



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:41 PM GMT

PDB ID : 1UR9  
Title : Interactions of a family 18 chitinase with the designed inhibitor HM508, and its degradation product, chitobiono-delta-lactone  
Authors : Vaaje-Kolstad, G.; Vasella, A.; Peter, M.G.; Netter, C.; Houston, D.R.; West-ereng, B.; Synstad, B.; Eijsink, V.G.H.; Van Aalten, D.M.F.  
Deposited on : 2003-10-27  
Resolution : 1.80 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.

---

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

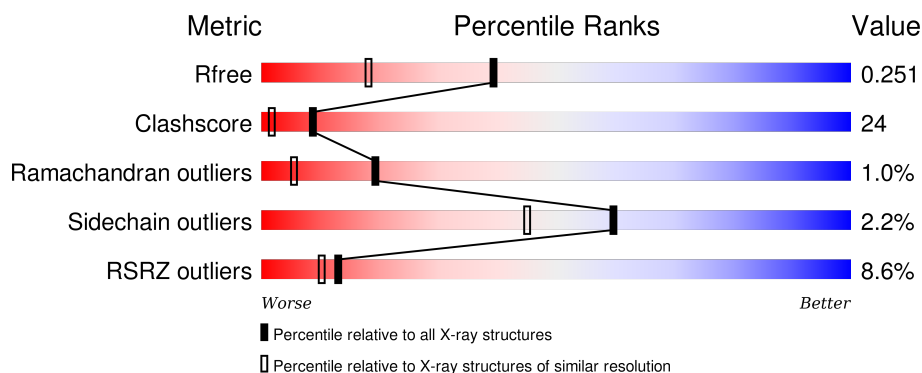
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	499	<div> <div>9%</div> <div>75%</div> <div>23%</div> </div>
1	B	499	<div> <div>8%</div> <div>74%</div> <div>24%</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
2	GOL	A	1500	-	-	X	X
2	GOL	A	1502	-	-	X	X
2	GOL	A	1503	-	-	-	X
2	GOL	A	1504	-	-	-	X
2	GOL	A	1505	-	-	X	-
2	GOL	A	1506	-	-	-	X
2	GOL	A	1507	-	-	X	-
2	GOL	A	1509	-	-	X	X
2	GOL	A	1511	-	-	-	X
2	GOL	A	1512	-	-	X	X
2	GOL	A	1513	-	-	X	X
2	GOL	A	1514	-	-	-	X
2	GOL	A	1516	-	-	-	X
2	GOL	A	1517	-	-	X	-
2	GOL	A	1519	-	-	-	X
2	GOL	A	1520	-	-	-	X
2	GOL	A	1521	-	-	X	-
2	GOL	A	1524	-	-	-	X
2	GOL	A	1525	-	-	X	X
2	GOL	A	1526	-	-	-	X
2	GOL	A	1527	-	-	X	-
2	GOL	A	1528	-	-	X	X
2	GOL	A	1538	-	-	-	X
2	GOL	B	1500	-	-	X	-
2	GOL	B	1501	-	-	-	X
2	GOL	B	1502	-	-	-	X
2	GOL	B	1503	-	-	X	X
2	GOL	B	1505	-	-	X	X
2	GOL	B	1506	-	-	-	X
2	GOL	B	1507	-	-	-	X
2	GOL	B	1508	-	-	X	-
2	GOL	B	1509	-	-	-	X
2	GOL	B	1510	-	-	-	X
2	GOL	B	1511	-	-	X	X
2	GOL	B	1512	-	-	-	X
2	GOL	B	1514	-	-	X	-
2	GOL	B	1515	-	-	X	X
2	GOL	B	1516	-	-	X	X
2	GOL	B	1520	-	-	-	X
2	GOL	B	1521	-	-	X	-
2	GOL	B	1522	-	-	X	X
2	GOL	B	1523	-	-	-	X
2	GOL	B	1524	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	1525	-	-	-	X
2	GOL	B	1526	-	-	-	X
2	GOL	B	1527	-	-	X	-
2	GOL	B	1528	-	-	-	X
2	GOL	B	1529	-	-	X	X
2	GOL	B	1531	-	-	X	-
2	GOL	B	1537	-	-	-	X
3	SO4	A	1533	-	-	X	-
3	SO4	B	1535	-	-	-	X
6	PHJ	A	2503	-	-	X	X
6	PHJ	B	2503	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9198 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.

