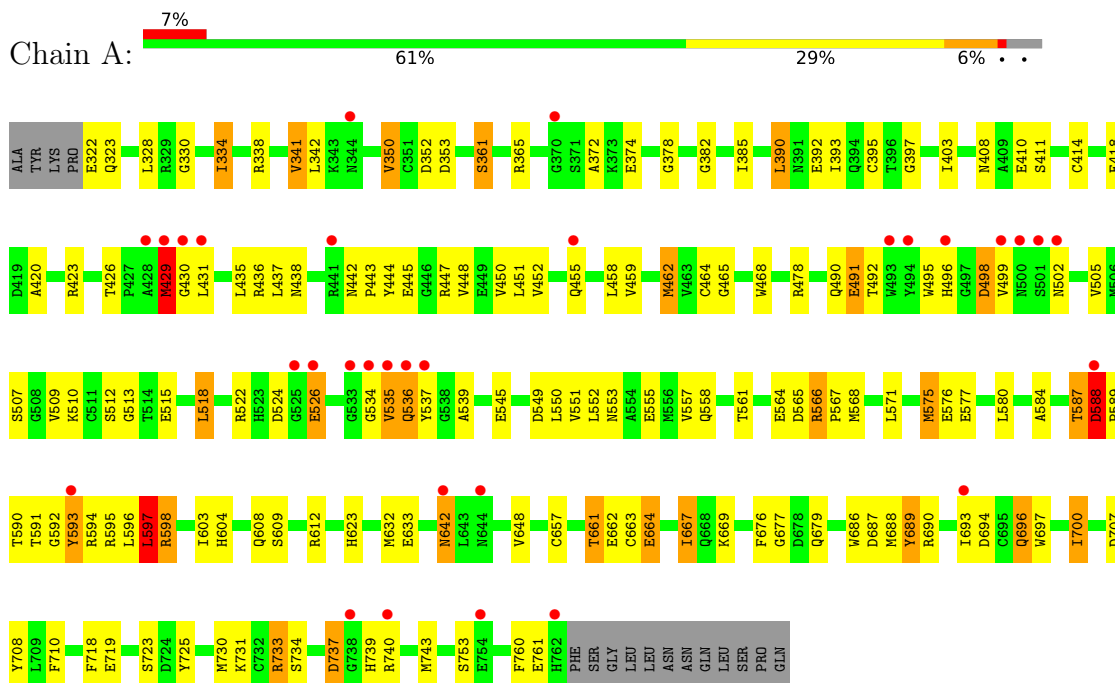
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	155	Total	O	0	0
			155	155		
6	B	47	Total	O	0	0
			47	47		

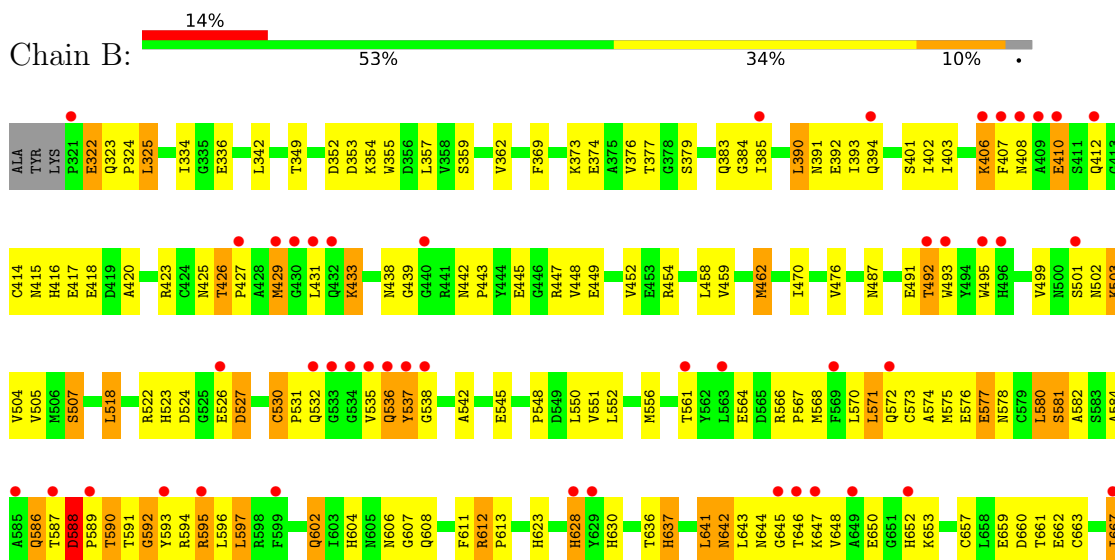
### 3 Residue-property plots

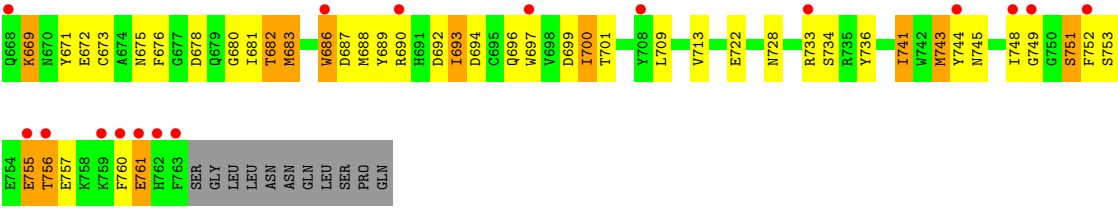
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lysyl oxidase homolog 2



