



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2024 – 12:07 pm GMT

PDB ID : 9GB9  
Title : Crystal structure of Lotus japonicus CERK6 kinase domain D460N  
Authors : Simonsen, B.W.; Gysel, K.  
Deposited on : 2024-07-30  
Resolution : 1.85 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 : 1.8.4, 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

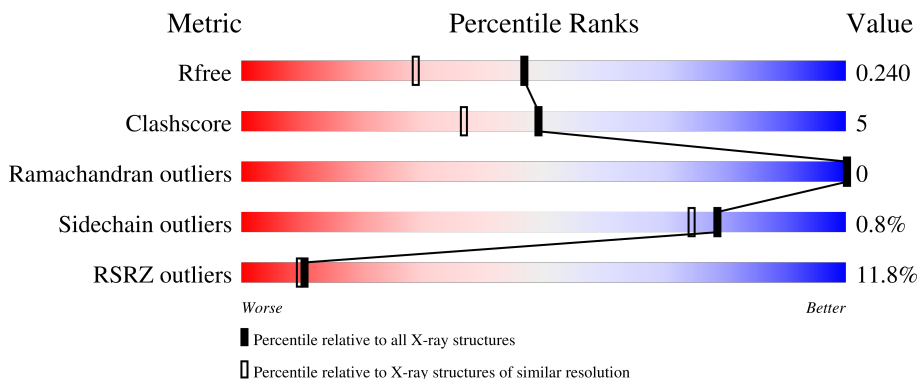
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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  $\geq 3$ , 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	297	
1	B	297	
1	C	297	
1	D	297	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9863 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 LysM type receptor kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2167	1382	372	406	7	0	1	0
1	B	283	2246	1429	384	426	7	0	5	0
1	C	282	2226	1419	382	418	7	0	4	0
1	D	277	2191	1397	378	409	7	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ASN	ASP	engineered mutation	UNP D3KTZ6
B	460	ASN	ASP	engineered mutation	UNP D3KTZ6
C	460	ASN	ASP	engineered mutation	UNP D3KTZ6
D	460	ASN	ASP	engineered mutation	UNP D3KTZ6

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



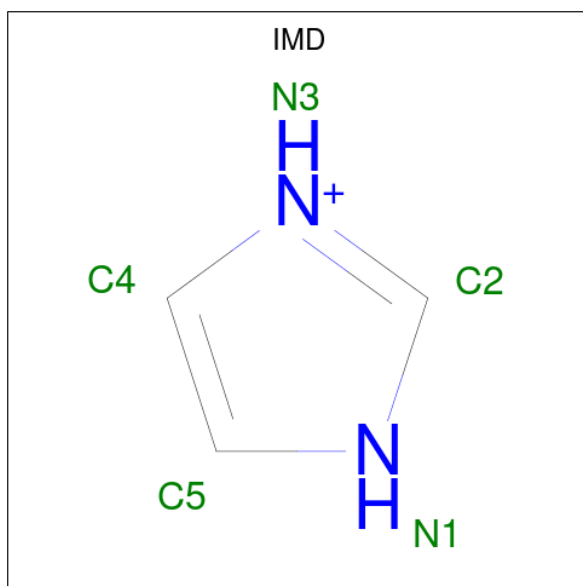
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	183	Total O 183 183	0	0

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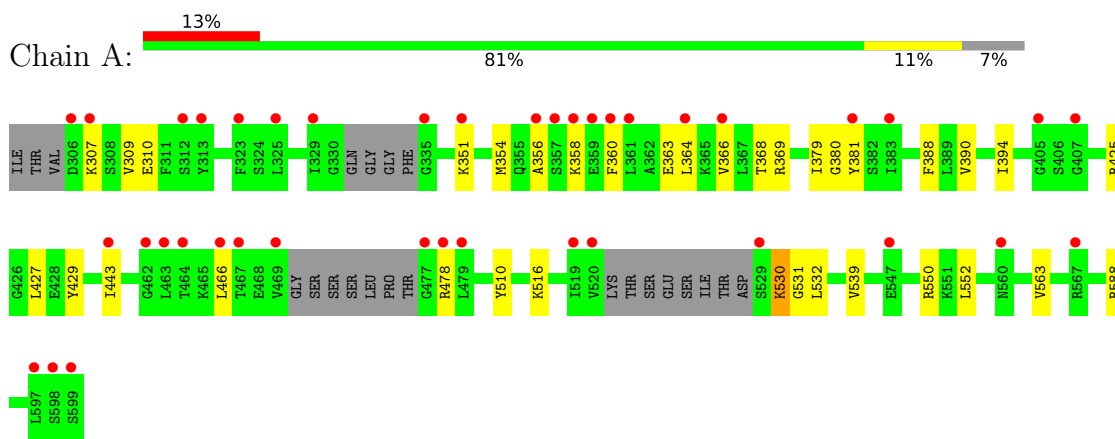
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	299	Total 299	O 299	0	0
4	C	285	Total 285	O 285	0	0
4	D	176	Total 176	O 176	0	0