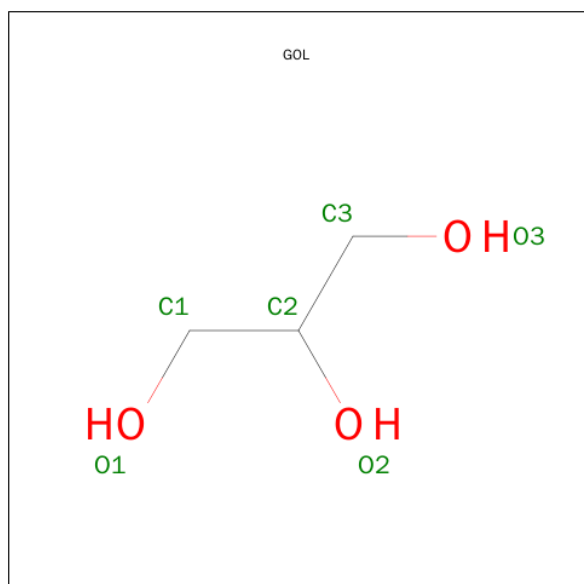
- Molecule 1 is a protein called CHITINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	2	1
			3904	2498	658	733	15			
1	B	498	Total	C	N	O	S	0	7	0
			3933	2513	664	741	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASN	ASP	ENGINEERED MUTATION	UNP Q54276
B	142	ASN	ASP	ENGINEERED MUTATION	UNP Q54276
A	499	ARG	ALA	CONFLICT	UNP Q54276
B	499	ARG	ALA	CONFLICT	UNP Q54276

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

*Continued from previous page...*

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

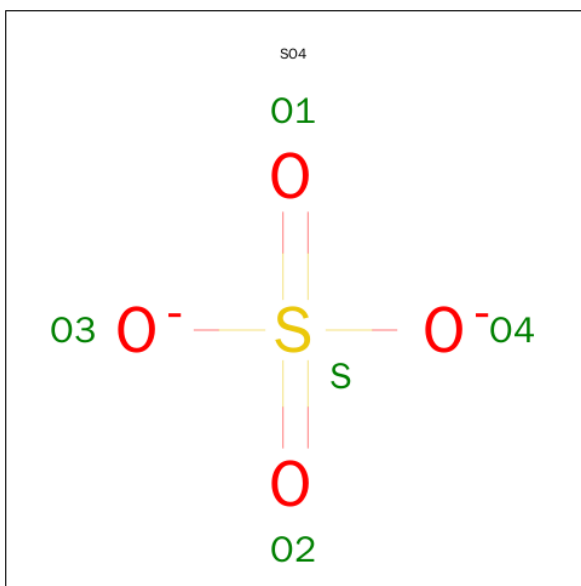
*Continued on next page...*

*Continued from previous page...*

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

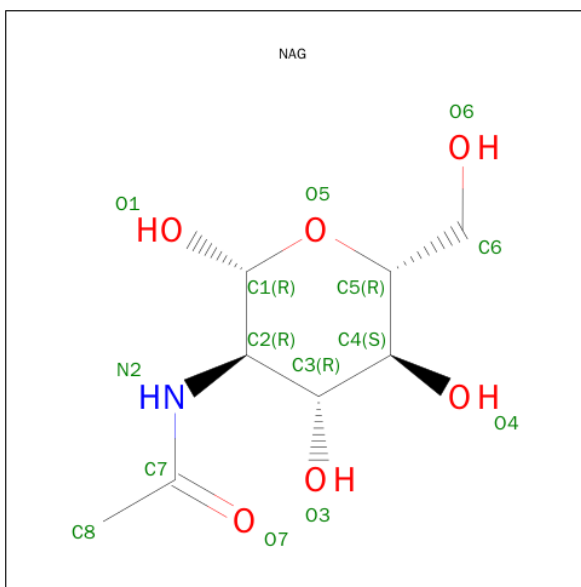


- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



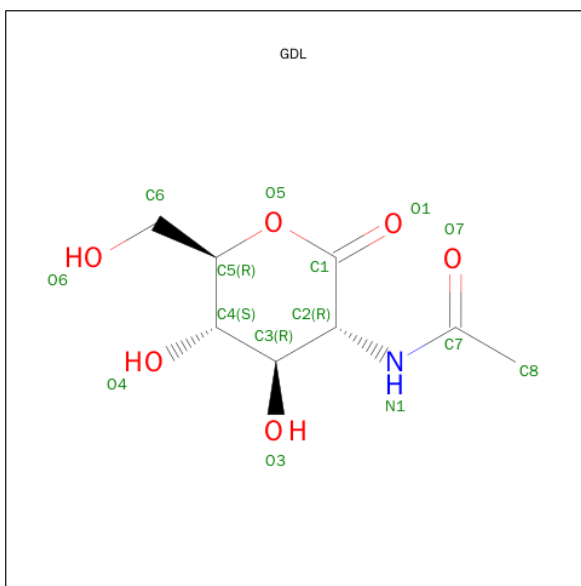
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $\text{C}_8\text{H}_{15}\text{NO}_6$ ).



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

- Molecule 5 is 2-ACETAMIDO-2-DEOXY-D-GLUCONO-1,5-LACTONE (three-letter code: GDL) (formula:  $C_8H_{13}NO_6$ ).



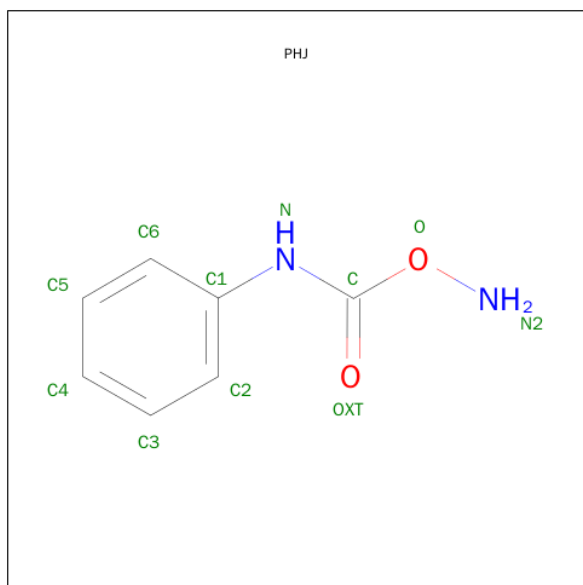
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

*Continued on next page...*

Continued from previous page...

