



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:18 AM UTC

PDB ID : 9PI6 / pdb\_00009pi6  
Title : Single stranded DNA-binding protein (ICP8) from Herpes simplex virus-1, apo form. Mutations: K166A, E167A, C254S, C455S  
Authors : Erlandsen, H.; Wright, D.; Weller, S.; Wilderman, R.; Krucinska, J.  
Deposited on : 2025-07-10  
Resolution : 2.75 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	:	4-5-2 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

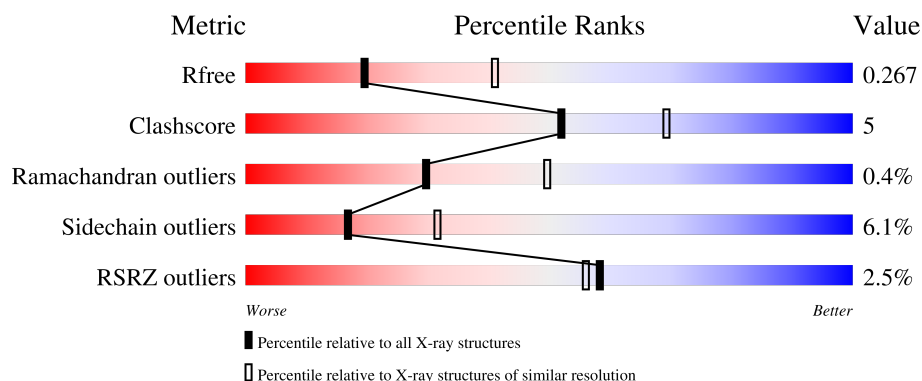
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	1136	 3% 75% 16% • 7%
1	B	1136	 2% 79% 14% • 6%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16294 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 Major DNA-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1051	Total	C	N	O	S	0	0	0
			8030	5079	1421	1483	47			
1	B	1071	Total	C	N	O	S	0	0	0
			8147	5146	1444	1511	46			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	LYS	engineered mutation	UNP P17470
A	167	ALA	GLU	engineered mutation	UNP P17470
A	254	SER	CYS	engineered mutation	UNP P17470
A	455	SER	CYS	engineered mutation	UNP P17470
B	166	ALA	LYS	engineered mutation	UNP P17470
B	167	ALA	GLU	engineered mutation	UNP P17470
B	254	SER	CYS	engineered mutation	UNP P17470
B	455	SER	CYS	engineered mutation	UNP P17470

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

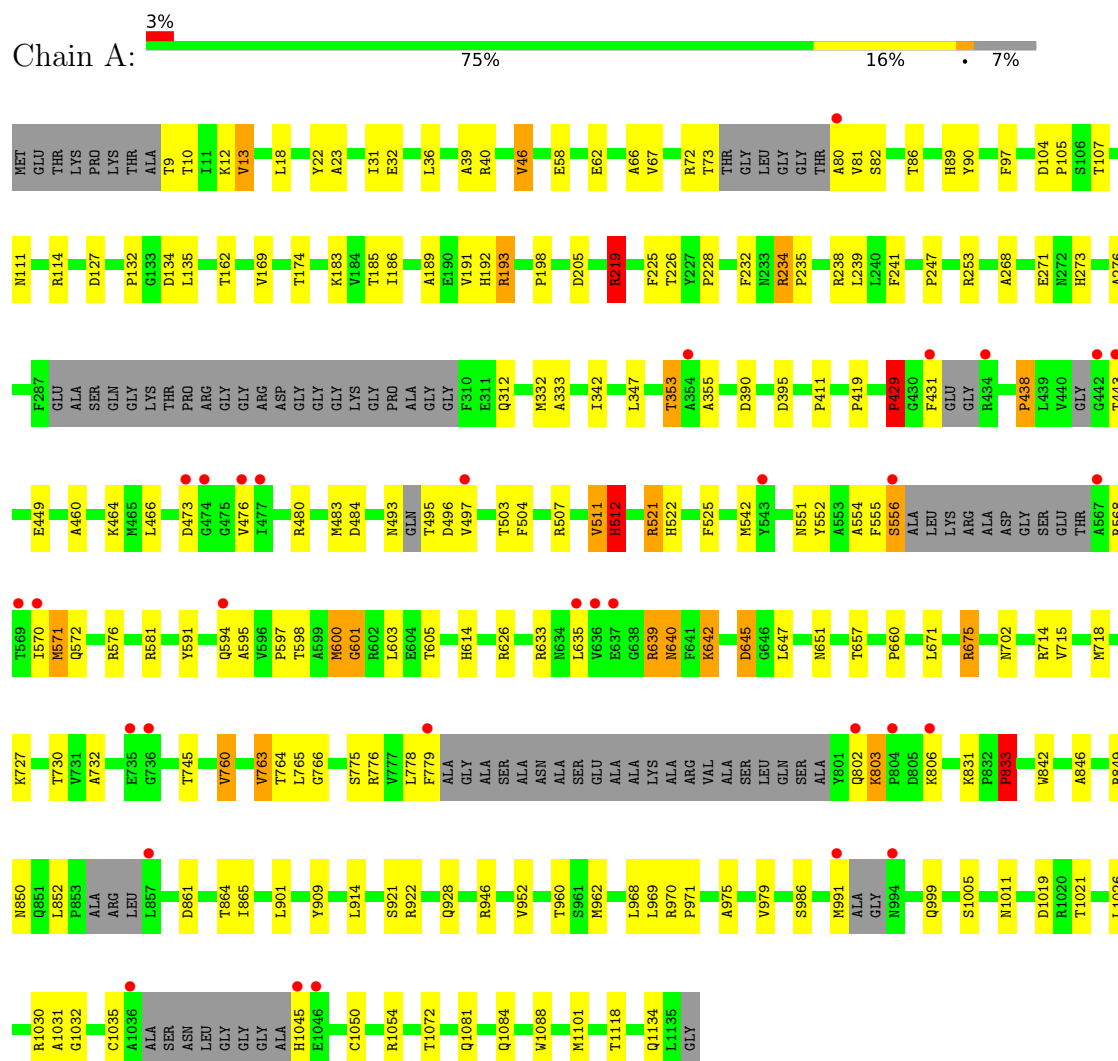
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total 35	O 35	0	0
5	B	69	Total 69	O 69	0	0