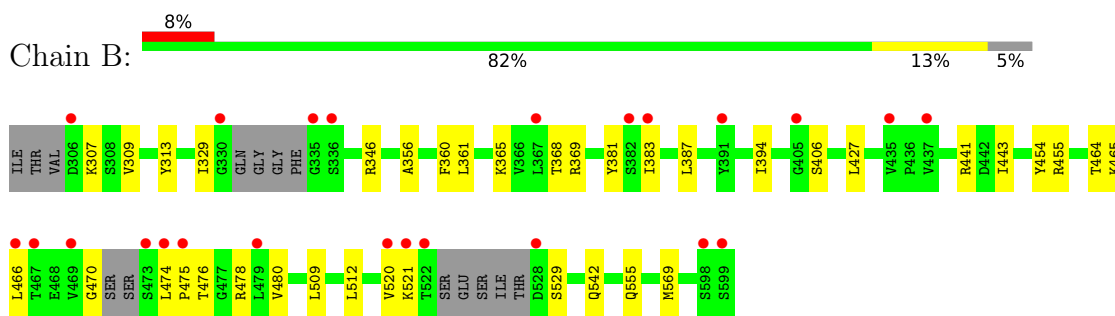
### 3 Residue-property plots [i](#)

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.

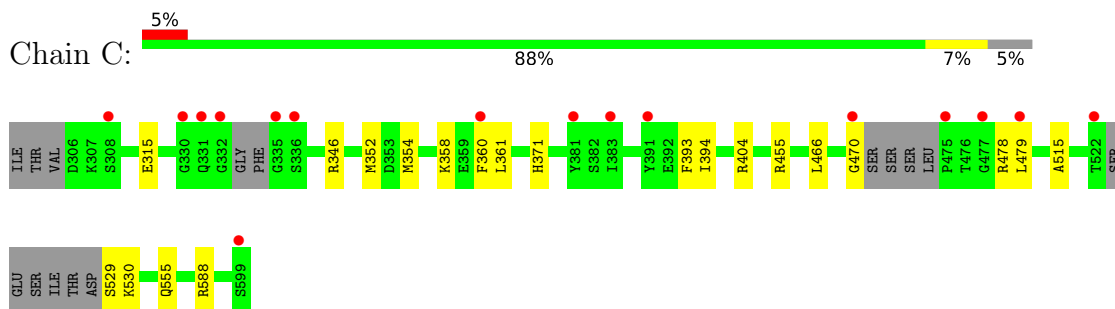
- Molecule 1: LysM type receptor kinase



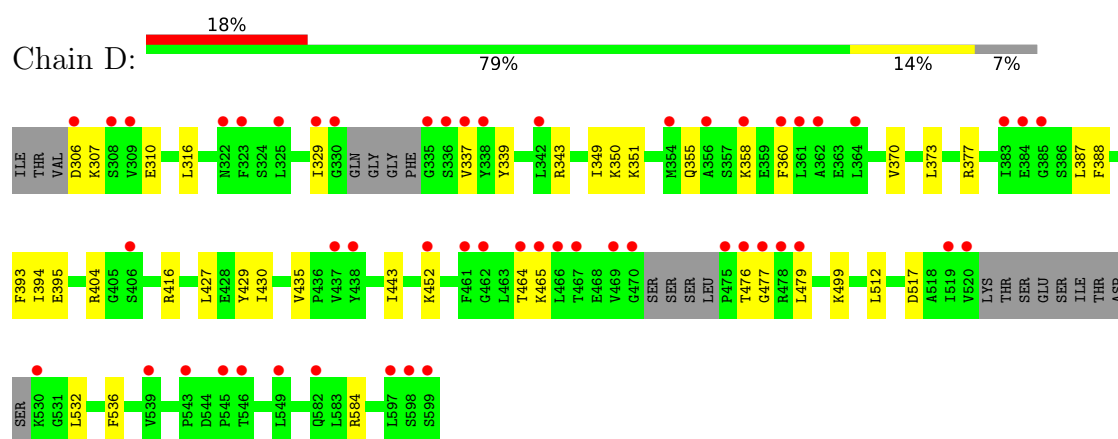
- Molecule 1: LysM type receptor kinase



- Molecule 1: LysM type receptor kinase



- Molecule 1: LysM type receptor kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.92Å 59.99Å 103.74Å 106.46° 97.31° 106.64°	Depositor
Resolution (Å)	48.45 – 1.85 48.45 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.45-1.85) 99.9 (48.45-1.85)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.86Å)	Xtrriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.209 , 0.242 0.207 , 0.240	Depositor DCC
$R_{free}$ test set	107409 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtrriage
Anisotropy	0.446	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-h-k-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.73% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.29	0/2205	0.53	0/2980
1	B	0.33	0/2288	0.56	0/3094
1	C	0.32	0/2274	0.56	0/3072
1	D	0.29	0/2236	0.53	0/3020
All	All	0.31	0/9003	0.54	0/12166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2167	0	2188	25	0
1	B	2246	0	2263	27	0
1	C	2226	0	2260	18	0
1	D	2191	0	2221	25	0
2	A	8	0	12	1	0
2	B	24	0	36	4	0
2	C	32	0	48	8	0
2	D	16	0	24	5	0
3	B	5	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	5	0	0
4	A	183	0	0	3	0
4	B	299	0	0	5	0
4	C	285	0	0	8	0
4	D	176	0	0	2	0
All	All	9863	0	9062	96	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 5.