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

- Molecule 6 is N-[(AMINOOXY)CARBONYL]-N-PHENYLAMINE (three-letter code: PHJ) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	7	2	2		
6	B	1	Total	C	N	O	0	0
			11	7	2	2		

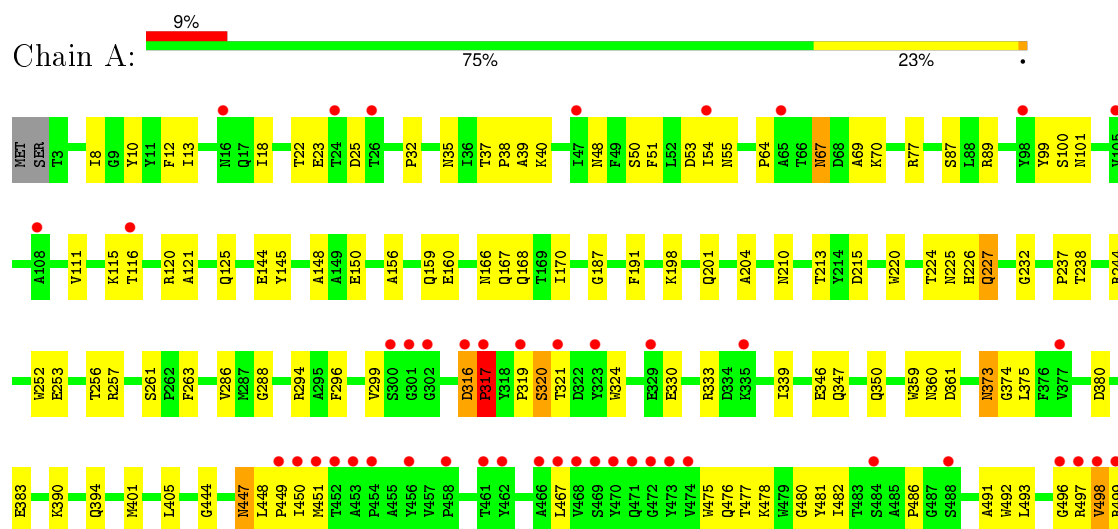
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	413	Total	O	0	0
			413	413		
7	B	441	Total	O	0	0
			441	441		

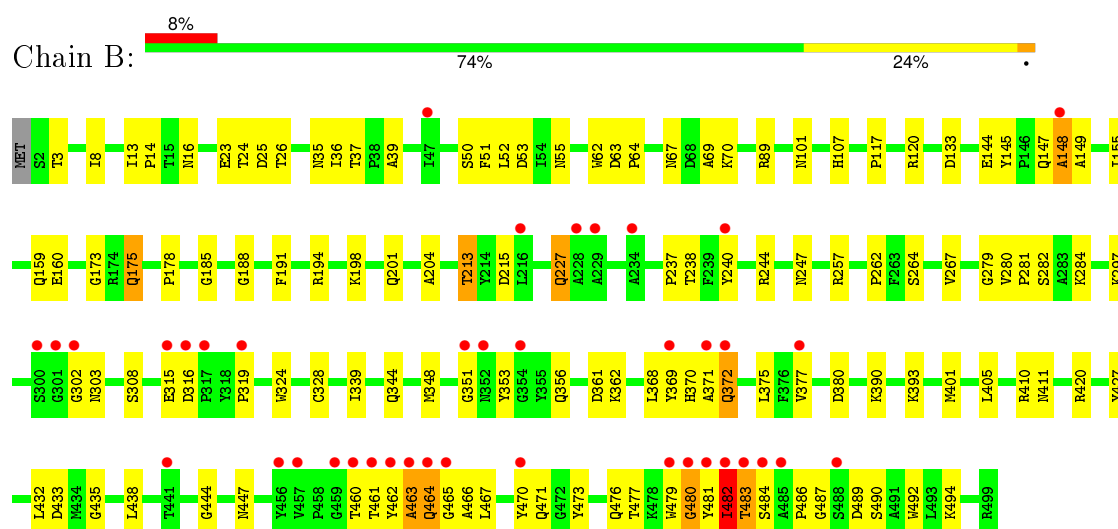
### 3 Residue-property plots

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: CHITINASE B



#### • Molecule 1: CHITINASE B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.52Å 104.18Å 185.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.88 – 1.80 24.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (24.88-1.80) 97.0 (24.87-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.255 0.204 , 0.251	Depositor DCC
$R_{free}$ test set	983 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 97882 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, GDL, NAG, PHJ

