



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K8K  
Title : Crystal structure of SusG  
Authors : Koropatkin, N.M.; Smith, T.J.  
Deposited on : 2009-10-14  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

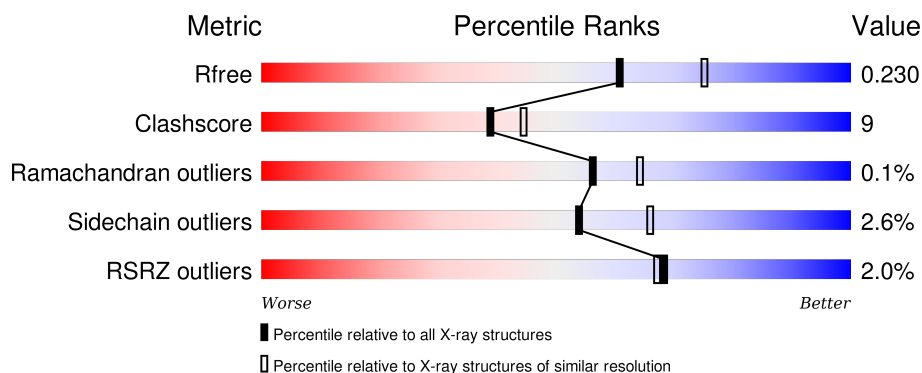
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	669	<div> <div></div> <div>82%</div> <div>13%</div> <div>••</div> </div>
1	B	669	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	904	-	-	-	X
4	EDO	A	908	-	-	-	X
4	EDO	A	910	-	-	-	X
5	PEG	A	951	-	-	-	X
6	ACT	A	961	-	-	-	X
6	ACT	A	962	-	-	-	X
6	ACT	A	973	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10894 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 Alpha-amylase, susG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	Se	0	0	0
			5178	3293	837	1032	5	11			
1	B	649	Total	C	N	O	S	Se	0	0	0
			5169	3288	835	1030	5	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 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
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

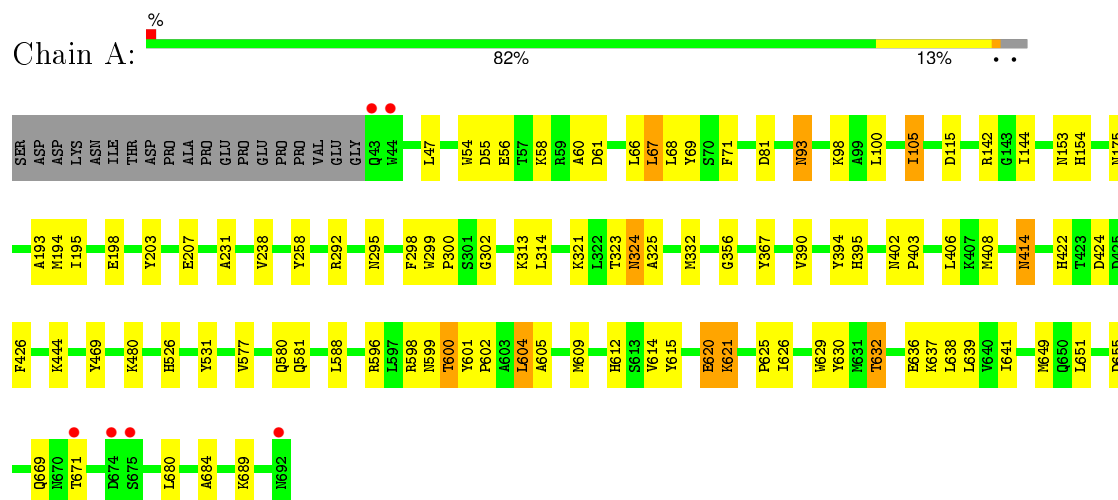
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	335	Total	O	0	0
			335	335		
7	B	129	Total	O	0	0
			129	129		

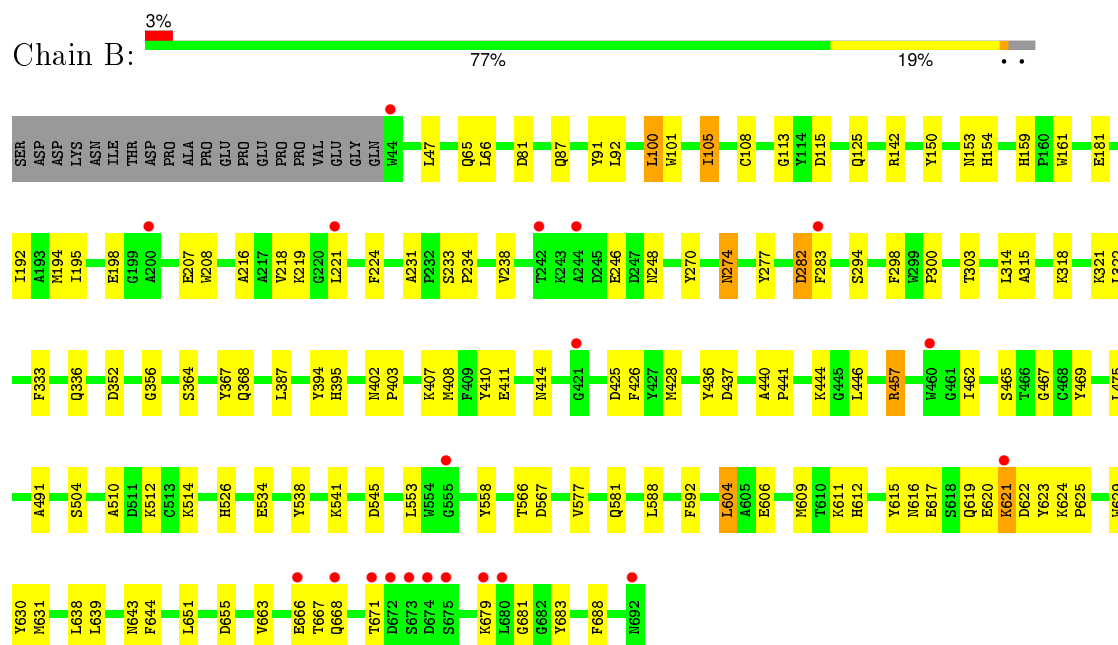
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Alpha-amylase, susG



- Molecule 1: Alpha-amylase, susG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.04Å 128.04Å 129.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 45.27 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.2 (50.00-2.20) 89.0 (45.27-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.99 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.196 , 0.230 0.197 , 0.230	Depositor DCC
$R_{free}$ test set	9435 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.7	EDS
Estimated twinning fraction	0.019 for -h,-l,-k 0.006 for -h,l,k 0.006 for l,-k,h 0.018 for -l,-k,-h 0.030 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 94658 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PEG, MG, ACT, CA, EDO

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	0.37	0/5306	0.60	0/7193
1	B	0.36	0/5297	0.56	0/7181
All	All	0.36	0/10603	0.58	0/14374

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	5178	0	4878	83	0
1	B	5169	0	4870	99	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	45	5	0
4	B	16	0	20	1	0
5	A	7	0	10	2	0
6	A	16	0	12	0	0
6	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	335	0	0	6	0
7	B	129	0	0	3	0
All	All	10894	0	9838	183	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 9.