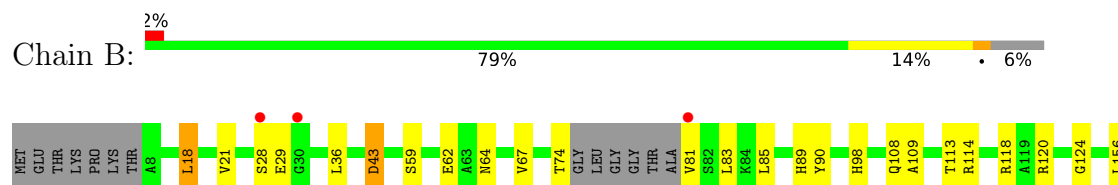
### 3 Residue-property plots [i](#)

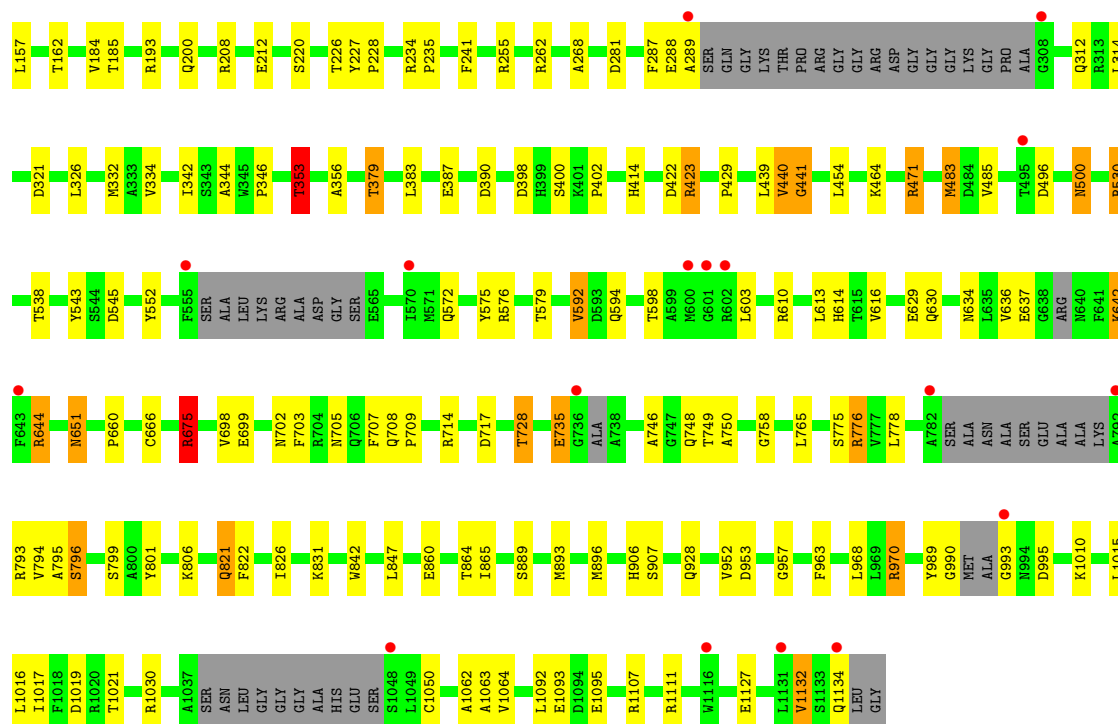
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



#### • Molecule 1: Major DNA-binding protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.35Å 139.78Å 98.87Å 90.00° 111.09° 90.00°	Depositor
Resolution (Å)	92.42 – 2.75 92.25 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.42-2.75) 100.0 (92.25-2.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.177 , 0.261 0.186 , 0.267	Depositor DCC
$R_{free}$ test set	2972 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: GOL, ZN, SO4

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	0.57	1/8202 (0.0%)	1.15	25/11138 (0.2%)
1	B	0.59	0/8320	1.15	25/11301 (0.2%)
All	All	0.58	1/16522 (0.0%)	1.15	50/22439 (0.2%)

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	13
1	B	0	11
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	HIS	CE1-NE2	-6.98	1.25	1.32