#### • Molecule 1: Lysyl oxidase homolog 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.09Å 61.49Å 137.88Å 90.00° 102.33° 90.00°	Depositor
Resolution (Å)	36.50 – 2.40 36.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	85.3 (36.50-2.40) 88.3 (36.50-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_2405: ???)	Depositor
R, $R_{free}$	0.217 , 0.239 0.224 , 0.236	Depositor DCC
$R_{free}$ test set	2361 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: SO4, CA, NAG, ZN

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	0.62	2/3529 (0.1%)	0.81	5/4773 (0.1%)
1	B	0.48	0/3543	0.72	6/4793 (0.1%)
All	All	0.55	2/7072 (0.0%)	0.77	11/9566 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	PRO	N-CD	5.23	1.55	1.47
1	A	589	PRO	N-CD	5.18	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	GLY	N-CA-C	7.32	131.40	113.10
1	A	593	TYR	CA-CB-CG	7.01	126.71	113.40
1	B	628	HIS	N-CA-C	-6.63	93.09	111.00
1	A	598	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	B	439	GLY	N-CA-C	-5.97	98.16	113.10
1	B	530	CYS	C-N-CD	-5.77	107.91	120.60
1	B	588	ASP	C-N-CD	5.73	140.43	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ASN	C-N-CD	5.51	139.98	128.40
1	A	597	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	588	ASP	C-N-CD	5.36	139.65	128.40
1	B	501	SER	N-CA-C	5.13	124.85	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	MET	Peptide
1	A	593	TYR	Peptide
1	B	693	ILE	Peptide

## 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	3451	0	3215	106	2
1	B	3463	0	3220	191	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	5	0	0	0	0
6	A	155	0	0	17	0
6	B	47	0	0	7	0
All	All	7153	0	6461	292	2

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 22.