All (183) 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:A:394:TYR:H	1:A:402:ASN:HD21	1.06	0.96
1:B:394:TYR:H	1:B:402:ASN:HD21	1.11	0.96
1:B:159:HIS:HD2	1:B:161:TRP:H	1.14	0.95
1:B:609:MSE:HB2	1:B:631:MSE:HE1	1.49	0.95
1:B:153:ASN:HD22	1:B:154:HIS:HD2	1.15	0.92
1:A:313:LYS:HE2	1:A:332:MSE:HE3	1.54	0.86
1:A:612:HIS:HD2	1:A:615:TYR:H	1.24	0.85
1:B:663:VAL:HG23	1:B:667:THR:HG21	1.60	0.83
1:A:422:HIS:NE2	4:A:910:EDO:H21	1.93	0.83
1:A:153:ASN:HD22	1:A:154:HIS:HD2	1.24	0.81
1:A:238:VAL:HG21	1:A:314:LEU:HD21	1.63	0.81
1:A:194:MSE:HE1	1:A:356:GLY:O	1.85	0.76
1:B:612:HIS:HD2	1:B:615:TYR:H	1.30	0.76
1:B:238:VAL:HG21	1:B:314:LEU:HD21	1.67	0.75
1:B:153:ASN:HD22	1:B:154:HIS:CD2	2.03	0.74
1:A:626:ILE:HD11	1:A:649:MSE:HE3	1.70	0.73
1:A:302:GLY:HA2	1:A:324:ASN:HD21	1.54	0.73
1:B:194:MSE:HE1	1:B:356:GLY:O	1.89	0.72
1:B:414:ASN:ND2	1:B:426:PHE:H	1.88	0.71
1:B:604:LEU:HD13	1:B:638:LEU:HD12	1.72	0.70
1:B:629:TRP:CD1	1:B:631:MSE:HE3	2.27	0.70
1:A:632:THR:HG23	7:A:722:HOH:O	1.92	0.68
1:A:596:ARG:O	1:A:600:THR:HG23	1.94	0.68
1:B:465:SER:HA	1:B:644:PHE:O	1.93	0.68
1:B:195:ILE:HG12	1:B:395:HIS:HB2	1.75	0.67
1:A:198:GLU:OE1	1:A:395:HIS:HD2	1.77	0.67
1:B:609:MSE:CB	1:B:631:MSE:HE1	2.23	0.67
1:B:621:LYS:HA	1:B:621:LYS:HE2	1.77	0.66
1:B:238:VAL:CG2	1:B:314:LEU:HD21	2.25	0.65
1:A:639:LEU:HD11	1:A:641:ILE:HD11	1.80	0.63
1:A:480:LYS:HE3	7:A:725:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:THR:HG21	1:A:637:LYS:NZ	2.13	0.63
1:A:671:THR:O	1:A:671:THR:HG22	1.99	0.63
1:B:444:LYS:HE3	7:B:813:HOH:O	1.98	0.63
1:B:300:PRO:O	1:B:303:THR:HB	1.98	0.63
1:B:234:PRO:HG2	1:B:322:LEU:HB2	1.82	0.62
1:A:203:TYR:OH	4:A:904:EDO:H21	2.01	0.61
1:B:666:GLU:HB3	1:B:681:GLY:HA3	1.84	0.60
1:A:604:LEU:HD13	1:A:638:LEU:HD12	1.83	0.60
1:B:629:TRP:NE1	1:B:631:MSE:HE3	2.17	0.60
1:B:462:ILE:HG22	1:B:512:LYS:HE3	1.83	0.60
1:B:159:HIS:CD2	1:B:161:TRP:H	2.06	0.59
1:A:612:HIS:CD2	1:A:615:TYR:H	2.15	0.58
1:A:100:LEU:HD13	1:A:144:ILE:HG21	1.84	0.58
1:A:596:ARG:HE	5:A:951:PEG:H21	1.67	0.58
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.69	0.58
1:A:620:GLU:OE2	1:A:621:LYS:HE2	2.04	0.58
1:A:58:LYS:O	1:A:98:LYS:HE3	2.03	0.58
1:A:469:TYR:OH	1:A:620:GLU:HG3	2.04	0.57
1:A:207:GLU:OE1	1:A:395:HIS:HE1	1.87	0.57
1:A:632:THR:HG21	1:A:637:LYS:HZ1	1.69	0.57