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	0.50	0/4023	0.78	4/5486 (0.1%)
1	B	0.50	0/4078	0.71	1/5558 (0.0%)
All	All	0.50	0/8101	0.75	5/11044 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	C-N-CD	-20.42	75.67	120.60
1	A	316	ASP	C-N-CA	13.40	178.27	122.00
1	B	482	ILE	N-CA-C	6.82	129.41	111.00
1	A	317	PRO	CA-N-CD	-5.73	103.48	111.50
1	A	100	SER	N-CA-C	5.17	124.97	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3904	0	3729	159	0
1	B	3933	0	3745	198	0
2	A	186	0	248	99	0
2	B	198	0	264	109	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	0	4	0
3	B	15	0	0	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	14	0	12	1	0
5	B	14	0	12	0	0
6	A	11	0	7	5	0
6	B	11	0	7	7	0
7	A	413	0	0	17	0
7	B	441	0	0	25	0
All	All	9198	0	8050	388	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 24.

All (388) 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:51:PHE:H	2:A:1524:GOL:H2	1.08	1.08
1:B:64:PRO:HD3	2:B:1511:GOL:H2	1.33	1.07
1:B:23:GLU:H	2:B:1510:GOL:H31	1.13	1.06
1:A:168:GLN:HE22	2:A:1521:GOL:H11	1.20	1.04
1:B:63:ASP:HA	2:B:1511:GOL:H12	1.40	1.01
1:A:361:ASP:H	2:A:1517:GOL:H32	1.19	1.01
1:A:261:SER:H	2:A:1500:GOL:H32	1.29	0.96
1:B:461:THR:HA	1:B:482:ILE:HG21	1.47	0.96
1:B:133:ASP:HA	2:B:1530:GOL:H2	1.48	0.96
1:B:35:ASN:HD21	1:B:410:ARG:HH11	1.14	0.93
1:A:480:GLY:H	2:B:1524:GOL:H31	1.36	0.91
1:A:39:ALA:HB2	2:A:1507:GOL:H32	1.54	0.89
1:B:461:THR:HA	1:B:482:ILE:CG2	2.03	0.89
1:B:188:GLY:H	2:B:1502:GOL:H31	1.37	0.88
1:A:350:GLN:HB2	2:A:1509:GOL:H2	1.53	0.88
1:B:264:SER:H	2:B:1509:GOL:H32	1.39	0.88
2:A:1501:GOL:H31	6:B:2503:PHJ:H4	1.54	0.87
1:B:482:ILE:O	1:B:484:SER:N	2.06	0.87
1:B:25:ASP:HA	2:B:1514:GOL:H32	1.56	0.86
1:B:460:THR:O	1:B:482:ILE:HG21	1.76	0.86
1:A:111:VAL:O	2:A:1525:GOL:O3	1.92	0.85
1:A:244:ARG:HH11	2:A:1500:GOL:H11	1.41	0.85
1:A:383:GLU:OE1	2:A:1510:GOL:H32	1.75	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:N	2:A:1524:GOL:H2	1.92	0.85
1:A:237:PRO:HA	2:A:1527:GOL:H32	1.60	0.83
2:B:1500:GOL:H12	7:B:2254:HOH:O	1.78	0.83
1:A:201:GLN:HG2	2:A:1512:GOL:H2	1.61	0.82
1:B:393:LYS:HZ3	2:B:1525:GOL:H32	1.45	0.81
1:B:62:TRP:O	2:B:1511:GOL:H32	1.80	0.81
2:A:1503:GOL:H32	7:A:2370:HOH:O	1.81	0.81
1:A:225:ASN:OD1	2:A:1502:GOL:H31	1.82	0.80
1:A:444:GLY:H	1:A:447:ASN:HD21	1.25	0.80
1:B:420[A]:ARG:HH21	2:B:1503:GOL:H11	1.46	0.80
1:B:282:SER:H	2:B:1500:GOL:C3	1.94	0.80
1:A:168:GLN:NE2	2:A:1521:GOL:H11	1.97	0.79
1:A:244:ARG:NH1	2:A:1500:GOL:H11	1.98	0.79
1:A:67:ASN:HD21	1:A:70:LYS:CG	1.95	0.79
1:B:64:PRO:HD3	2:B:1511:GOL:C2	2.13	0.78
1:B:284:LYS:NZ	2:B:1508:GOL:H2	1.99	0.78
2:A:1525:GOL:H32	7:A:2394:HOH:O	1.85	0.77