All (292) 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:492:THR:OG1	1:B:536:GLN:HB3	1.27	1.31
1:B:567:PRO:HA	1:B:592:GLY:O	1.36	1.22
1:B:369:PHE:CD1	1:B:426:THR:CG2	2.25	1.18
1:B:642:ASN:OD1	1:B:648:VAL:CG2	1.97	1.12
1:B:426:THR:HB	1:B:427:PRO:HD2	1.24	1.10
1:B:749:GLY:O	1:B:757:GLU:OE2	1.68	1.10
1:B:426:THR:HB	1:B:427:PRO:CD	1.89	1.02
1:B:588:ASP:OD1	1:B:590:THR:OG1	1.77	1.00
1:B:442:ASN:HB2	1:B:443:PRO:HD2	1.43	0.97
1:B:369:PHE:CD1	1:B:426:THR:HG21	1.98	0.96
1:B:429:MET:HA	1:B:429:MET:CE	1.94	0.96
1:B:369:PHE:HD1	1:B:426:THR:CG2	1.75	0.96
1:B:661:THR:O	1:B:669:LYS:NZ	1.98	0.95
1:B:369:PHE:HD1	1:B:426:THR:HG22	1.28	0.95
1:A:568:MET:HG3	1:A:587:THR:HG22	1.50	0.93
1:B:642:ASN:OD1	1:B:648:VAL:HG22	1.67	0.91
1:B:391:ASN:ND2	1:B:410:GLU:OE1	2.06	0.88
1:B:734:SER:CB	1:B:743:MET:SD	2.63	0.87
1:B:607:GLY:O	1:B:683:MET:HE3	1.75	0.86
1:B:734:SER:HB2	1:B:743:MET:SD	2.15	0.86
1:A:558:GLN:NE2	1:A:743:MET:O	2.09	0.85
1:B:369:PHE:CE1	1:B:426:THR:HG21	2.11	0.85
1:A:689:TYR:HB3	1:A:696:GLN:NE2	1.90	0.84
1:A:492:THR:O	6:A:901:HOH:O	1.95	0.84
1:B:390:LEU:HD23	1:B:393:ILE:HD11	1.58	0.84
1:B:608:GLN:HA	1:B:683:MET:HE3	1.60	0.83
1:A:612:ARG:NH1	1:A:679:GLN:O	2.12	0.83
1:B:462:MET:HE2	1:B:538:GLY:HA3	1.59	0.82
1:A:633:GLU:OE2	6:A:902:HOH:O	1.96	0.82
1:B:584:ALA:HB2	1:B:594:ARG:CZ	2.10	0.82
1:A:661:THR:HG21	1:A:688:MET:H	1.43	0.81
1:A:430:GLY:O	1:A:431:LEU:HD22	1.81	0.81
1:B:567:PRO:CA	1:B:592:GLY:O	2.25	0.80
1:B:392:GLU:HB2	1:B:408:ASN:HB2	1.63	0.80
1:B:448:VAL:O	6:B:903:HOH:O	1.99	0.79
1:B:536:GLN:HA	1:B:536:GLN:OE1	1.82	0.77
1:B:571:LEU:HB2	1:B:574:ALA:HB3	1.67	0.76
1:B:734:SER:HB3	1:B:743:MET:SD	2.25	0.76
1:B:336:GLU:HG3	1:B:423:ARG:HG2	1.68	0.75
1:B:523:HIS:ND1	1:B:524:ASP:O	2.19	0.75
1:A:590:THR:HG23	1:A:591:THR:HG23	1.69	0.75
1:B:550:LEU:HA	1:B:604:HIS:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:GLN:HA	1:B:683:MET:CE	2.16	0.75
1:A:608:GLN:NE2	6:A:908:HOH:O	2.15	0.74
1:B:325:LEU:HD12	1:B:325:LEU:N	2.03	0.73
1:B:661:THR:HG21	1:B:688:MET:H	1.52	0.73
1:B:429:MET:HA	1:B:429:MET:HE3	1.69	0.73
1:B:748:ILE:O	1:B:751:SER:OG	2.06	0.72
1:A:382:GLY:O	6:A:903:HOH:O	2.07	0.72
1:A:719:GLU:OE2	6:A:905:HOH:O	2.07	0.72
1:B:492:THR:OG1	1:B:536:GLN:CB	2.23	0.71
1:A:734:SER:OG	1:A:743:MET:SD	2.49	0.70
1:A:395:CYS:O	6:A:904:HOH:O	2.07	0.70
1:B:426:THR:CB	1:B:427:PRO:CD	2.60	0.70
1:B:354:LYS:HB3	1:B:394:GLN:HE22	1.56	0.70
1:A:664:GLU:OE1	6:A:906:HOH:O	2.09	0.69
1:B:492:THR:HG22	6:B:901:HOH:O	1.91	0.69
1:B:342:LEU:C	1:B:342:LEU:HD23	2.13	0.69
1:B:643:LEU:O	1:B:644:ASN:C	2.29	0.69
1:B:566:ARG:HD3	1:B:571:LEU:HD23	1.75	0.69
1:B:573:CYS:O	1:B:576:GLU:N	2.26	0.68
1:A:669:LYS:NZ	6:A:915:HOH:O	2.26	0.68
1:B:728:ASN:O	6:B:905:HOH:O	2.13	0.67
1:A:568:MET:HG3	1:A:587:THR:CG2	2.23	0.67
1:B:568:MET:HB2	1:B:589:PRO:HA	1.76	0.66
1:B:406:LYS:O	1:B:406:LYS:HG2	1.95	0.66
1:B:499:VAL:CG1	1:B:536:GLN:HG3	2.26	0.66
1:B:671:TYR:CG	1:B:680:GLY:O	2.49	0.66
1:B:733:ARG:O	1:B:744:TYR:HB3	1.96	0.66
1:B:383:GLN:O	6:B:906:HOH:O	2.14	0.65
1:A:438:ASN:HD21	1:A:498:ASP:H	1.43	0.65
1:A:575:MET:HG2	1:A:580:LEU:HD12	1.78	0.65
1:B:594:ARG:NH2	1:B:699:ASP:OD1	2.28	0.65