All (96) 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:394:ILE:H	3:B:606:IMD:HN1	1.20	0.89
1:A:356:ALA:HB1	1:A:358:LYS:HG2	1.68	0.75
1:D:377:ARG:NH2	4:D:701:HOH:O	2.19	0.75
1:B:512:LEU:HB2	1:B:569:MET:HE1	1.71	0.72
1:B:307:LYS:NZ	4:B:702:HOH:O	2.25	0.68
1:D:404:ARG:HD2	2:D:603:EDO:H12	1.76	0.67
1:D:307:LYS:HA	1:D:310:GLU:HB3	1.77	0.66
1:A:369:ARG:NH2	4:A:805:HOH:O	2.29	0.65
1:D:329:ILE:HD11	1:D:339:TYR:HB2	1.79	0.65
1:D:394:ILE:H	2:D:601:EDO:H11	1.64	0.62
1:A:360:PHE:HA	1:A:363:GLU:HB2	1.83	0.61
1:D:427:LEU:HD21	1:D:443:ILE:HD11	1.84	0.59
1:B:368:THR:OG1	1:B:369:ARG:NH1	2.36	0.58
1:C:358:LYS:HA	1:C:361:LEU:HD12	1.85	0.58
1:A:427:LEU:HD21	1:A:443[B]:ILE:HD11	1.86	0.58
1:A:550:ARG:HH21	1:A:563:VAL:HG21	1.68	0.57
1:A:379:ILE:HB	1:A:390:VAL:HG23	1.85	0.57
1:B:454:TYR:CZ	2:B:607:EDO:H12	2.39	0.57
1:B:361:LEU:HD22	1:B:383:ILE:HG12	1.85	0.57
1:B:365:LYS:HG2	1:B:381:TYR:OH	2.05	0.56
1:B:356:ALA:HB2	1:B:387:LEU:HD22	1.87	0.56
1:C:371:HIS:HD2	2:C:604:EDO:H21	1.72	0.55
1:B:520:VAL:HG12	1:B:521:LYS:H	1.71	0.55
1:B:464:THR:HG23	1:B:480:VAL:HG21	1.88	0.55
1:D:355:GLN:HB2	1:D:387:LEU:N	2.22	0.55
1:B:476:THR:HG21	1:B:478:ARG:HH21	1.72	0.54
1:C:346:ARG:NH1	4:C:710:HOH:O	2.36	0.54
1:D:427:LEU:HD23	1:D:430:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:GLU:HG3	1:D:452:LYS:HG3	1.90	0.53
1:C:529:SER:O	1:C:530:LYS:HD2	2.09	0.53
1:A:425:ARG:HD3	4:C:702:HOH:O	2.09	0.52
1:A:360:PHE:O	1:A:364:LEU:N	2.38	0.52
1:C:455:ARG:NH2	4:C:713:HOH:O	2.44	0.51
1:B:465:LYS:O	1:B:470:GLY:N	2.44	0.51
1:B:542:GLN:NE2	4:B:701:HOH:O	2.22	0.51
1:D:306:ASP:O	1:D:310:GLU:N	2.43	0.51
1:B:474:LEU:HD12	1:B:475:PRO:HD2	1.93	0.51
1:D:517:ASP:HA	2:D:603:EDO:H11	1.92	0.50
1:A:309:VAL:HG22	1:A:380:GLY:HA2	1.92	0.50
1:C:394:ILE:H	2:C:601:EDO:C1	2.25	0.49
1:B:313:TYR:H	2:B:605:EDO:H11	1.78	0.49
1:C:315:GLU:OE1	4:C:701:HOH:O	2.20	0.49
1:D:393:PHE:HA	2:D:601:EDO:H12	1.95	0.49
1:C:352:MET:O	1:C:354:MET:N	2.46	0.49
1:D:316:LEU:HG	1:D:349:ILE:HD13	1.94	0.49
1:C:393:PHE:HA	2:C:601:EDO:H12	1.95	0.48
1:C:394:ILE:H	2:C:601:EDO:H12	1.79	0.48
1:A:364:LEU:O	1:A:368:THR:HG23	2.14	0.48
1:B:427:LEU:HD21	1:B:443:ILE:HD11	1.95	0.47