1:A:39:ALA:CB	2:A:1507:GOL:H32	2.15	0.76
1:B:462:TYR:H	1:B:482:ILE:CG2	1.98	0.76
1:B:89:ARG:HH22	2:B:1515:GOL:H2	1.51	0.76
1:A:160:GLU:HG2	7:A:2149:HOH:O	1.85	0.76
2:A:1521:GOL:H32	7:A:2127:HOH:O	1.86	0.75
1:A:294:ARG:NH1	1:A:339:ILE:HD11	2.02	0.75
1:A:32:PRO:HD2	1:A:35:ASN:HD21	1.51	0.75
1:B:185:GLY:HA2	7:B:2192:HOH:O	1.87	0.75
1:B:393:LYS:NZ	2:B:1525:GOL:H32	2.02	0.75
1:A:237:PRO:CA	2:A:1527:GOL:H32	2.17	0.75
1:A:324:TRP:HB2	2:A:1528:GOL:H31	1.68	0.75
2:A:1503:GOL:H31	7:A:2369:HOH:O	1.88	0.74
2:B:1501:GOL:H11	7:B:2071:HOH:O	1.86	0.73
1:B:482:ILE:HG12	1:B:483:THR:N	2.03	0.73
1:B:35:ASN:HD21	1:B:410:ARG:NH1	1.86	0.73
1:A:150:GLU:HA	2:A:1525:GOL:O2	1.88	0.73
1:A:32:PRO:HD2	1:A:35:ASN:ND2	2.04	0.73
1:B:464:GLN:NE2	1:B:464:GLN:HA	2.03	0.72
1:B:479:TRP:CD1	1:B:480:GLY:N	2.56	0.72
1:A:198:LYS:NZ	2:A:1518:GOL:H11	2.04	0.72
1:B:23:GLU:N	2:B:1510:GOL:H31	1.98	0.72
1:A:115:LYS:HA	2:A:1525:GOL:H12	1.72	0.72
1:B:282:SER:H	2:B:1500:GOL:H31	1.53	0.72
1:A:198:LYS:HZ1	2:A:1518:GOL:H11	1.54	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ASN:ND2	7:B:2365:HOH:O	2.22	0.72
1:A:330:GLU:HG2	2:A:1520:GOL:H12	1.72	0.71
1:B:67:ASN:HD22	1:B:70:LYS:H	1.37	0.71
1:A:244:ARG:HH11	2:A:1500:GOL:C1	2.04	0.71
1:B:461:THR:HG23	1:B:481:TYR:HB3	1.73	0.71
1:B:420[A]:ARG:NH2	2:B:1503:GOL:H11	2.05	0.70
1:B:37:THR:HG21	2:B:1505:GOL:H11	1.72	0.70
1:B:464:GLN:HE21	1:B:464:GLN:HA	1.57	0.70
1:B:479:TRP:HD1	1:B:480:GLY:N	1.90	0.70
1:B:240:TYR:HE1	7:B:2223:HOH:O	1.74	0.70
1:A:350:GLN:HB2	2:A:1509:GOL:C2	2.20	0.70
1:B:482:ILE:HG12	1:B:483:THR:H	1.56	0.70
1:B:25:ASP:HA	2:B:1514:GOL:C3	2.22	0.69
1:A:324:TRP:HB2	2:A:1528:GOL:C3	2.23	0.69
1:B:215:ASP:HB3	6:B:2503:PHJ:H2	1.75	0.69
1:A:67:ASN:HD21	1:A:70:LYS:HG3	1.57	0.68
1:A:215:ASP:HB3	6:A:2503:PHJ:H2	1.75	0.68
1:B:247:ASN:ND2	2:B:1527:GOL:H12	2.09	0.68
1:B:370:HIS:HE1	1:B:372:GLN:HE21	1.40	0.68
2:A:1509:GOL:O3	2:A:1526:GOL:H11	1.94	0.68
1:A:167:GLN:O	2:A:1513:GOL:H11	1.92	0.68
1:A:204:ALA:HB3	2:A:1512:GOL:H31	1.75	0.67
1:A:225:ASN:HD21	2:A:1502:GOL:H31	1.59	0.67
1:B:257:ARG:HD2	7:B:2239:HOH:O	1.94	0.67
1:A:373:ASN:N	1:A:373:ASN:HD22	1.90	0.67
2:A:1504:GOL:H2	6:A:2503:PHJ:C1	2.25	0.67
1:A:204:ALA:HB3	2:A:1512:GOL:C3	2.25	0.66
1:B:461:THR:CA	1:B:482:ILE:HG21	2.23	0.66
6:B:2503:PHJ:H6	6:B:2503:PHJ:OXT	1.94	0.66
1:A:170:ILE:HD13	2:A:1513:GOL:H31	1.77	0.66
1:A:225:ASN:ND2	2:A:1502:GOL:H31	2.11	0.66
1:A:361:ASP:N	2:A:1517:GOL:H32	2.02	0.65
1:B:420[A]:ARG:HH21	2:B:1503:GOL:C1	2.09	0.65
1:A:201:GLN:HA	2:A:1512:GOL:C2	2.27	0.65
1:B:369:TYR:CE2	1:B:371:ALA:HB2	2.31	0.65
1:B:64:PRO:CD	2:B:1511:GOL:H2	2.21	0.65
1:B:24:THR:C	2:B:1514:GOL:H12	2.17	0.65