1:A:361:SER:HB2	1:A:372:ALA:H	1.60	0.65
1:B:671:TYR:CD2	1:B:680:GLY:O	2.50	0.65
1:A:661:THR:HB	6:A:921:HOH:O	1.96	0.64
1:B:342:LEU:HD23	1:B:342:LEU:O	1.97	0.64
1:A:390:LEU:HB3	1:A:393:ILE:HD11	1.79	0.64
1:A:566:ARG:HD3	1:A:571:LEU:HD21	1.80	0.64
1:A:330:GLY:O	6:A:907:HOH:O	2.15	0.64
1:B:442:ASN:HB2	1:B:443:PRO:CD	2.26	0.63
1:B:748:ILE:HD12	1:B:748:ILE:N	2.14	0.63
1:B:507:SER:HB3	1:B:524:ASP:OD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ASN:OD1	1:B:648:VAL:HG21	1.94	0.62
1:A:350:VAL:HG22	1:A:420:ALA:HB3	1.80	0.62
1:B:325:LEU:HD12	1:B:325:LEU:H	1.63	0.62
1:B:392:GLU:HB2	1:B:408:ASN:CB	2.29	0.61
1:B:429:MET:HA	1:B:429:MET:HE2	1.81	0.61
1:A:689:TYR:HB3	1:A:696:GLN:HE22	1.62	0.61
1:B:753:SER:OG	1:B:756:THR:OG1	2.19	0.61
1:A:447:ARG:NH1	6:A:901:HOH:O	2.31	0.61
1:A:661:THR:CG2	1:A:688:MET:H	2.12	0.61
1:B:755:GLU:O	1:B:755:GLU:HG2	2.00	0.61
1:B:662:GLU:HG2	1:B:663:CYS:H	1.66	0.60
1:A:642:ASN:ND2	1:A:648:VAL:HG21	2.16	0.60
1:B:584:ALA:HB2	1:B:594:ARG:NE	2.17	0.59
1:B:641:LEU:CB	1:B:646:THR:O	2.50	0.59
1:A:411:SER:O	1:A:414:CYS:HB2	2.02	0.59
1:B:689:TYR:HD2	1:B:696:GLN:HE22	1.50	0.59
1:B:652:HIS:HE1	1:B:699:ASP:H	1.50	0.59
1:A:478:ARG:NH2	1:A:513:GLY:O	2.30	0.58
1:B:641:LEU:HB2	1:B:646:THR:O	2.04	0.58
1:B:492:THR:CB	1:B:536:GLN:HB3	2.32	0.58
1:A:429:MET:HB3	1:B:433:LYS:HB3	1.84	0.57
1:B:412:GLN:HA	1:B:412:GLN:OE1	2.04	0.57
1:B:527:ASP:OD1	1:B:527:ASP:N	2.37	0.57
1:B:608:GLN:CA	1:B:683:MET:HE3	2.32	0.57
1:A:430:GLY:C	1:A:431:LEU:HD22	2.25	0.57
1:B:354:LYS:HB3	1:B:394:GLN:NE2	2.17	0.57
1:B:561:THR:HG21	1:B:743:MET:HG2	1.87	0.57
1:B:493:TRP:N	6:B:901:HOH:O	1.87	0.56
1:B:662:GLU:HB3	1:B:686:TRP:CZ2	2.40	0.56
1:A:491:GLU:HB3	1:A:534:GLY:O	2.05	0.56
1:A:492:THR:O	1:A:537:TYR:HB3	2.06	0.56
1:B:369:PHE:CD1	1:B:426:THR:HG23	2.34	0.56
1:B:595:ARG:HB3	1:B:700:ILE:HG22	1.86	0.56
1:B:694:ASP:C	6:B:907:HOH:O	2.43	0.56
1:B:681:ILE:HD13	1:B:687:ASP:HB2	1.88	0.55
1:A:536:GLN:O	1:A:536:GLN:HG3	2.07	0.55
1:B:643:LEU:O	1:B:645:GLY:N	2.40	0.55
1:A:510:LYS:HE2	6:A:1028:HOH:O	2.06	0.55
1:A:588:ASP:OD1	1:A:588:ASP:N	2.40	0.55
1:A:512:SER:HB3	1:B:526:GLU:HG3	1.88	0.55
1:B:568:MET:O	1:B:572:GLN:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:TYR:OH	1:A:545:GLU:OE2	2.18	0.54
1:B:581:SER:OG	1:B:582:ALA:N	2.40	0.54
1:B:641:LEU:O	1:B:709:LEU:N	2.34	0.54
1:B:577:GLU:HG2	1:B:623:HIS:NE2	2.22	0.54
1:A:564:GLU:OE1	1:A:566:ARG:HG3	2.08	0.54
1:B:462:MET:CE	1:B:538:GLY:HA3	2.34	0.53
1:B:596:LEU:HD13	1:B:697:TRP:CE3	2.44	0.53
1:A:694:ASP:OD2	6:A:909:HOH:O	2.19	0.53
1:B:661:THR:CG2	1:B:688:MET:H	2.20	0.53
1:A:429:MET:HA	1:B:433:LYS:HG2	1.91	0.53
1:B:641:LEU:HA	1:B:648:VAL:HG23	1.91	0.53
1:B:659:GLU:HG3	1:B:672:GLU:HA	1.90	0.53
1:B:416:HIS:C	1:B:418:GLU:H	2.12	0.52
1:B:752:PHE:HB2	1:B:757:GLU:HG2	1.92	0.52
1:A:663:CYS:HB3	1:A:667:ILE:HB	1.92	0.52
1:A:445:GLU:HG3	1:A:495:TRP:CZ2	2.45	0.52
1:A:661:THR:CG2	1:A:687:ASP:HA	2.40	0.52
1:B:401:SER:OG	1:B:403:ILE:HD12	2.10	0.51
1:A:737:ASP:HB3	1:A:739:HIS:H	1.76	0.51
1:B:487:ASN:HB2	1:B:542:ALA:HB3	1.91	0.51
1:B:383:GLN:HB2	1:B:606:ASN:HB3	1.92	0.51
1:B:671:TYR:CB	1:B:680:GLY:O	2.59	0.51