1:A:238:VAL:CG2	1:A:314:LEU:HD21	2.34	0.57
1:A:367:TYR:CZ	1:A:408:MSE:HE3	2.39	0.57
1:B:91:TYR:OH	1:B:534:GLU:OE1	2.22	0.57
1:B:504:SER:OG	1:B:538:TYR:HB2	2.04	0.57
1:A:60:ALA:H	1:A:599:ASN:HD22	1.51	0.56
1:A:444:LYS:HG2	7:A:822:HOH:O	2.04	0.56
1:B:541:LYS:HE3	1:B:545:ASP:OD1	2.06	0.56
1:A:47:LEU:HD22	1:A:669:GLN:HE21	1.70	0.56
1:A:612:HIS:CD2	1:A:614:VAL:H	2.23	0.55
1:A:67:LEU:HD22	1:A:531:TYR:HE2	1.71	0.55
1:A:100:LEU:HD13	1:A:144:ILE:CG2	2.37	0.55
1:A:302:GLY:CA	1:A:324:ASN:HD21	2.19	0.54
1:A:680:LEU:HD22	1:A:684:ALA:HB3	1.89	0.54
1:A:321:LYS:H	1:A:321:LYS:HD2	1.72	0.54
1:B:125:GLN:NE2	4:B:905:EDO:O2	2.41	0.54
4:A:911:EDO:O2	1:B:321:LYS:HE2	2.09	0.53
1:A:323:THR:HG22	1:A:325:ALA:H	1.73	0.53
1:B:92:LEU:HD13	1:B:100:LEU:HD11	1.89	0.53
1:B:663:VAL:HG21	1:B:667:THR:OG1	2.09	0.52
1:B:510:ALA:O	1:B:514:LYS:HG3	2.10	0.52
1:A:414:ASN:ND2	1:A:426:PHE:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:HIS:CE1	4:A:910:EDO:H21	2.45	0.52
1:A:47:LEU:HD22	1:A:669:GLN:NE2	2.25	0.52
1:B:153:ASN:ND2	1:B:154:HIS:HD2	1.96	0.51
1:A:402:ASN:HB2	1:A:403:PRO:HD3	1.93	0.51
1:B:577:VAL:O	1:B:581:GLN:HG3	2.11	0.51
1:A:612:HIS:HE1	1:A:655:ASP:OD2	1.94	0.51
1:B:440:ALA:HB3	1:B:441:PRO:HD3	1.93	0.50
1:B:394:TYR:H	1:B:402:ASN:ND2	1.94	0.50
1:A:67:LEU:HD22	1:A:531:TYR:CE2	2.45	0.50
1:B:364:SER:O	1:B:368:GLN:HG3	2.12	0.50
1:A:298:PHE:O	1:A:300:PRO:HD3	2.11	0.50
1:A:596:ARG:O	1:A:600:THR:CG2	2.60	0.50
1:B:616:ASN:HB2	1:B:617:GLU:OE1	2.12	0.50
1:A:612:HIS:HD2	1:A:615:TYR:N	2.03	0.49
1:B:387:LEU:HD11	1:B:428:MSE:HE3	1.94	0.49
1:B:410:TYR:HB2	1:B:428:MSE:HE2	1.94	0.49
1:A:636:GLU:HG3	1:A:689:LYS:NZ	2.27	0.49
1:A:67:LEU:HG	1:A:69:TYR:OH	2.13	0.49
1:B:315:ALA:HB3	1:B:318:LYS:HD2	1.93	0.49
1:B:609:MSE:HE2	1:B:629:TRP:CD2	2.48	0.49
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.78	0.49
1:A:195:ILE:HG12	1:A:395:HIS:HB2	1.95	0.48
1:B:553:LEU:O	1:B:577:VAL:HG23	2.13	0.48
1:B:298:PHE:O	1:B:300:PRO:HD3	2.13	0.48
1:B:87:GLN:NE2	1:B:558:TYR:OH	2.46	0.48
1:A:55:ASP:O	1:A:56:GLU:HB2	2.14	0.48
1:B:231:ALA:HA	1:B:233:SER:N	2.27	0.48
1:B:108:CYS:SG	1:B:113:GLY:HA2	2.53	0.48
4:A:910:EDO:H22	7:A:702:HOH:O	2.14	0.48
1:A:66:LEU:C	1:A:66:LEU:HD12	2.34	0.48
1:B:105:ILE:HG23	7:B:769:HOH:O	2.14	0.48
1:A:626:ILE:CD1	1:A:649:MSE:HE3	2.40	0.48