1:D:358:LYS:C	1:D:360:PHE:H	2.17	0.47
1:A:539:VAL:HG21	1:A:552:LEU:HD11	1.96	0.47
1:C:555:GLN:HG2	4:C:859:HOH:O	2.13	0.47
1:D:343:ARG:NH1	4:D:705:HOH:O	2.45	0.47
1:B:394:ILE:N	3:B:606:IMD:HN1	2.02	0.47
1:C:358:LYS:NZ	4:C:716:HOH:O	2.47	0.46
1:A:307:LYS:HA	1:A:310:GLU:HB2	1.96	0.46
1:D:476:THR:HG23	1:D:477:GLY:O	2.16	0.46
1:C:455:ARG:HG3	2:C:603:EDO:H11	1.97	0.45
1:A:516:LYS:HB2	1:A:532:LEU:HD21	1.99	0.45
1:D:370:VAL:HG13	1:D:429:TYR:HE2	1.82	0.44
1:A:358:LYS:HG3	1:A:360:PHE:H	1.82	0.44
1:D:464:THR:OG1	1:D:465:LYS:NZ	2.51	0.44
1:A:530:LYS:NZ	1:A:531:GLY:H	2.16	0.44
1:B:360:PHE:CZ	1:B:466:LEU:HG	2.52	0.44
1:A:351:LYS:HG2	1:A:388:PHE:CE2	2.53	0.44
1:A:354:MET:SD	1:A:466:LEU:HD22	2.57	0.44
1:A:588:ARG:HG3	1:C:588:ARG:HG3	2.00	0.44
1:B:521:LYS:HB2	1:B:529:SER:HA	2.00	0.44
1:B:455:ARG:HG3	2:B:602:EDO:H11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLU:HG2	1:A:381:TYR:CE1	2.54	0.43
1:A:510:TYR:HB3	1:A:532:LEU:HD13	2.01	0.43
1:B:346:ARG:NH1	4:B:717:HOH:O	2.51	0.43
1:B:509:LEU:HD22	1:B:569:MET:HE2	2.00	0.43
1:D:394:ILE:H	2:D:601:EDO:C1	2.32	0.43
1:D:416:ARG:HB3	1:D:512:LEU:HD22	2.01	0.43
1:B:309:VAL:HG13	1:B:368:THR:HG21	2.00	0.42
1:C:360:PHE:CE2	1:C:466:LEU:HD13	2.54	0.42
2:C:604:EDO:H22	4:C:714:HOH:O	2.18	0.42
1:B:542:GLN:HG2	4:B:810:HOH:O	2.19	0.42
1:A:358:LYS:HD2	1:A:360:PHE:HB2	2.01	0.42
1:A:429:TYR:OH	4:A:801:HOH:O	2.21	0.42
1:B:441:ARG:NH1	1:B:464:THR:HG21	2.34	0.42
1:A:363:GLU:OE2	4:A:802:HOH:O	2.22	0.42
1:D:499[A]:LYS:HD2	1:D:584:ARG:HB2	2.02	0.41
1:D:337:VAL:HG22	1:D:350:LYS:HD2	2.01	0.41
2:C:602:EDO:H11	4:C:900:HOH:O	2.20	0.41
1:A:530:LYS:HD3	1:A:531:GLY:N	2.35	0.41
1:C:404:ARG:NE	1:C:515:ALA:O	2.53	0.41
1:B:406:SER:HB2	4:B:894:HOH:O	2.21	0.41
1:D:532:LEU:HD22	1:D:536:PHE:HE1	1.86	0.41
1:C:371:HIS:CD2	2:C:604:EDO:H21	2.54	0.40
1:D:351:LYS:HB2	1:D:388:PHE:CE2	2.55	0.40
1:D:479:LEU:HD23	1:D:479:LEU:HA	1.95	0.40
1:B:454:TYR:CE2	2:B:607:EDO:H12	2.55	0.40
1:A:394:ILE:HG12	2:A:701:EDO:H21	2.04	0.40
1:C:470:GLY:C	1:C:478:ARG:HH12	2.25	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	268/297 (90%)	254 (95%)	14 (5%)	0	100	100
1	B	280/297 (94%)	274 (98%)	6 (2%)	0	100	100