1:B:492:THR:HG1	1:B:536:GLN:HB3	1.64	0.51
1:B:682:THR:CG2	1:B:683:MET:N	2.73	0.51
1:A:342:LEU:HD21	1:A:753:SER:HB3	1.93	0.51
1:A:526:GLU:N	1:A:526:GLU:OE1	2.43	0.51
1:A:552:LEU:HD12	1:A:730:MET:HG3	1.93	0.51
1:B:493:TRP:HE3	1:B:493:TRP:O	1.94	0.51
1:B:662:GLU:HB3	1:B:686:TRP:CH2	2.46	0.51
1:B:682:THR:HG23	1:B:683:MET:H	1.76	0.51
1:B:392:GLU:HB2	1:B:408:ASN:CG	2.31	0.51
1:B:458:LEU:N	6:B:904:HOH:O	2.04	0.50
1:A:595:ARG:HG2	1:A:700:ILE:HG22	1.92	0.50
1:B:602:GLN:HG3	1:B:688:MET:CE	2.41	0.50
1:A:365:ARG:NH2	1:A:397:GLY:O	2.44	0.50
1:B:499:VAL:HG11	1:B:536:GLN:CG	2.42	0.49
1:B:349:THR:HG21	1:B:384:GLY:HA3	1.93	0.49
1:B:566:ARG:CD	1:B:571:LEU:HD23	2.42	0.49
1:B:503:LYS:HG3	1:B:504:VAL:H	1.77	0.49
1:B:671:TYR:HB2	1:B:680:GLY:O	2.13	0.49
1:A:567:PRO:HA	1:A:592:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:HIS:NE2	1:A:740:ARG:NH1	2.60	0.49
1:A:341:VAL:HG13	1:A:403:ILE:HD11	1.94	0.48
1:A:662:GLU:HB3	1:A:686:TRP:CZ2	2.48	0.48
1:B:369:PHE:CD1	1:B:426:THR:HG22	2.10	0.48
1:B:612:ARG:HG3	1:B:613:PRO:HD2	1.94	0.48
1:B:641:LEU:HB3	1:B:647:LYS:HA	1.95	0.48
1:B:352:ASP:HB2	1:B:377:THR:HG22	1.95	0.48
1:B:415:ASN:OD1	1:B:417:GLU:HB2	2.13	0.48
1:B:593:TYR:O	1:B:594:ARG:HD2	2.13	0.48
1:A:353:ASP:O	1:A:392:GLU:HA	2.13	0.48
1:B:391:ASN:OD1	1:B:392:GLU:N	2.46	0.48
1:B:492:THR:HG22	1:B:493:TRP:H	1.78	0.48
1:B:353:ASP:O	1:B:392:GLU:HA	2.13	0.48
1:B:499:VAL:CG1	1:B:536:GLN:CG	2.91	0.48
1:A:577:GLU:HG2	1:A:623:HIS:NE2	2.29	0.48
1:B:577:GLU:HG2	1:B:623:HIS:CE1	2.49	0.48
1:B:667:ILE:N	1:B:667:ILE:HD13	2.29	0.48
1:B:415:ASN:O	1:B:418:GLU:HB2	2.13	0.47
1:B:748:ILE:N	1:B:748:ILE:CD1	2.77	0.47
1:A:710:PHE:O	1:A:731:LYS:HA	2.13	0.47
1:A:550:LEU:HA	1:A:604:HIS:O	2.14	0.47
1:A:555:GLU:O	1:A:558:GLN:HB3	2.14	0.47
1:A:677:GLY:O	6:A:910:HOH:O	2.20	0.47
1:B:607:GLY:O	1:B:683:MET:CE	2.53	0.47
1:B:476:VAL:HG22	1:B:518:LEU:HG	1.95	0.47
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.76	0.47
1:A:733:ARG:NH1	6:A:929:HOH:O	2.47	0.47
1:B:571:LEU:HD12	1:B:571:LEU:O	2.15	0.47
1:A:498:ASP:OD1	1:A:498:ASP:N	2.49	0.46
1:B:667:ILE:N	1:B:667:ILE:CD1	2.78	0.46
1:A:568:MET:CG	1:A:587:THR:CG2	2.91	0.46
1:A:561:THR:HG21	1:A:743:MET:HG3	1.97	0.46
1:B:582:ALA:N	1:B:650:GLU:OE1	2.48	0.46
1:A:464:CYS:HB2	1:A:507:SER:HB2	1.97	0.46
1:A:642:ASN:HD22	1:A:642:ASN:HA	1.58	0.46
1:B:570:LEU:HD23	1:B:570:LEU:HA	1.76	0.46
1:B:661:THR:HG23	1:B:687:ASP:HA	1.98	0.46
1:B:659:GLU:HG2	1:B:660:ASP:N	2.30	0.46
1:A:451:LEU:HD12	1:A:459:VAL:O	2.16	0.45
1:B:594:ARG:CZ	1:B:701:THR:HB	2.46	0.45
1:A:435:LEU:HD12	1:A:450:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:CYS:SG	1:B:537:TYR:HB3	2.56	0.45
1:A:648:VAL:HG11	1:A:708:TYR:CE1	2.51	0.45
1:B:692:ASP:OD1	1:B:692:ASP:N	2.45	0.45
1:A:429:MET:HE2	1:B:433:LYS:HG2	1.98	0.45
1:A:438:ASN:HD21	1:A:498:ASP:N	2.13	0.45
1:B:492:THR:O	1:B:493:TRP:CG	2.70	0.45
1:B:594:ARG:NH2	1:B:701:THR:HB	2.32	0.45
1:B:642:ASN:OD1	1:B:648:VAL:HG23	2.04	0.45
1:A:568:MET:CG	1:A:587:THR:HG22	2.35	0.45
1:B:503:LYS:HG3	1:B:504:VAL:N	2.31	0.45
1:A:465:GLY:HA3	1:A:490:GLN:O	2.17	0.45
1:B:492:THR:O	1:B:493:TRP:CD1	2.70	0.44
1:A:642:ASN:CG	1:A:648:VAL:CG2	2.86	0.44