1:B:216:ALA:O	1:B:336:GLN:HG2	2.14	0.48
1:B:671:THR:O	1:B:671:THR:HG22	2.14	0.48
1:B:620:GLU:N	1:B:620:GLU:OE1	2.46	0.48
1:B:207:GLU:OE1	1:B:395:HIS:HE1	1.96	0.47
1:B:643:ASN:O	1:B:683:TYR:HA	2.14	0.47
1:B:66:LEU:C	1:B:66:LEU:HD12	2.34	0.47
1:A:625:PRO:HD2	1:A:649:MSE:HE1	1.95	0.47
1:B:294:SER:HB3	1:B:303:THR:HG21	1.97	0.47
1:B:231:ALA:HA	1:B:234:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:MSE:HE2	1:B:446:LEU:CD2	2.45	0.47
1:A:394:TYR:H	1:A:402:ASN:ND2	1.91	0.46
1:B:231:ALA:HA	1:B:233:SER:H	1.81	0.46
1:B:668:GLN:OE1	1:B:679:LYS:HD3	2.15	0.46
1:B:663:VAL:HG23	1:B:667:THR:CG2	2.40	0.46
1:B:142:ARG:HG3	1:B:142:ARG:NH1	2.30	0.46
1:B:624:LYS:NZ	1:B:624:LYS:HB2	2.30	0.46
1:A:54:TRP:CZ2	1:A:56:GLU:HA	2.50	0.45
1:B:367:TYR:CZ	1:B:408:MSE:HE3	2.51	0.45
1:B:491:ALA:HA	1:B:526:HIS:O	2.15	0.45
1:B:248:ASN:HA	1:B:270:TYR:OH	2.17	0.45
1:A:580:GLN:HG2	7:A:896:HOH:O	2.16	0.45
1:A:71:PHE:HB3	7:A:733:HOH:O	2.16	0.45
1:A:577:VAL:O	1:A:581:GLN:HG3	2.17	0.45
1:A:153:ASN:HD22	1:A:154:HIS:CD2	2.16	0.44
1:B:219:LYS:HA	1:B:283:PHE:O	2.17	0.44
1:A:596:ARG:NE	5:A:951:PEG:H11	2.32	0.44
1:B:402:ASN:HB2	1:B:403:PRO:HD3	1.99	0.44
1:B:619:GLN:HB3	1:B:623:TYR:HB2	1.99	0.44
1:A:323:THR:HG22	1:A:324:ASN:N	2.33	0.44
1:B:198:GLU:OE1	1:B:395:HIS:HD2	1.99	0.44
1:A:609:MSE:HA	1:A:630:TYR:O	2.18	0.44
1:B:609:MSE:HA	1:B:631:MSE:HE2	2.00	0.43
1:A:198:GLU:OE1	1:A:395:HIS:CD2	2.64	0.43
1:B:566:THR:HG22	1:B:567:ASP:N	2.33	0.43
1:B:457:ARG:HD3	1:B:457:ARG:HA	1.83	0.43
1:A:598:ARG:O	1:A:605:ALA:HB2	2.18	0.43
1:B:277:TYR:CD2	1:B:277:TYR:N	2.85	0.43
1:B:630:TYR:O	1:B:631:MSE:HE2	2.19	0.43
1:B:414:ASN:HD21	1:B:425:ASP:HA	1.84	0.43
1:B:274:ASN:HD22	1:B:274:ASN:HA	1.54	0.43
1:B:436:TYR:CG	1:B:437:ASP:N	2.87	0.43
1:B:629:TRP:CD1	1:B:631:MSE:CE	2.99	0.43
1:A:54:TRP:CD1	1:A:600:THR:HG22	2.54	0.43
1:A:258:TYR:CE1	1:A:295:ASN:HB3	2.53	0.43
1:A:54:TRP:CE2	1:A:56:GLU:HA	2.53	0.43
1:A:60:ALA:H	1:A:599:ASN:ND2	2.16	0.42
1:B:623:TYR:CE1	1:B:651:LEU:HD23	2.54	0.42
1:B:101:TRP:C	1:B:101:TRP:CD1	2.93	0.42
1:B:609:MSE:CB	1:B:631:MSE:CE	2.95	0.42
1:B:624:LYS:HB3	1:B:625:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:LEU:HG	1:B:592:PHE:CE2	2.55	0.42
1:A:93:ASN:HD22	1:A:93:ASN:HA	1.64	0.42
1:A:626:ILE:HD12	1:A:651:LEU:HD11	2.02	0.42