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1132	VAL	N-CA-CB	-9.04	102.27	112.21
1	A	429	PRO	N-CA-CB	-8.95	93.85	103.25
1	B	379	THR	CA-CB-OG1	-8.33	97.11	109.60
1	A	833	PRO	N-CA-CB	-7.62	95.25	103.25
1	B	43	ASP	CB-CA-C	-7.13	96.99	110.67
1	A	1045	HIS	CA-CB-CG	6.84	120.64	113.80
1	A	1084	GLN	CB-CA-C	6.75	122.93	110.24
1	B	185	THR	CA-CB-OG1	-6.68	99.58	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	THR	CA-CB-OG1	-6.65	99.63	109.60
1	A	512	HIS	ND1-CE1-NE2	-6.62	101.78	108.40
1	B	321	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	225	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	226	THR	CA-CB-OG1	-6.46	99.91	109.60
1	A	1081	GLN	N-CA-CB	-6.45	100.64	110.12
1	A	429	PRO	N-CA-C	6.36	125.57	112.47
1	A	512	HIS	CE1-NE2-CD2	6.32	115.32	109.00
1	B	423	ARG	N-CA-CB	-6.28	100.55	110.22
1	A	18	LEU	N-CA-CB	-6.20	100.75	110.30
1	B	1019	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	43	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	353	THR	CA-CB-OG1	-6.13	100.41	109.60
1	B	963	PHE	CA-CB-CG	6.08	119.88	113.80
1	B	287	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	219	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	B	387	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	1019	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	241	PHE	N-CA-CB	-5.85	100.89	110.14
1	A	104	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	241	PHE	CA-CB-CG	5.83	119.62	113.80
1	B	728	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	390	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	1118	THR	CA-CB-OG1	-5.63	101.15	109.60
1	B	705	ASN	CB-CA-C	-5.62	100.24	110.63
1	B	821	GLN	N-CA-CB	5.60	118.13	110.01
1	B	821	GLN	CB-CA-C	-5.56	102.14	110.88
1	A	134	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	500	ASN	CB-CA-C	-5.46	100.18	110.01
1	B	62	GLU	CB-CA-C	5.40	119.72	110.81
1	B	281	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	114	ARG	CB-CA-C	-5.35	101.91	110.79
1	B	21	VAL	N-CA-CB	5.25	117.97	111.41
1	B	312	GLN	N-CA-CB	-5.22	102.44	110.01
1	A	438	PRO	N-CA-CB	-5.15	97.84	103.25
1	A	127	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	312	GLN	N-CA-CB	-5.13	102.56	110.16
1	A	228	PRO	N-CA-C	5.11	119.08	111.41
1	B	538	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	395	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	205	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	605	THR	CA-CB-OG1	-5.01	102.09	109.60

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1030	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	234	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	626	ARG	Sidechain
1	A	675	ARG	Sidechain
1	A	714	ARG	Sidechain
1	A	776	ARG	Sidechain
1	A	946	ARG	Sidechain
1	B	1030	ARG	Sidechain
1	B	1107	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	193	ARG	Sidechain
1	B	262	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	471	ARG	Sidechain
1	B	530	ARG	Sidechain
1	B	644	ARG	Sidechain
1	B	675	ARG	Sidechain
1	B	970	ARG	Sidechain