1:B:323:GLN:HG3	1:B:324:PRO:O	2.18	0.44
1:B:407:PHE:N	1:B:407:PHE:CD1	2.85	0.44
1:B:642:ASN:OD1	1:B:642:ASN:N	2.49	0.44
1:B:566:ARG:O	1:B:592:GLY:O	2.34	0.44
1:B:342:LEU:HD11	1:B:753:SER:HB3	1.98	0.44
1:B:659:GLU:HB2	1:B:673:CYS:SG	2.58	0.44
1:B:643:LEU:C	1:B:645:GLY:N	2.71	0.44
1:A:430:GLY:C	1:A:431:LEU:CD2	2.85	0.44
1:A:597:LEU:HB3	1:A:700:ILE:HD13	1.99	0.44
1:A:584:ALA:HA	1:A:594:ARG:NH1	2.33	0.44
1:B:586:GLN:H	1:B:586:GLN:HG3	1.58	0.44
1:A:535:VAL:O	1:A:535:VAL:HG13	2.18	0.43
1:B:392:GLU:CB	1:B:408:ASN:OD1	2.66	0.43
1:B:573:CYS:O	1:B:575:MET:N	2.51	0.43
1:B:660:ASP:HB3	1:B:669:LYS:HB3	1.99	0.43
1:A:408:ASN:OD1	1:A:410:GLU:HG2	2.19	0.43
1:A:458:LEU:O	6:A:911:HOH:O	2.21	0.43
1:B:493:TRP:O	1:B:493:TRP:CE3	2.70	0.43
1:B:608:GLN:HA	1:B:683:MET:HE1	1.99	0.43
1:B:414:CYS:HA	1:B:418:GLU:OE1	2.19	0.43
1:A:549:ASP:HB2	1:A:723:SER:OG	2.19	0.43
1:B:392:GLU:HB2	1:B:408:ASN:OD1	2.19	0.43
1:B:323:GLN:HG3	1:B:324:PRO:N	2.30	0.42
1:A:552:LEU:HD13	1:A:553:ASN:N	2.34	0.42
1:B:499:VAL:HG11	1:B:536:GLN:HG2	2.02	0.42
1:B:637:HIS:HB2	1:B:713:VAL:HB	2.02	0.42
1:A:509:VAL:HG11	1:A:518:LEU:HD21	2.01	0.42
1:B:342:LEU:C	1:B:342:LEU:CD2	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LEU:N	1:B:643:LEU:HD23	2.34	0.42
1:A:575:MET:HE3	1:A:580:LEU:HB2	2.02	0.42
1:B:573:CYS:O	1:B:574:ALA:C	2.57	0.42
1:B:752:PHE:HB2	1:B:757:GLU:CG	2.49	0.42
1:A:352:ASP:OD2	1:A:378:GLY:N	2.41	0.42
1:A:468:TRP:CD1	1:A:539:ALA:HB1	2.54	0.42
1:B:636:THR:HA	1:B:713:VAL:O	2.19	0.42
1:A:436:ARG:NH2	6:A:917:HOH:O	2.28	0.42
1:A:462:MET:CE	1:A:502:ASN:HA	2.50	0.42
1:B:374:GLU:OE1	1:B:376:VAL:HG22	2.19	0.42
1:A:328:LEU:HA	1:A:338:ARG:O	2.19	0.42
1:B:355:TRP:CE2	1:B:420:ALA:HB1	2.54	0.42
1:A:334:ILE:H	1:A:334:ILE:HG12	1.61	0.42
1:A:452:VAL:HG11	1:A:505:VAL:HG13	2.01	0.41
1:B:690:ARG:HD2	1:B:692:ASP:OD1	2.20	0.41
1:A:429:MET:HB3	1:B:433:LYS:CB	2.50	0.41
1:A:512:SER:N	1:A:515:GLU:OE2	2.37	0.41
1:A:718:PHE:HE1	1:A:725:TYR:HB3	1.86	0.41
1:B:548:PRO:HG3	1:B:611:PHE:HA	2.02	0.41
1:A:414:CYS:HA	1:A:418:GLU:OE1	2.21	0.41
1:B:394:GLN:O	1:B:406:LYS:HD3	2.21	0.41
1:B:628:HIS:CD2	1:B:628:HIS:C	2.93	0.41
1:B:736:TYR:HA	1:B:741:ILE:HD12	2.03	0.41
1:B:336:GLU:CG	1:B:423:ARG:HG2	2.45	0.41
1:B:623:HIS:CG	1:B:630:HIS:CE1	3.08	0.41
1:B:761:GLU:H	1:B:761:GLU:HG3	1.65	0.41
1:B:575:MET:HE2	1:B:580:LEU:HD12	2.02	0.41
1:A:603:ILE:N	1:A:603:ILE:HD12	2.36	0.41
1:A:429:MET:CA	1:A:429:MET:HE3	2.51	0.41
1:B:447:ARG:NE	1:B:449:GLU:OE2	2.50	0.41
1:A:566:ARG:HD2	1:A:598:ARG:HH11	1.86	0.41
1:A:595:ARG:HE	1:A:595:ARG:HB2	1.75	0.41
1:B:359:SER:O	1:B:362:VAL:HB	2.20	0.41
1:B:548:PRO:O	1:B:722:GLU:HA	2.21	0.41
1:B:597:LEU:HB2	1:B:700:ILE:HD12	2.02	0.41
1:B:744:TYR:O	1:B:745:ASN:HB2	2.20	0.41
1:B:573:CYS:C	1:B:575:MET:N	2.73	0.41
1:A:374:GLU:HB2	1:A:423:ARG:HB2	2.03	0.40
1:A:596:LEU:HD13	1:A:697:TRP:CE3	2.57	0.40
1:A:552:LEU:HD11	1:A:557:VAL:HG11	2.04	0.40
1:B:641:LEU:HB3	1:B:646:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:ND2	1:A:648:VAL:CG2	2.83	0.40
1:B:641:LEU:H	1:B:641:LEU:HG	1.80	0.40
1:B:416:HIS:C	1:B:418:GLU:N	2.74	0.40
1:B:595:ARG:CZ	1:B:595:ARG:HB2	2.50	0.40