1:B:224:PHE:CD2	1:B:238:VAL:HG22	2.55	0.42
1:B:407:LYS:O	1:B:411:GLU:HG3	2.20	0.42
1:A:61:ASP:OD2	1:A:526:HIS:HD2	2.02	0.42
1:A:258:TYR:CZ	1:A:295:ASN:HB3	2.54	0.42
1:A:390:VAL:HB	1:A:406:LEU:HD11	2.01	0.42
1:B:221:LEU:HD23	1:B:282:ASP:HA	2.01	0.42
1:A:302:GLY:HA2	1:A:324:ASN:ND2	2.28	0.42
1:B:192:ILE:HD13	1:B:208:TRP:CH2	2.55	0.42
1:A:601:TYR:HA	1:A:602:PRO:HD3	1.94	0.42
1:A:292:ARG:HD2	1:A:299:TRP:CH2	2.55	0.42
1:B:303:THR:CG2	7:B:796:HOH:O	2.67	0.41
1:A:609:MSE:HE2	1:A:629:TRP:CD2	2.54	0.41
1:B:639:LEU:HB3	1:B:688:PHE:HB2	2.01	0.41
1:B:612:HIS:HE1	1:B:655:ASP:OD2	2.04	0.41
1:A:193:ALA:C	1:A:194:MSE:HE2	2.41	0.41
1:A:636:GLU:HG3	1:A:689:LYS:HZ1	1.84	0.41
1:B:192:ILE:HD13	1:B:208:TRP:HH2	1.85	0.41
1:A:68:LEU:HD11	1:A:105:ILE:HG22	2.03	0.41
1:B:609:MSE:HE2	1:B:629:TRP:CE2	2.56	0.41
1:A:580:GLN:NE2	1:A:588:LEU:H	2.19	0.41
1:B:475:LEU:CD1	1:B:611:LYS:HG3	2.51	0.41
1:B:47:LEU:HD12	1:B:667:THR:HB	2.02	0.41
1:B:65:GLN:HG3	1:B:101:TRP:CE3	2.56	0.41
1:B:467:GLY:C	1:B:469:TYR:H	2.24	0.40
1:B:218:VAL:HG21	1:B:333:PHE:CD2	2.56	0.40
1:B:428:MSE:CE	1:B:446:LEU:CD2	2.99	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	648/669 (97%)	625 (96%)	22 (3%)	1 (0%)	52	59
1	B	647/669 (97%)	605 (94%)	42 (6%)	0	100	100
All	All	1295/1338 (97%)	1230 (95%)	64 (5%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA

### 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	551/557 (99%)	537 (98%)	14 (2%)	55	67
1	B	550/557 (99%)	535 (97%)	15 (3%)	52	64
All	All	1101/1114 (99%)	1072 (97%)	29 (3%)	54	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	81	ASP
1	A	93	ASN
1	A	105	ILE
1	A	115	ASP
1	A	175	ASN
1	A	324	ASN
1	A	414	ASN
1	A	424	ASP
1	A	600	THR
1	A	604	LEU
1	A	620	GLU
1	A	621	LYS
1	A	632	THR
1	B	81	ASP

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Mol	Chain	Res	Type
1	B	100	LEU
1	B	105	ILE
1	B	115	ASP
1	B	150	TYR
1	B	181	GLU
1	B	246	GLU
1	B	274	ASN
1	B	282	ASP
1	B	352	ASP
1	B	457	ARG
1	B	604	LEU
1	B	606	GLU
1	B	621	LYS
1	B	622	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	106	HIS
1	A	154	HIS
1	A	274	ASN
1	A	324	ASN
1	A	337	GLN
1	A	395	HIS
1	A	402	ASN
1	A	414	ASN
1	A	526	HIS
1	A	543	ASN
1	A	561	ASN
1	A	580	GLN
1	A	589	ASN
1	A	599	ASN
1	A	612	HIS
1	A	669	GLN
1	B	87	GLN
1	B	94	GLN
1	B	125	GLN