## 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	8030	0	7918	85	0
1	B	8147	0	8032	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	35	0	0	1	0
5	B	69	0	0	2	0
All	All	16294	0	15958	164	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 (164) 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:440:VAL:O	1:B:441:GLY:O	1.76	1.02
1:B:353:THR:HG22	1:B:356:ALA:H	1.38	0.87
1:A:36:LEU:O	1:A:464:LYS:NZ	2.14	0.81
1:B:471:ARG:NH1	1:B:957:GLY:O	2.17	0.77
1:B:675:ARG:HG2	1:B:675:ARG:HH11	1.52	0.73
1:A:46:VAL:CG1	1:A:239:LEU:HD13	2.21	0.70
1:B:990:GLY:O	1:B:993:GLY:N	2.26	0.69
1:B:614:HIS:HE1	1:B:864:THR:OG1	1.78	0.66
1:A:594:GLN:O	1:A:595:ALA:HB3	1.97	0.65
1:A:715:VAL:HA	1:A:718:MET:HE2	1.79	0.65
1:B:634:ASN:HA	1:B:637:GLU:HG2	1.81	0.61
1:A:600:MET:O	1:A:601:GLY:C	2.43	0.60
1:A:62:GLU:HA	1:A:62:GLU:OE1	2.02	0.59
1:B:1015:LEU:O	1:B:1017:ILE:HD12	2.02	0.59
1:A:922:ARG:HB3	1:A:962:MET:HE1	1.83	0.59
1:A:493:ASN:C	1:A:495:THR:N	2.61	0.58
1:B:592:VAL:CG2	1:B:889:SER:OG	2.51	0.58
1:A:186:ILE:HD12	1:A:191:VAL:HG21	1.84	0.58
1:A:89:HIS:CE1	1:A:660:PRO:HG3	2.39	0.58
1:A:591:TYR:O	1:A:603:LEU:HD11	2.04	0.57
1:B:483:MET:HE2	1:B:485:VAL:HG12	1.86	0.57
1:A:521:ARG:NH1	1:A:1011:ASN:O	2.32	0.56
1:A:1072:THR:HG21	1:A:1088:TRP:CH2	2.40	0.56
1:A:715:VAL:HA	1:A:718:MET:CE	2.36	0.56
1:B:464:LYS:HE3	1:B:666:CYS:SG	2.47	0.55
1:B:610:ARG:NH1	1:B:864:THR:OG1	2.39	0.55
1:A:23:ALA:HB3	1:A:192:HIS:HB2	1.88	0.55
1:B:67:VAL:O	1:B:85:LEU:HA	2.07	0.55
1:B:288:GLU:HG3	1:B:289:ALA:N	2.23	0.55
1:B:1062:ALA:HB1	1:B:1132:VAL:HG12	1.89	0.54
1:A:9:THR:N	5:A:1301:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:ARG:NH2	1:B:860:GLU:HB3	2.22	0.54
1:B:579:THR:HG22	1:B:896:MET:CE	2.38	0.54
1:A:46:VAL:HG22	1:A:97:PHE:HA	1.89	0.53
1:B:579:THR:HG22	1:B:896:MET:HE1	1.90	0.53
1:A:1050:CYS:SG	1:A:1054:ARG:NH1	2.82	0.53
1:A:597:PRO:HG3	1:A:971:PRO:HG2	1.91	0.52
1:B:530:ARG:NH2	5:B:1302:HOH:O	2.42	0.52
1:B:651:ASN:HB3	1:B:776:ARG:HA	1.91	0.52
1:A:226:THR:OG1	1:A:745:THR:O	2.22	0.51
1:A:333:ALA:HA	1:A:765:LEU:HD21	1.93	0.51
1:A:572:GLN:O	1:A:581:ARG:NH2	2.43	0.51
1:B:43:ASP:OD2	1:B:113:THR:HB	2.09	0.51
1:A:568:ARG:HA	1:A:571:MET:HE2	1.93	0.51
1:B:1111:ARG:HH11	1:B:1111:ARG:HG3	1.76	0.51
1:A:647:LEU:HD21	1:A:901:LEU:HD23	1.93	0.51
1:B:118:ARG:HH12	1:B:500:ASN:HB2	1.76	0.50
1:A:90:TYR:HA	1:A:162:THR:HA	1.94	0.50
1:A:846:ALA:HB3	1:A:852:LEU:HD13	1.95	0.49
1:B:85:LEU:HD12	1:B:85:LEU:N	2.28	0.49
1:B:1111:ARG:NH2	1:B:1127:GLU:OE2	2.45	0.49
1:B:545:ASP:HA	1:B:576:ARG:HH22	1.78	0.49
1:A:975:ALA:HA	1:A:1031:ALA:HB3	1.95	0.49
1:B:268:ALA:HA	1:B:332:MET:HE3	1.95	0.48
1:A:914:LEU:HB2	1:A:969:LEU:HD13	1.94	0.48
1:B:353:THR:HG22	1:B:356:ALA:N	2.17	0.48
1:B:614:HIS:HE1	1:B:864:THR:HG1	1.60	0.48
1:A:353:THR:O	1:A:355:ALA:N	2.45	0.48
1:A:803:LYS:HB3	1:A:803:LYS:HE3	1.60	0.48
1:A:13:VAL:HG12	1:A:66:ALA:HB2	1.95	0.48
1:A:1032:GLY:N	1:A:1035:CYS:O	2.47	0.47
1:B:847:LEU:HD11	1:B:865:ILE:HD13	1.96	0.47
1:B:89:HIS:CE1	1:B:660:PRO:HG2	2.49	0.47
1:A:268:ALA:HA	1:A:332:MET:HE3	1.97	0.47
1:B:893:MET:HA	1:B:893:MET:HE2	1.96	0.47
1:A:73:THR:HA	1:A:80:ALA:O	2.15	0.47
1:B:228:PRO:HB3	1:B:748:GLN:HB3	1.97	0.47
1:B:98:HIS:HB3	1:B:157:LEU:HB2	1.97	0.46
1:B:390:ASP:OD1	1:B:390:ASP:C	2.56	0.46
1:A:271:GLU:H	1:A:271:GLU:CD	2.23	0.46
1:B:398:ASP:OD1	1:B:400:SER:CB	2.63	0.46
1:B:485:VAL:CG2	1:B:928:GLN:HE21	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HA	1:A:189:ALA:O	2.16	0.46
1:B:1010:LYS:HE2	1:B:1016:LEU:O	2.15	0.46
1:A:411:PRO:HB3	1:A:525:PHE:CD1	2.51	0.46
1:A:576:ARG:CG	1:A:970:ARG:HH22	2.28	0.46
1:A:645:ASP:N	1:A:645:ASP:OD1	2.49	0.46
1:A:1088:TRP:CE3	1:A:1101:MET:HG3	2.51	0.46
1:B:383:LEU:HB3	1:B:454:LEU:HG	1.98	0.46
1:A:778:LEU:O	1:A:779:PHE:C	2.59	0.45
1:B:200:GLN:OE1	1:B:200:GLN:N	2.42	0.45
1:A:842:TRP:HB2	1:B:1132:VAL:HG13	1.98	0.45