1	C	278/297 (94%)	272 (98%)	6 (2%)	0	100	100
1	D	272/297 (92%)	262 (96%)	10 (4%)	0	100	100
All	All	1098/1188 (92%)	1062 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	235/253 (93%)	232 (99%)	3 (1%)	65	55
1	B	246/253 (97%)	244 (99%)	2 (1%)	79	74
1	C	243/253 (96%)	242 (100%)	1 (0%)	89	88
1	D	238/253 (94%)	236 (99%)	2 (1%)	79	74
All	All	962/1012 (95%)	954 (99%)	8 (1%)	79	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	VAL
1	A	478	ARG
1	A	530	LYS
1	B	329	ILE
1	B	555	GLN
1	C	479	LEU
1	D	373	LEU
1	D	435	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	371	HIS
1	C	418	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 ligands 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	$\# Z  > 2$
2	EDO	B	602	-	3,3,3	0.29	0	2,2,2	0.25	0
2	EDO	C	603	-	3,3,3	0.30	0	2,2,2	0.23	0
2	EDO	C	601	-	3,3,3	0.28	0	2,2,2	0.49	0
2	EDO	B	605	-	3,3,3	0.27	0	2,2,2	0.19	0
2	EDO	C	604	-	3,3,3	0.33	0	2,2,2	0.16	0
2	EDO	C	606	-	3,3,3	0.26	0	2,2,2	0.20	0
2	EDO	C	608	-	3,3,3	0.21	0	2,2,2	0.40	0
3	IMD	B	606	-	3,5,5	0.18	0	4,5,5	1.13	0
2	EDO	B	604	-	3,3,3	0.28	0	2,2,2	0.04	0
2	EDO	A	701	-	3,3,3	0.25	0	2,2,2	0.17	0
2	EDO	A	702	-	3,3,3	0.27	0	2,2,2	0.23	0
2	EDO	C	602	-	3,3,3	0.28	0	2,2,2	0.37	0
2	EDO	B	607	-	3,3,3	0.27	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	D	604	-	3,3,3	0.26	0	2,2,2	0.31	0
2	EDO	C	605	-	3,3,3	0.27	0	2,2,2	0.24	0
2	EDO	B	601	-	3,3,3	0.27	0	2,2,2	0.43	0
2	EDO	B	603	-	3,3,3	0.29	0	2,2,2	0.41	0
2	EDO	C	609	-	3,3,3	0.27	0	2,2,2	0.26	0
3	IMD	C	607	-	3,5,5	0.14	0	4,5,5	0.89	0
2	EDO	D	601	-	3,3,3	0.20	0	2,2,2	0.13	0
2	EDO	D	602	-	3,3,3	0.27	0	2,2,2	0.13	0
2	EDO	D	603	-	3,3,3	0.25	0	2,2,2	0.32	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
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	B	605	-	-	0/1/1/1	-
2	EDO	C	604	-	-	0/1/1/1	-
2	EDO	C	606	-	-	0/1/1/1	-
2	EDO	C	608	-	-	1/1/1/1	-
3	IMD	B	606	-	-	-	0/1/1/1
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	A	702	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	B	607	-	-	1/1/1/1	-
2	EDO	D	604	-	-	1/1/1/1	-
2	EDO	C	605	-	-	0/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	C	609	-	-	0/1/1/1	-
3	IMD	C	607	-	-	-	0/1/1/1