1	B	154	HIS
1	B	159	HIS
1	B	274	ASN
1	B	395	HIS

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Mol	Chain	Res	Type
1	B	402	ASN
1	B	414	ASN
1	B	561	ASN
1	B	589	ASN
1	B	612	HIS
1	B	650	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	EDO	A	900	-	3,3,3	2.22	1 (33%)	2,2,2	0.41	0
4	EDO	A	901	-	3,3,3	2.18	1 (33%)	2,2,2	0.41	0
4	EDO	A	902	-	3,3,3	2.11	1 (33%)	2,2,2	0.36	0
4	EDO	A	903	-	3,3,3	2.16	1 (33%)	2,2,2	0.38	0
4	EDO	A	904	-	3,3,3	2.16	1 (33%)	2,2,2	0.36	0
4	EDO	A	908	-	3,3,3	2.14	1 (33%)	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	909	-	3,3,3	2.11	1 (33%)	2,2,2	0.36	0
4	EDO	A	910	-	3,3,3	2.14	1 (33%)	2,2,2	0.37	0
4	EDO	A	911	-	3,3,3	2.14	1 (33%)	2,2,2	0.44	0
5	PEG	A	951	-	6,6,6	0.91	0	5,5,5	2.28	3 (60%)
6	ACT	A	961	-	1,3,3	1.58	0	0,3,3	0.00	-
6	ACT	A	962	-	1,3,3	1.28	0	0,3,3	0.00	-
6	ACT	A	972	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
6	ACT	A	973	-	1,3,3	1.66	0	0,3,3	0.00	-
4	EDO	B	905	-	3,3,3	2.15	1 (33%)	2,2,2	0.41	0
4	EDO	B	906	-	3,3,3	2.17	1 (33%)	2,2,2	0.42	0
4	EDO	B	907	-	3,3,3	2.16	1 (33%)	2,2,2	0.40	0
4	EDO	B	912	-	3,3,3	2.15	1 (33%)	2,2,2	0.34	0
6	ACT	B	971	-	1,3,3	1.70	0	0,3,3	0.00	-

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	EDO	A	900	-	-	0/1/1/1	0/0/0/0
4	EDO	A	901	-	-	0/1/1/1	0/0/0/0
4	EDO	A	902	-	-	0/1/1/1	0/0/0/0
4	EDO	A	903	-	-	0/1/1/1	0/0/0/0
4	EDO	A	904	-	-	0/1/1/1	0/0/0/0
4	EDO	A	908	-	-	0/1/1/1	0/0/0/0
4	EDO	A	909	-	-	0/1/1/1	0/0/0/0
4	EDO	A	910	-	-	0/1/1/1	0/0/0/0
4	EDO	A	911	-	-	0/1/1/1	0/0/0/0
5	PEG	A	951	-	-	0/4/4/4	0/0/0/0
6	ACT	A	961	-	-	0/0/0/0	0/0/0/0
6	ACT	A	962	-	-	0/0/0/0	0/0/0/0
6	ACT	A	972	-	-	0/0/0/0	0/0/0/0
6	ACT	A	973	-	-	0/0/0/0	0/0/0/0
4	EDO	B	905	-	-	0/1/1/1	0/0/0/0
4	EDO	B	906	-	-	0/1/1/1	0/0/0/0
4	EDO	B	907	-	-	0/1/1/1	0/0/0/0
4	EDO	B	912	-	-	0/1/1/1	0/0/0/0
6	ACT	B	971	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	EDO	O1-C1	-3.65	1.22	1.42
4	A	901	EDO	O1-C1	-3.61	1.22	1.42
4	B	906	EDO	O1-C1	-3.56	1.22	1.42
4	A	911	EDO	O1-C1	-3.54	1.22	1.42
4	A	908	EDO	O1-C1	-3.54	1.22	1.42
4	A	904	EDO	O1-C1	-3.54	1.22	1.42
4	A	903	EDO	O1-C1	-3.53	1.23	1.42
4	B	905	EDO	O1-C1	-3.53	1.23	1.42
4	B	907	EDO	O1-C1	-3.53	1.23	1.42
4	B	912	EDO	O1-C1	-3.51	1.23	1.42
4	A	910	EDO	O1-C1	-3.49	1.23	1.42
4	A	902	EDO	O1-C1	-3.44	1.23	1.42