1:A:600:MET:HE3	1:A:600:MET:HB3	1.60	0.45
1:A:642:LYS:HD2	1:A:642:LYS:HA	1.47	0.45
1:A:861:ASP:O	1:A:865:ILE:HG12	2.16	0.45
1:B:36:LEU:O	1:B:464:LYS:NZ	2.46	0.45
1:B:576:ARG:HD3	1:B:970:ARG:HH22	1.81	0.45
1:A:921:SER:O	1:A:962:MET:CE	2.65	0.45
1:B:821:GLN:HB2	1:B:822:PHE:CD2	2.52	0.45
1:A:727:LYS:O	1:A:766:GLY:HA2	2.17	0.44
1:A:594:GLN:O	1:A:595:ALA:CB	2.62	0.44
1:B:714:ARG:NH2	5:B:1307:HOH:O	2.50	0.44
1:A:10:THR:HA	1:A:730:THR:O	2.18	0.44
1:A:576:ARG:HG2	1:A:970:ARG:HH22	1.81	0.44
1:B:778:LEU:HD11	1:B:906:HIS:CE1	2.53	0.44
1:B:485:VAL:HG22	1:B:928:GLN:HE21	1.82	0.44
1:A:614:HIS:HE1	1:A:864:THR:OG1	2.01	0.44
1:B:592:VAL:HG21	1:B:889:SER:OG	2.18	0.44
1:A:183:LYS:HE3	1:A:192:HIS:CE1	2.53	0.44
1:A:46:VAL:HG13	1:A:239:LEU:HD13	1.99	0.43
1:B:234:ARG:HB3	1:B:235:PRO:HD3	2.00	0.43
1:A:58:GLU:HA	1:A:186:ILE:HG12	2.01	0.43
1:A:484:ASP:HA	1:A:928:GLN:NE2	2.33	0.43
1:B:801:TYR:CE1	1:B:1021:THR:HG22	2.54	0.43
1:B:708:GLN:N	1:B:709:PRO:CD	2.81	0.43
1:B:728:THR:HA	1:B:765:LEU:O	2.18	0.43
1:A:111:ASN:HD22	1:A:114:ARG:HH21	1.67	0.43
1:A:466:LEU:HD21	1:A:511:VAL:HG13	2.01	0.43
1:A:979:VAL:HA	1:A:1026:LEU:O	2.19	0.43
1:B:847:LEU:C	1:B:847:LEU:HD23	2.44	0.43
1:B:402:PRO:HG3	1:B:989:TYR:HE2	1.84	0.42
1:A:521:ARG:O	1:A:522:HIS:C	2.62	0.42
1:A:921:SER:HA	1:A:960:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ASP:OD1	1:B:422:ASP:C	2.62	0.42
1:A:551:ASN:O	1:A:552:TYR:C	2.61	0.42
1:A:169:VAL:HG22	1:A:174:THR:HG21	2.01	0.42
1:A:232:PHE:CD1	1:A:232:PHE:C	2.97	0.42
1:B:90:TYR:HA	1:B:162:THR:HA	1.99	0.42
1:A:31:ILE:HD12	1:A:31:ILE:HA	1.86	0.42
1:A:273:HIS:HE1	1:A:276:ALA:O	2.03	0.42
1:A:507:ARG:HG3	1:A:512:HIS:HE1	1.84	0.42
1:B:344:ALA:O	1:B:346:PRO:HD3	2.19	0.42
1:A:968:LEU:O	1:A:971:PRO:HD2	2.20	0.42
1:B:18:LEU:C	1:B:18:LEU:HD12	2.44	0.42
1:B:698:VAL:HA	1:B:703:PHE:CD1	2.54	0.42
1:A:12:LYS:HA	1:A:732:ALA:O	2.20	0.42
1:A:39:ALA:HB1	1:A:460:ALA:O	2.20	0.42
1:B:124:GLY:O	1:B:255:ARG:HD3	2.19	0.42
1:B:314:LEU:HD21	1:B:703:PHE:CD2	2.55	0.41
1:B:793:ARG:C	1:B:795:ALA:N	2.78	0.41
1:A:132:PRO:HA	1:A:135:LEU:HD23	2.02	0.41
1:A:419:PRO:HA	1:A:431:PHE:CD1	2.56	0.41
1:B:746:ALA:HB1	1:B:750:ALA:CB	2.50	0.41
1:A:503:THR:O	1:A:504:PHE:C	2.63	0.41
1:B:642:LYS:HD3	1:B:642:LYS:HA	1.51	0.41
1:A:72:ARG:O	1:A:81:VAL:HA	2.21	0.41
1:A:105:PRO:HB2	1:A:107:THR:O	2.21	0.41
1:B:326:LEU:HD12	1:B:326:LEU:HA	1.92	0.41
1:A:760:VAL:HG13	1:A:763:VAL:HG13	2.03	0.41
1:A:849:ARG:O	1:A:850:ASN:C	2.63	0.41
1:B:831:LYS:O	1:B:842:TRP:CZ3	2.74	0.41
1:A:32:GLU:H	1:A:32:GLU:CD	2.29	0.41
1:B:83:LEU:O	1:B:758:GLY:HA2	2.21	0.41
1:B:108:GLN:O	1:B:109:ALA:C	2.60	0.41
1:B:613:LEU:HD22	1:B:826:ILE:HD13	2.03	0.41
1:B:1063:ALA:O	1:B:1064:VAL:C	2.64	0.41
1:A:22:TYR:CZ	1:A:193:ARG:HD2	2.56	0.40
1:A:554:ALA:O	1:A:556:SER:N	2.53	0.40
1:A:647:LEU:HD21	1:A:901:LEU:CD2	2.51	0.40
1:B:227:TYR:HA	1:B:228:PRO:HD3	1.90	0.40
1:B:703:PHE:CE1	1:B:707:PHE:CD2	3.09	0.40
1:B:778:LEU:CD1	1:B:906:HIS:CE1	3.04	0.40
1:B:793:ARG:O	1:B:796:SER:N	2.51	0.40
1:B:288:GLU:HG2	1:B:439:LEU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:TYR:O	1:B:575:TYR:HB3	2.21	0.40
1:B:968:LEU:HD23	1:B:968:LEU:HA	1.92	0.40
1:B:1062:ALA:HB1	1:B:1132:VAL:CG1	2.50	0.40
1:B:1092:LEU:O	1:B:1093:GLU:HB2	2.20	0.40
1:A:568:ARG:O	1:A:572:GLN:NE2	2.55	0.40
1:A:986:SER:O	1:A:999:GLN:HA	2.21	0.40
1:A:833:PRO:HB2	1:B:1134:GLN:NE2	2.36	0.40
1:A:247:PRO:HB3	1:A:671:LEU:HD11	2.04	0.40
1:A:639:ARG:O	1:A:640:ASN:C	2.64	0.40
1:B:735:GLU:H	1:B:735:GLU:HG2	1.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1029/1136 (91%)	967 (94%)	56 (5%)	6 (1%)	21	38
1	B	1053/1136 (93%)	1007 (96%)	44 (4%)	2 (0%)	43	64
All	All	2082/2272 (92%)	1974 (95%)	100 (5%)	8 (0%)	30	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	PRO
1	A	601	GLY
1	A	833	PRO
1	B	441	GLY
1	A	1134	GLN
1	A	555	PHE
1	B	794	VAL
1	A	476	VAL