All (2) 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:322:GLU:CG	1:B:322:GLU:OE1[1_545]	1.38	0.82
1:A:322:GLU:CB	1:B:322:GLU:OE1[1_545]	1.95	0.25

## 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	439/457 (96%)	420 (96%)	19 (4%)	0	100	100
1	B	441/457 (96%)	407 (92%)	32 (7%)	2 (0%)	25	38
All	All	880/914 (96%)	827 (94%)	51 (6%)	2 (0%)	44	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	531	PRO
1	B	693	ILE

### 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	370/384 (96%)	321 (87%)	49 (13%)	3	4
1	B	371/384 (97%)	294 (79%)	77 (21%)	1	1
All	All	741/768 (96%)	615 (83%)	126 (17%)	1	2

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	A	334	ILE
1	A	341	VAL
1	A	350	VAL
1	A	361	SER
1	A	385	ILE
1	A	390	LEU
1	A	426	THR
1	A	429	MET
1	A	437	LEU
1	A	448	VAL
1	A	455	GLN
1	A	462	MET
1	A	491	GLU
1	A	496	HIS
1	A	498	ASP
1	A	499	VAL
1	A	518	LEU
1	A	522	ARG
1	A	524	ASP
1	A	526	GLU
1	A	535	VAL
1	A	536	GLN
1	A	551	VAL
1	A	565	ASP
1	A	566	ARG
1	A	575	MET
1	A	576	GLU
1	A	587	THR
1	A	588	ASP
1	A	597	LEU
1	A	609	SER
1	A	632	MET

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Mol	Chain	Res	Type
1	A	642	ASN
1	A	657	CYS
1	A	661	THR
1	A	664	GLU
1	A	667	ILE
1	A	676	PHE
1	A	689	TYR
1	A	690	ARG
1	A	693	ILE
1	A	696	GLN
1	A	700	ILE
1	A	707	ASP
1	A	733	ARG
1	A	737	ASP
1	A	760	PHE
1	A	761	GLU
1	B	322	GLU
1	B	325	LEU
1	B	334	ILE
1	B	357	LEU
1	B	373	LYS
1	B	379	SER
1	B	385	ILE
1	B	390	LEU
1	B	402	ILE
1	B	406	LYS
1	B	410	GLU
1	B	425	ASN
1	B	426	THR
1	B	429	MET
1	B	431	LEU
1	B	433	LYS
1	B	438	ASN
1	B	445	GLU
1	B	452	VAL
1	B	454	ARG
1	B	459	VAL
1	B	462	MET
1	B	470	ILE
1	B	491	GLU
1	B	492	THR
1	B	495	TRP

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Mol	Chain	Res	Type
1	B	502	ASN
1	B	503	LYS
1	B	505	VAL
1	B	507	SER
1	B	518	LEU
1	B	522	ARG
1	B	527	ASP
1	B	532	GLN
1	B	535	VAL
1	B	536	GLN
1	B	537	TYR
1	B	545	GLU
1	B	551	VAL
1	B	552	LEU
1	B	556	MET
1	B	564	GLU
1	B	571	LEU
1	B	577	GLU
1	B	578	ASN
1	B	580	LEU
1	B	581	SER
1	B	586	GLN
1	B	587	THR
1	B	588	ASP
1	B	590	THR
1	B	591	THR
1	B	595	ARG
1	B	597	LEU
1	B	602	GLN
1	B	612	ARG
1	B	637	HIS
1	B	641	LEU
1	B	642	ASN
1	B	653	LYS
1	B	657	CYS
1	B	667	ILE
1	B	669	LYS
1	B	675	ASN
1	B	676	PHE
1	B	678	ASP
1	B	682	THR
1	B	683	MET