2	EDO	D	601	-	-	1/1/1/1	-
2	EDO	D	602	-	-	0/1/1/1	-
2	EDO	D	603	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	EDO	O1-C1-C2-O2
2	D	603	EDO	O1-C1-C2-O2
2	D	601	EDO	O1-C1-C2-O2
2	A	702	EDO	O1-C1-C2-O2
2	B	607	EDO	O1-C1-C2-O2
2	B	601	EDO	O1-C1-C2-O2
2	C	603	EDO	O1-C1-C2-O2
2	C	608	EDO	O1-C1-C2-O2
2	D	604	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	EDO	1	0
2	C	603	EDO	1	0
2	C	601	EDO	3	0
2	B	605	EDO	1	0
2	C	604	EDO	3	0
3	B	606	IMD	2	0
2	A	701	EDO	1	0
2	C	602	EDO	1	0
2	B	607	EDO	2	0
2	D	601	EDO	3	0
2	D	603	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	275/297 (92%)	0.81	40 (14%) <b>7</b> <b>6</b>	16, 49, 97, 139	1 (0%)
1	B	283/297 (95%)	0.36	24 (8%) <b>18</b> <b>19</b>	15, 36, 89, 123	5 (1%)
1	C	282/297 (94%)	0.25	16 (5%) <b>30</b> <b>32</b>	14, 35, 83, 128	4 (1%)
1	D	277/297 (93%)	0.92	52 (18%) <b>4</b> <b>3</b>	19, 53, 109, 142	3 (1%)
All	All	1117/1188 (94%)	0.58	132 (11%) <b>10</b> <b>10</b>	14, 42, 96, 142	13 (1%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	597	LEU	8.1
1	B	383	ILE	6.3
1	D	469	VAL	5.7
1	D	476	THR	5.6
1	D	520	VAL	4.9
1	B	330	GLY	4.9
1	A	469	VAL	4.9
1	B	437[A]	VAL	4.6
1	A	383	ILE	4.4
1	A	599	SER	4.2
1	A	360	PHE	4.2
1	D	356	ALA	4.1
1	D	466	LEU	4.0
1	D	475	PRO	4.0
1	D	470	GLY	3.9
1	D	360	PHE	3.9
1	D	358	LYS	3.9
1	C	331	GLN	3.8
1	A	356	ALA	3.8
1	D	335	GLY	3.7
1	D	477	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	522	THR	3.7
1	C	330	GLY	3.7
1	A	335	GLY	3.6
1	B	598	SER	3.6
1	C	332	GLY	3.5
1	B	469	VAL	3.5
1	A	351	LYS	3.4
1	A	529	SER	3.4
1	B	335	GLY	3.4
1	A	479	LEU	3.4
1	D	383	ILE	3.4
1	C	335	GLY	3.3
1	D	597	LEU	3.3
1	D	336	SER	3.3
1	A	464	THR	3.3
1	A	477	GLY	3.3
1	C	391	TYR	3.3
1	D	361	LEU	3.2
1	B	475	PRO	3.2
1	A	520	VAL	3.1
1	C	383	ILE	3.1
1	A	466	LEU	3.1
1	A	358	LYS	3.1
1	D	325	LEU	3.1
1	D	479	LEU	3.1
1	D	438	TYR	3.0
1	D	330	GLY	3.0
1	B	521	LYS	3.0
1	D	323	PHE	3.0
1	A	361	LEU	2.9
1	D	309	VAL	2.9
1	D	598	SER	2.9
1	A	364	LEU	2.9
1	C	308	SER	2.9
1	D	362	ALA	2.8
1	D	462	GLY	2.8
1	A	598	SER	2.7
1	A	329	ILE	2.7
1	D	364	LEU	2.7
1	D	478	ARG	2.6
1	D	322	ASN	2.6
1	D	546	THR	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	549	LEU	2.6