### 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	839/885 (95%)	787 (94%)	52 (6%)	16	31
1	B	846/885 (96%)	795 (94%)	51 (6%)	17	32
All	All	1685/1770 (95%)	1582 (94%)	103 (6%)	17	31

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	46	VAL
1	A	67	VAL
1	A	82	SER
1	A	86	THR
1	A	198	PRO
1	A	219	ARG
1	A	234	ARG
1	A	235	PRO
1	A	342	ILE
1	A	347	LEU
1	A	353	THR
1	A	429	PRO
1	A	438	PRO
1	A	443	THR
1	A	449	GLU
1	A	473	ASP
1	A	483	MET
1	A	496	ASP
1	A	497	VAL
1	A	511	VAL
1	A	512	HIS
1	A	521	ARG
1	A	542	MET
1	A	556	SER
1	A	570	ILE
1	A	571	MET

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Mol	Chain	Res	Type
1	A	598	THR
1	A	600	MET
1	A	633	ARG
1	A	635	LEU
1	A	639	ARG
1	A	640	ASN
1	A	642	LYS
1	A	645	ASP
1	A	651	ASN
1	A	675	ARG
1	A	702	ASN
1	A	760	VAL
1	A	763	VAL
1	A	764	THR
1	A	775	SER
1	A	802	GLN
1	A	803	LYS
1	A	806	LYS
1	A	831	LYS
1	A	833	PRO
1	A	909	TYR
1	A	952	VAL
1	A	991	MET
1	A	1005	SER
1	A	1021	THR
1	B	18	LEU
1	B	28	SER
1	B	29	GLU
1	B	59	SER
1	B	64	ASN
1	B	74	THR
1	B	81	VAL
1	B	156	LEU
1	B	184	VAL
1	B	208	ARG
1	B	212	GLU
1	B	220	SER
1	B	334	VAL
1	B	342	ILE
1	B	353	THR
1	B	379	THR
1	B	414	HIS

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Mol	Chain	Res	Type
1	B	429	PRO
1	B	440	VAL
1	B	483	MET
1	B	496	ASP
1	B	543	TYR
1	B	572	GLN
1	B	592	VAL
1	B	594	GLN
1	B	598	THR
1	B	603	LEU
1	B	616	VAL
1	B	629	GLU
1	B	630	GLN
1	B	636	VAL
1	B	642	LYS
1	B	644	ARG
1	B	651	ASN
1	B	675	ARG
1	B	699	GLU
1	B	702	ASN
1	B	717	ASP
1	B	735	GLU
1	B	749	THR
1	B	775	SER
1	B	776	ARG
1	B	796	SER
1	B	799	SER
1	B	806	LYS
1	B	907	SER
1	B	952	VAL
1	B	953	ASP
1	B	995	ASP
1	B	1050	CYS
1	B	1095	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	89	HIS
1	A	111	ASN
1	A	137	HIS

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Mol	Chain	Res	Type
1	A	192	HIS
1	A	273	HIS
1	A	572	GLN
1	A	614	HIS
1	A	619	ASN
1	A	706	GLN
1	A	841	GLN
1	A	886	ASN
1	A	928	GLN
1	A	936	GLN
1	A	955	HIS
1	A	1002	ASN
1	A	1052	GLN
1	A	1134	GLN
1	B	64	ASN
1	B	89	HIS
1	B	98	HIS
1	B	111	ASN
1	B	172	ASN
1	B	192	HIS
1	B	237	ASN
1	B	399	HIS
1	B	420	GLN
1	B	444	GLN
1	B	590	GLN
1	B	614	HIS
1	B	640	ASN
1	B	702	ASN
1	B	705	ASN
1	B	720	ASN
1	B	836	ASN
1	B	851	GLN
1	B	928	GLN
1	B	967	ASN
1	B	1134	GLN