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Mol	Chain	Res	Type
1	B	686	TRP
1	B	700	ILE
1	B	741	ILE
1	B	743	MET
1	B	751	SER
1	B	755	GLU
1	B	756	THR
1	B	760	PHE
1	B	761	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	A	432	GLN
1	A	438	ASN
1	A	532	GLN
1	A	536	GLN
1	A	642	ASN
1	B	389	HIS
1	B	394	GLN
1	B	438	ASN
1	B	572	GLN
1	B	586	GLN
1	B	652	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
5	SO4	B	802	-	4,4,4	0.15	0	6,6,6	0.11	0
3	NAG	B	803	1	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	A	802	1	14,14,15	0.29	0	17,19,21	0.61	0

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
3	NAG	B	803	1	-	1/6/23/26	0/1/1/1
3	NAG	A	802	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	NAG	O5-C5-C6-O6
3	A	802	NAG	C4-C5-C6-O6
3	A	802	NAG	C8-C7-N2-C2
3	A	802	NAG	O7-C7-N2-C2
3	B	803	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	441/457 (96%)	0.27	31 (7%) 24 22	15, 35, 82, 113	0
1	B	443/457 (96%)	0.96	63 (14%) 7 6	30, 63, 112, 152	0
All	All	884/914 (96%)	0.61	94 (10%) 13 11	15, 51, 102, 152	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	534	GLY	7.3
1	A	534	GLY	6.4
1	B	537	TYR	6.1
1	A	501	SER	5.6
1	B	760	PHE	5.1
1	B	533	GLY	5.0
1	B	535	VAL	5.0
1	B	532	GLN	4.9
1	B	431	LEU	4.9
1	B	429	MET	4.5
1	A	500	ASN	4.5
1	A	496	HIS	4.4
1	B	430	GLY	4.2
1	B	569	PHE	4.2
1	B	585	ALA	4.1
1	B	536	GLN	4.1
1	B	763	PHE	4.0
1	A	499	VAL	3.7
1	B	408	ASN	3.6
1	A	493	TRP	3.5
1	A	533	GLY	3.4
1	B	762	HIS	3.4
1	B	412	GLN	3.3
1	A	428	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	538	GLY	3.3
1	B	385	ILE	3.3
1	A	431	LEU	3.2
1	A	502	ASN	3.2
1	A	536	GLN	3.2
1	A	441	ARG	3.2
1	B	733	ARG	3.2
1	B	652	HIS	3.1
1	A	455	GLN	3.1
1	B	593	TYR	3.1
1	B	595	ARG	3.0
1	B	759	LYS	2.9
1	A	429	MET	2.8
1	B	526	GLU	2.8
1	B	427	PRO	2.8
1	B	407	PHE	2.8
1	B	321	PRO	2.8
1	A	754	GLU	2.8
1	A	588	ASP	2.8
1	B	667	ILE	2.7
1	A	593	TYR	2.7
1	B	756	THR	2.7
1	B	409	ALA	2.6
1	A	537	TYR	2.6
1	B	599	PHE	2.6
1	B	432	GLN	2.6
1	A	430	GLY	2.6
1	B	561	THR	2.6
1	A	535	VAL	2.5
1	A	526	GLU	2.5
1	B	686	TRP	2.5
1	B	646	THR	2.5
1	A	738	GLY	2.5
1	B	496	HIS	2.4
1	B	587	THR	2.4
1	B	572	GLN	2.4
1	B	563	LEU	2.3
1	A	642	ASN	2.3
1	B	410	GLU	2.3
1	B	440	GLY	2.3
1	B	645	GLY	2.3
1	B	394	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	749	GLY	2.3
1	A	762	HIS	2.3
1	B	752	PHE	2.3
1	B	493	TRP	2.3
1	B	755	GLU	2.3
1	B	761	GLU	2.3
1	B	649	ALA	2.2
1	B	492	THR	2.2
1	A	740	ARG	2.2
1	B	501	SER	2.2
1	B	495	TRP	2.2
1	B	406	LYS	2.2
1	B	744	TYR	2.1
1	B	708	TYR	2.1
1	B	690	ARG	2.1
1	A	344	ASN	2.1
1	A	644	ASN	2.1
1	A	693	ILE	2.1
1	B	629	TYR	2.1
1	A	525	GLY	2.0
1	B	697	TRP	2.0
1	A	494	TYR	2.0
1	A	370	GLY	2.0
1	B	647	LYS	2.0
1	B	589	PRO	2.0
1	B	668	GLN	2.0
1	B	628	HIS	2.0
1	B	748	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	802	14/15	0.52	0.20	94,102,107,110	0
3	NAG	B	803	14/15	0.64	0.16	92,102,121,125	0
5	SO4	B	802	5/5	0.87	0.15	75,89,92,94	0
4	ZN	B	804	1/1	0.95	0.06	57,57,57,57	0
2	CA	A	801	1/1	0.98	0.06	28,28,28,28	0
2	CA	B	801	1/1	0.98	0.04	40,40,40,40	0
4	ZN	A	803	1/1	1.00	0.02	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.