1:B:175:GLN:HE21	1:B:175:GLN:H	1.43	0.65
1:B:26:THR:HG23	2:B:1514:GOL:H11	1.78	0.64
1:B:282:SER:H	2:B:1500:GOL:H32	1.62	0.64
1:B:14:PRO:HB3	2:B:1517:GOL:H32	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD21	2:A:1528:GOL:H32	1.80	0.64
1:B:284:LYS:HZ3	2:B:1508:GOL:H2	1.63	0.64
1:A:256:THR:HG23	2:A:1500:GOL:O2	1.98	0.63
1:B:463:ALA:HA	1:B:477:THR:CB	2.28	0.63
1:B:463:ALA:HB2	1:B:481:TYR:HA	1.79	0.63
2:A:1524:GOL:H31	7:A:2011:HOH:O	1.98	0.63
1:B:433:ASP:OD2	7:B:2353:HOH:O	2.15	0.63
1:A:498:VAL:HG12	1:A:499:ARG:N	2.14	0.63
1:B:328:CYS:HB2	1:B:348[B]:MET:HE1	1.79	0.63
1:B:133:ASP:CA	2:B:1530:GOL:H2	2.27	0.63
2:B:1523:GOL:H31	7:B:2121:HOH:O	1.99	0.63
1:A:170:ILE:HD13	2:A:1513:GOL:C3	2.29	0.62
1:B:37:THR:OG1	2:B:1505:GOL:H12	1.99	0.62
1:A:498:VAL:HG12	1:A:499:ARG:H	1.64	0.62
1:A:467:LEU:HD23	1:A:476:GLN:HB2	1.80	0.62
1:A:39:ALA:H	2:A:1507:GOL:H32	1.64	0.62
2:A:1501:GOL:H31	6:B:2503:PHJ:C4	2.30	0.62
1:A:69:ALA:HA	7:A:2072:HOH:O	1.98	0.62
2:A:1505:GOL:H12	3:A:1533:SO4:O4	1.99	0.61
1:B:370:HIS:CE1	1:B:372:GLN:HE21	2.17	0.61
1:B:63:ASP:CA	2:B:1511:GOL:H12	2.25	0.61
1:B:438:LEU:HD13	2:B:1509:GOL:H12	1.83	0.61
1:B:63:ASP:HA	2:B:1511:GOL:C1	2.26	0.61
1:B:89:ARG:HH12	2:B:1515:GOL:H2	1.66	0.61
1:B:351:GLY:HA3	1:B:353:TYR:CE2	2.36	0.61
1:A:383:GLU:HG2	7:A:2284:HOH:O	2.01	0.61
1:B:159[A]:GLN:HB2	2:B:1506:GOL:H32	1.83	0.61
2:A:1529:GOL:H31	7:A:2012:HOH:O	2.01	0.60
1:B:284:LYS:HZ1	2:B:1508:GOL:H2	1.66	0.60
1:B:462:TYR:O	1:B:463:ALA:HB3	2.01	0.60
1:B:344:GLN:HG3	1:B:348[B]:MET:CE	2.32	0.60
1:A:39:ALA:HB2	2:A:1507:GOL:C3	2.29	0.60
1:A:18:ILE:O	1:A:70:LYS:HB3	2.01	0.60
1:B:284:LYS:HZ1	2:B:1508:GOL:C2	2.15	0.60
1:A:346:GLU:O	1:A:350:GLN:HG2	2.01	0.60
1:A:225:ASN:CG	2:A:1502:GOL:H31	2.22	0.60
1:B:432:LEU:HD12	2:B:1512:GOL:H11	1.84	0.60
1:A:115:LYS:HA	2:A:1525:GOL:C1	2.32	0.59
1:A:360:ASN:HA	2:A:1517:GOL:H31	1.84	0.59
1:A:383:GLU:HG3	2:A:1510:GOL:O3	2.02	0.59
1:B:279:GLY:CA	2:B:1518:GOL:H31	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLU:N	2:B:1506:GOL:H31	2.18	0.59
1:B:264:SER:N	2:B:1509:GOL:H32	2.14	0.59
1:B:175:GLN:NE2	1:B:175:GLN:H	2.00	0.59
1:B:487:GLY:O	2:B:1522:GOL:H31	2.03	0.59
1:A:447:ASN:HD22	1:A:447:ASN:H	1.51	0.58
6:A:2503:PHJ:OXT	6:A:2503:PHJ:H6	2.01	0.58
1:A:299:VAL:HG22	1:A:374:GLY:O	2.03	0.58
1:B:328:CYS:HB2	1:B:348[B]:MET:CE	2.33	0.58
1:A:350:GLN:HB3	2:A:1526:GOL:H32	1.84	0.58
1:A:447:ASN:N	1:A:447:ASN:HD22	2.01	0.58
1:B:369:TYR:CE2	2:B:1529:GOL:H11	2.39	0.58
1:A:167:GLN:HG2	2:A:1513:GOL:O2	2.04	0.58
1:A:201:GLN:HA	2:A:1512:GOL:H32	1.85	0.57
1:B:284:LYS:NZ	2:B:1508:GOL:C2	2.67	0.57
1:A:238:THR:OG1	2:A:1527:GOL:H11	2.03	0.57
1:B:281:PRO:HA	2:B:1500:GOL:H11	1.85	0.57