### 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
4	GOL	B	1201	-	5,5,5	0.12	0	5,5,5	0.26	0
3	SO4	A	1202	-	4,4,4	0.28	0	6,6,6	0.21	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
4	GOL	B	1201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1201	GOL	O1-C1-C2-O2
4	B	1201	GOL	C1-C2-C3-O3
4	B	1201	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	1201	GOL	O2-C2-C3-O3

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](#)

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	1051/1136 (92%)	0.06	32 (3%) 52 50	18, 39, 68, 103	0
1	B	1071/1136 (94%)	-0.20	20 (1%) 66 64	13, 30, 67, 100	0
All	All	2122/2272 (93%)	-0.07	52 (2%) 58 56	13, 35, 68, 103	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	GLY	4.7
1	B	600	MET	4.5
1	A	567	ALA	4.1
1	A	779	PHE	4.0
1	B	782	ALA	3.9
1	A	477	ILE	3.7
1	B	643	PHE	3.5
1	A	570	ILE	3.5
1	B	28	SER	3.4
1	B	555	PHE	3.3
1	B	289	ALA	3.3
1	A	806	LYS	3.3
1	B	792	ALA	3.0
1	A	1045	HIS	3.0
1	B	495	THR	3.0
1	A	80	ALA	2.9
1	A	476	VAL	2.9
1	B	308	GLY	2.7
1	A	474	GLY	2.7
1	B	81	VAL	2.7
1	A	1046	GLU	2.7
1	B	601	GLY	2.6
1	A	636	VAL	2.5
1	A	443	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	ASP	2.5
1	B	1048	SER	2.5
1	A	354	ALA	2.4
1	A	635	LEU	2.4
1	B	570	ILE	2.4
1	A	431	PHE	2.4
1	B	993	GLY	2.3
1	A	802	GLN	2.3
1	B	1131	LEU	2.2
1	A	991	MET	2.2
1	A	569	THR	2.2
1	A	434	ARG	2.2
1	B	736	GLY	2.2
1	A	497	VAL	2.2
1	B	1116	TRP	2.2
1	A	804	PRO	2.2
1	A	594	GLN	2.2
1	A	994	ASN	2.1
1	B	602	ARG	2.1
1	B	1134	GLN	2.1
1	A	556	SER	2.1
1	A	735	GLU	2.1
1	A	1036	ALA	2.0
1	A	736	GLY	2.0
1	A	543	TYR	2.0
1	A	637	GLU	2.0
1	A	857	LEU	2.0
1	B	30	GLY	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 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,



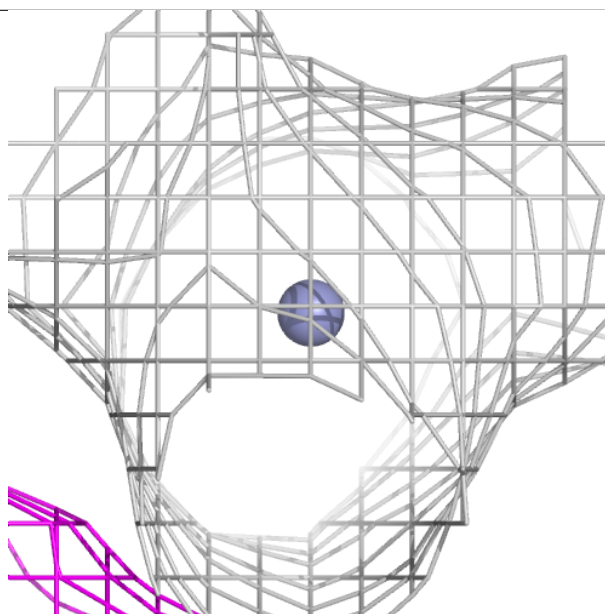
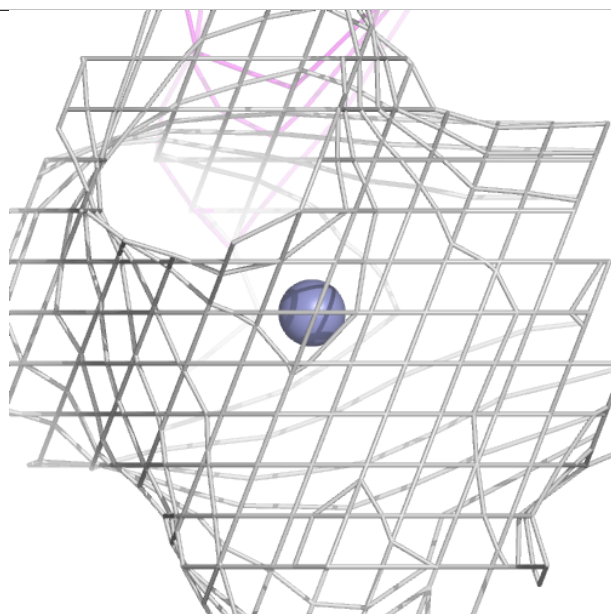
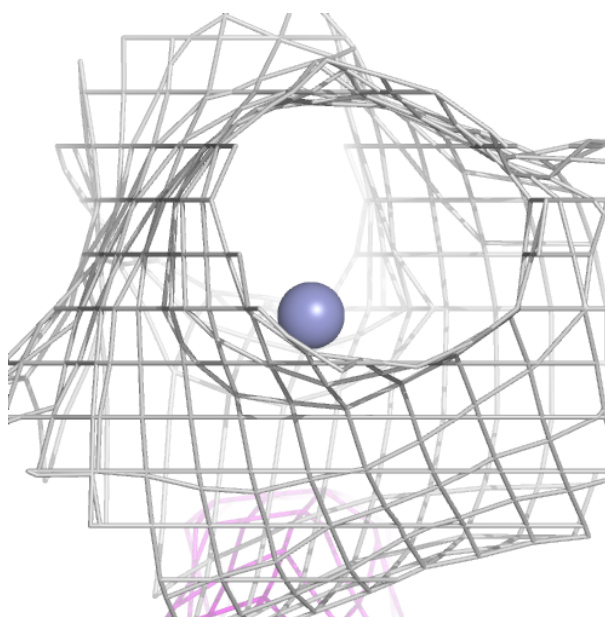
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1202	5/5	0.92	0.23	69,76,82,98	0
4	GOL	B	1201	6/6	0.94	0.10	32,35,35,36	0
2	ZN	A	1201	1/1	0.99	0.02	41,41,41,41	0
2	ZN	B	1202	1/1	0.99	0.01	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