4	A	909	EDO	O1-C1	-3.44	1.23	1.42
6	A	972	ACT	CH3-C	2.61	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	951	PEG	O2-C3-C4	2.58	122.30	110.43
5	A	951	PEG	O2-C2-C1	2.67	122.73	110.43
5	A	951	PEG	C3-O2-C2	3.17	126.92	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	EDO	1	0
4	A	910	EDO	3	0
4	A	911	EDO	1	0
5	A	951	PEG	2	0
4	B	905	EDO	1	0

## 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	639/669 (95%)	-0.32	6 (0%) 85 85	22, 37, 52, 65	0
1	B	638/669 (95%)	-0.03	20 (3%) 52 51	31, 48, 59, 66	0
All	All	1277/1338 (95%)	-0.18	26 (2%) 68 67	22, 42, 57, 66	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	674	ASP	4.3
1	B	675	SER	3.5
1	B	666	GLU	3.5
1	B	680	LEU	3.4
1	B	692	ASN	3.2
1	A	692	ASN	3.1
1	B	672	ASP	3.1
1	B	671	THR	3.0
1	A	44	TRP	3.0
1	B	421	GLY	2.8
1	A	43	GLN	2.6
1	B	44	TRP	2.6
1	B	673	SER	2.5
1	B	460	TRP	2.4
1	A	675	SER	2.3
1	B	668	GLN	2.3
1	A	674	ASP	2.3
1	B	621	LYS	2.3
1	B	221	LEU	2.2
1	B	283	PHE	2.1
1	B	200	ALA	2.1
1	B	679	LYS	2.1
1	A	671	THR	2.0
1	B	242	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	244	ALA	2.0
1	B	555	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	A	910	4/4	0.74	0.23	17.63	61,61,61,62	0
5	PEG	A	951	7/7	0.92	0.28	7.05	49,50,54,58	0
6	ACT	A	962	4/4	0.90	0.22	6.42	50,52,53,55	0
6	ACT	A	961	4/4	0.91	0.24	6.06	53,54,55,57	0
4	EDO	A	904	4/4	0.81	0.16	4.59	48,51,52,52	0
6	ACT	A	973	4/4	0.92	0.29	4.03	59,62,63,64	0
4	EDO	A	908	4/4	0.97	0.17	3.31	47,52,53,56	0
4	EDO	A	901	4/4	0.99	0.16	1.81	42,43,44,45	0
4	EDO	A	903	4/4	0.93	0.13	1.09	46,48,49,49	0
4	EDO	A	911	4/4	0.92	0.12	0.65	59,60,60,64	0
6	ACT	B	971	4/4	0.98	0.13	0.52	53,55,55,56	0
2	MG	B	800	1/1	0.95	0.11	0.35	53,53,53,53	0
4	EDO	B	905	4/4	0.85	0.14	0.03	58,58,58,60	0
3	CA	A	710	1/1	1.00	0.11	-0.47	31,31,31,31	0
3	CA	B	810	1/1	0.99	0.09	-0.68	38,38,38,38	0
4	EDO	A	900	4/4	0.97	0.09	-1.32	43,46,48,50	0
2	MG	A	700	1/1	0.96	0.04	-3.33	36,36,36,36	0
4	EDO	B	906	4/4	0.97	0.10	-3.42	50,50,52,52	0
6	ACT	A	972	4/4	0.91	0.13	-	55,55,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	909	4/4	0.86	0.14	-	55,58,58,58	0
4	EDO	B	907	4/4	0.91	0.27	-	60,60,61,61	0
4	EDO	A	902	4/4	0.95	0.09	-	54,55,56,57	0
4	EDO	B	912	4/4	0.79	0.17	-	57,57,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.