1:B:201:GLN:HG3	7:B:2198:HOH:O	2.03	0.57
1:A:237:PRO:CB	2:A:1527:GOL:H32	2.35	0.57
2:A:1509:GOL:O3	2:A:1526:GOL:C1	2.53	0.57
1:B:462:TYR:O	1:B:481:TYR:HD1	1.88	0.56
1:B:487:GLY:O	2:B:1522:GOL:H11	2.05	0.56
1:B:198:LYS:NZ	2:B:1527:GOL:H2	2.20	0.56
1:A:225:ASN:ND2	1:A:226:HIS:H	2.03	0.56
1:A:168:GLN:HE22	2:A:1521:GOL:C1	2.08	0.56
1:A:263:PHE:HB2	2:A:1506:GOL:H31	1.87	0.56
1:A:38:PRO:HB2	2:A:1507:GOL:H2	1.87	0.56
1:B:481:TYR:O	1:B:482:ILE:CG2	2.54	0.56
2:A:1506:GOL:H32	7:A:2374:HOH:O	2.06	0.56
2:B:1537:GOL:H11	7:B:2426:HOH:O	2.06	0.56
1:A:67:ASN:HD21	1:A:70:LYS:HG2	1.71	0.55
1:B:147:GLN:HB3	1:B:194:ARG:HD3	1.87	0.55
1:A:22:THR:HA	2:A:1523:GOL:H31	1.88	0.55
1:B:53:ASP:HB3	2:B:1511:GOL:H11	1.88	0.55
1:B:463:ALA:HA	1:B:477:THR:HB	1.88	0.55
1:B:486:PRO:HA	1:B:492:TRP:CD1	2.41	0.55
1:B:302:GLY:C	2:B:1529:GOL:H31	2.27	0.55
1:B:344:GLN:HG3	1:B:348[B]:MET:HE3	1.87	0.55
1:A:166:ASN:O	1:A:170:ILE:HD12	2.07	0.55
1:B:16[A]:ASN:ND2	7:B:2016:HOH:O	2.39	0.55
1:B:89:ARG:NH2	2:B:1515:GOL:H2	2.20	0.54
1:B:279:GLY:C	2:B:1518:GOL:H31	2.28	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HH22	2:B:1515:GOL:C2	2.19	0.54
1:B:237:PRO:HA	2:B:1519:GOL:H2	1.89	0.54
1:B:470:TYR:CD2	1:B:471:GLN:HG3	2.43	0.54
1:A:225:ASN:HD21	2:A:1502:GOL:C3	2.21	0.54
1:A:64:PRO:HD3	7:A:2066:HOH:O	2.08	0.54
1:B:53:ASP:CB	2:B:1511:GOL:H11	2.38	0.53
1:B:55:ASN:HB3	2:B:1511:GOL:O3	2.08	0.53
1:B:67:ASN:ND2	1:B:70:LYS:H	2.06	0.53
1:A:39:ALA:N	2:A:1507:GOL:H32	2.22	0.53
2:A:1538:GOL:H31	7:A:2410:HOH:O	2.08	0.53
1:B:204:ALA:O	2:B:1508:GOL:H2	2.08	0.53
1:A:156:ALA:HA	1:A:159:GLN:NE2	2.24	0.53
1:A:263:PHE:HB2	2:A:1506:GOL:C3	2.39	0.53
1:B:120:ARG:NH1	2:B:1523:GOL:O2	2.42	0.53
1:A:448:LEU:O	1:A:497:ARG:NH1	2.42	0.53
1:A:55:ASN:HA	2:A:1516:GOL:H31	1.91	0.53
1:B:461:THR:HA	1:B:482:ILE:HG23	1.88	0.53
1:A:201:GLN:HA	2:A:1512:GOL:C3	2.39	0.52
1:A:261:SER:N	2:A:1500:GOL:H32	2.11	0.52
1:A:497:ARG:HG2	1:A:497:ARG:HH11	1.74	0.52
1:B:481:TYR:HB2	2:B:1531:GOL:H12	1.91	0.52
1:A:316:ASP:OD1	1:A:317:PRO:HD3	2.10	0.52
2:B:1537:GOL:H31	7:B:2084:HOH:O	2.08	0.52
1:A:191:PHE:CE2	6:A:2503:PHJ:C5	2.93	0.52
1:B:159[A]:GLN:HB2	2:B:1506:GOL:C3	2.40	0.52
1:A:201:GLN:HA	2:A:1512:GOL:H2	1.92	0.52
1:B:53:ASP:OD2	2:B:1511:GOL:H11	2.10	0.52
1:A:324:TRP:CB	2:A:1528:GOL:H31	2.40	0.51
1:B:473:TYR:CE2	1:B:494:LYS:HD3	2.46	0.51
1:B:481:TYR:HD2	2:B:1531:GOL:H32	1.75	0.51
1:A:10:TYR:HA	1:A:48:ASN:HB2	1.92	0.51
1:B:482:ILE:CG1	1:B:483:THR:N	2.72	0.51
1:A:449:PRO:O	1:A:451:MET:HG3	2.11	0.51
1:B:215:ASP:H	1:B:227:GLN:HE21	1.60	0.50
1:B:284:LYS:HZ1	2:B:1508:GOL:C3	2.24	0.50
1:A:252:TRP:HZ2	2:B:1528:GOL:H31	1.76	0.50