1	D	599	SER	2.6
1	C	360	PHE	2.6
1	B	473	SER	2.6
1	B	467	THR	2.6
1	A	313	TYR	2.5
1	A	478	ARG	2.5
1	B	435	VAL	2.5
1	B	466	LEU	2.5
1	C	470	GLY	2.5
1	D	354	MET	2.5
1	D	530	LYS	2.5
1	B	336	SER	2.5
1	A	463	LEU	2.5
1	C	522	THR	2.5
1	D	539	VAL	2.5
1	A	312	SER	2.4
1	D	467	THR	2.4
1	D	545	PRO	2.4
1	A	306	ASP	2.4
1	B	306	ASP	2.4
1	A	381	TYR	2.4
1	D	385	GLY	2.4
1	A	467	THR	2.4
1	D	306	ASP	2.4
1	B	367	LEU	2.4
1	D	329	ILE	2.4
1	D	406	SER	2.4
1	A	462	GLY	2.4
1	A	547	GLU	2.4
1	A	519	ILE	2.3
1	C	336	SER	2.3
1	C	599	SER	2.3
1	B	391	TYR	2.3
1	D	342	LEU	2.3
1	D	384	GLU	2.3
1	D	437	VAL	2.3
1	D	452	LYS	2.3
1	A	405	GLY	2.3
1	A	307	LYS	2.3
1	A	357	SER	2.3
1	A	560	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	465	LYS	2.2
1	B	599	SER	2.2
1	A	325	LEU	2.2
1	A	407	GLY	2.2
1	D	519	ILE	2.2
1	C	475	PRO	2.2
1	B	479	LEU	2.2
1	C	479	LEU	2.2
1	D	338	TYR	2.2
1	A	443[A]	ILE	2.2
1	A	567	ARG	2.2
1	B	528	ASP	2.1
1	D	308	SER	2.1
1	D	337	VAL	2.1
1	C	477	GLY	2.1
1	A	359	GLU	2.1
1	D	461	PHE	2.1
1	D	464	THR	2.1
1	B	520	VAL	2.1
1	B	405	GLY	2.1
1	A	366	VAL	2.1
1	A	323	PHE	2.1
1	B	474	LEU	2.1
1	D	543	PRO	2.0
1	B	382	SER	2.0
1	C	381	TYR	2.0
1	D	582	GLN	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
2	EDO	B	605	4/4	0.63	0.20	69,69,72,83	0
2	EDO	B	604	4/4	0.69	0.19	46,64,74,83	0
2	EDO	B	607	4/4	0.72	0.18	47,54,56,57	0
2	EDO	D	602	4/4	0.73	0.20	54,62,63,67	0
2	EDO	C	605	4/4	0.74	0.18	69,80,82,85	0
2	EDO	B	603	4/4	0.74	0.14	51,54,65,79	0
2	EDO	C	606	4/4	0.76	0.15	69,76,77,78	0
2	EDO	A	702	4/4	0.77	0.18	52,55,59,59	0
2	EDO	B	602	4/4	0.78	0.16	44,45,50,55	0
2	EDO	C	603	4/4	0.79	0.15	45,50,51,56	0
2	EDO	D	604	4/4	0.79	0.15	64,65,67,77	0
2	EDO	B	601	4/4	0.80	0.17	44,45,45,50	0
2	EDO	C	609	4/4	0.81	0.14	69,76,77,77	0
3	IMD	B	606	5/5	0.82	0.14	27,28,39,41	0
2	EDO	C	601	4/4	0.83	0.19	23,35,37,48	0
2	EDO	C	602	4/4	0.84	0.10	47,51,58,61	0
2	EDO	A	701	4/4	0.84	0.15	31,39,42,61	0
2	EDO	C	604	4/4	0.84	0.17	43,46,48,55	0
2	EDO	D	603	4/4	0.85	0.13	59,64,65,67	0
2	EDO	D	601	4/4	0.89	0.10	37,38,48,54	0
2	EDO	C	608	4/4	0.90	0.17	38,45,51,52	0
3	IMD	C	607	5/5	0.93	0.10	33,35,45,53	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.