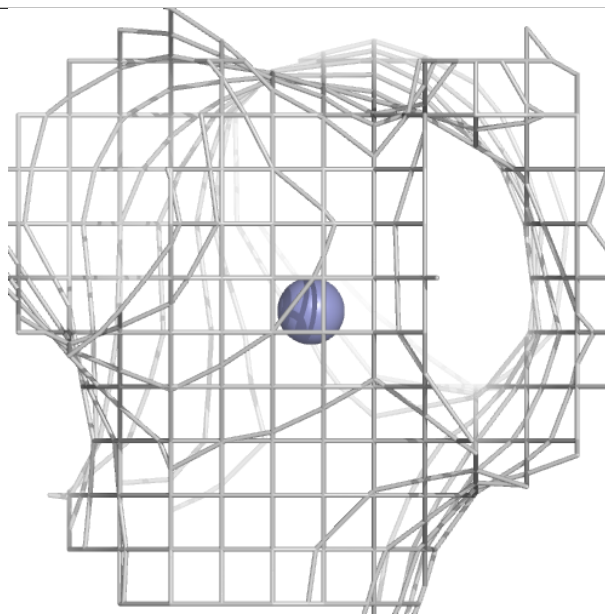
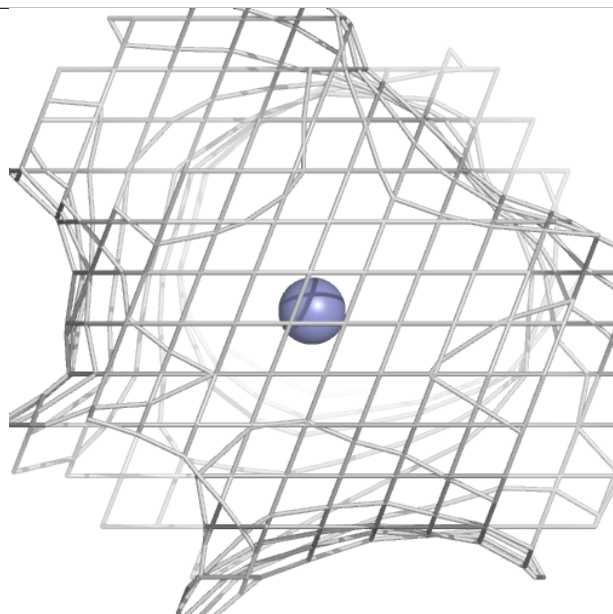
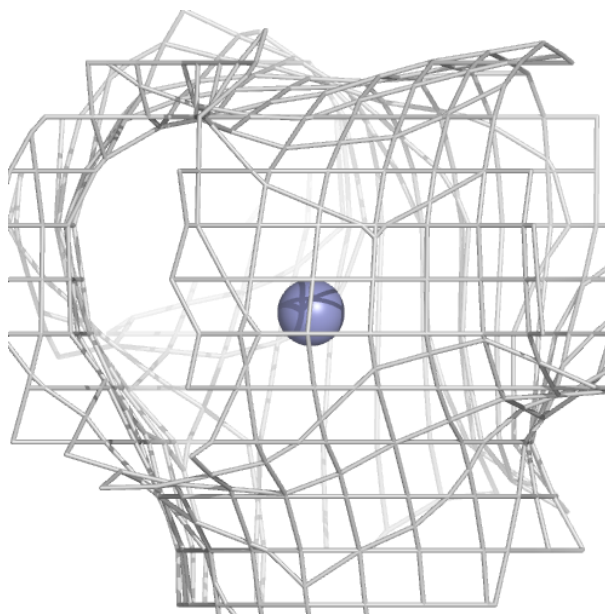
**Electron density around ZN A 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN B 1202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.