1:A:480:GLY:N	2:B:1524:GOL:H31	2.17	0.50
1:A:225:ASN:HD21	2:A:1502:GOL:C2	2.24	0.50
1:A:210:ASN:HD22	1:A:286:VAL:HB	1.77	0.50
1:A:204:ALA:HB3	2:A:1512:GOL:H32	1.94	0.50
2:A:1505:GOL:H32	5:A:2502:GDL:O6	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:TRP:HD1	1:B:480:GLY:CA	2.24	0.50
1:B:280:VAL:N	2:B:1518:GOL:H31	2.26	0.50
1:B:460:THR:O	1:B:482:ILE:HG13	2.11	0.50
1:B:462:TYR:O	1:B:463:ALA:CB	2.59	0.50
1:A:360:ASN:HA	2:A:1517:GOL:C3	2.42	0.50
1:B:462:TYR:HB3	1:B:466:ALA:CB	2.41	0.49
1:B:481:TYR:C	1:B:482:ILE:HG23	2.31	0.49
1:B:215:ASP:H	1:B:227:GLN:NE2	2.09	0.49
2:B:1503:GOL:H31	7:B:2343:HOH:O	2.11	0.49
1:B:117:PRO:HG3	2:B:1521:GOL:H11	1.93	0.49
1:B:444:GLY:N	1:B:447:ASN:OD1	2.39	0.49
1:A:451:MET:SD	1:A:496:GLY:HA3	2.52	0.49
1:A:482:ILE:HD12	1:A:491:ALA:CB	2.43	0.49
1:B:303:ASN:HB2	7:B:2260:HOH:O	2.12	0.49
1:A:148:ALA:HB1	3:A:1537:SO4:O3	2.12	0.49
1:B:117:PRO:HD3	2:B:1521:GOL:H31	1.93	0.49
1:B:147:GLN:O	1:B:149:ALA:N	2.46	0.49
1:A:204:ALA:CB	2:A:1512:GOL:H31	2.42	0.49
1:B:198:LYS:CE	2:B:1527:GOL:H2	2.43	0.49
1:B:247:ASN:HD22	2:B:1527:GOL:H12	1.75	0.49
1:A:167:GLN:HA	2:A:1513:GOL:H11	1.94	0.49
1:A:252:TRP:CZ2	2:B:1528:GOL:H31	2.48	0.48
1:A:477:THR:HG23	1:A:492:TRP:CZ3	2.48	0.48
1:B:173:GLY:HA2	1:B:175:GLN:HE22	1.78	0.48
1:A:319:PRO:O	1:A:320:SER:HB2	2.13	0.48
1:A:475:TRP:CD2	1:A:486:PRO:HB3	2.48	0.48
1:B:247:ASN:HB3	7:B:2226:HOH:O	2.14	0.48
2:B:1526:GOL:H31	7:B:2431:HOH:O	2.14	0.48
6:B:2503:PHJ:C6	6:B:2503:PHJ:OXT	2.60	0.48
1:A:478:LYS:HE2	1:A:493:LEU:HB2	1.96	0.48
1:B:482:ILE:HA	7:B:2389:HOH:O	2.13	0.48
1:B:26:THR:H	2:B:1514:GOL:H31	1.78	0.48
1:B:479:TRP:C	1:B:479:TRP:CD1	2.86	0.48
1:B:120:ARG:HH22	2:B:1521:GOL:H31	1.79	0.48
1:B:487:GLY:HA2	7:B:2427:HOH:O	2.13	0.48
1:A:215:ASP:H	1:A:227:GLN:HE21	1.61	0.47
1:A:191:PHE:CE2	6:A:2503:PHJ:H5	2.49	0.47
1:A:253:GLU:O	1:A:257:ARG:HG3	2.14	0.47
1:B:482:ILE:CG1	1:B:483:THR:H	2.25	0.47
1:B:39:ALA:HB3	2:B:1505:GOL:H12	1.96	0.47
1:B:3:THR:HA	3:B:1536:SO4:O3	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:THR:O	1:B:482:ILE:CG2	2.56	0.47
1:A:361:ASP:H	2:A:1517:GOL:C3	2.08	0.47
1:B:37:THR:OG1	2:B:1505:GOL:C1	2.63	0.47
1:B:479:TRP:HH2	1:B:490:SER:HB2	1.80	0.47
1:B:120:ARG:HH22	2:B:1521:GOL:C3	2.28	0.47
1:B:302:GLY:H	2:B:1529:GOL:H12	1.79	0.47
1:A:299:VAL:HG22	1:A:374:GLY:C	2.36	0.47
1:B:473:TYR:CD2	1:B:494:LYS:HD3	2.50	0.47
1:B:361:ASP:O	2:B:1516:GOL:H11	2.15	0.47
1:A:294:ARG:HG2	1:A:339:ILE:CD1	2.45	0.47
1:B:362:LYS:HD3	2:B:1516:GOL:O1	2.15	0.46
1:B:144:GLU:HA	1:B:145:TYR:CG	2.50	0.46
1:B:89:ARG:NH1	2:B:1515:GOL:H2	2.30	0.46
1:A:319:PRO:O	1:A:320:SER:CB	2.63	0.46
1:A:121:ALA:O	1:A:125:GLN:HG3	2.15	0.46
1:B:466:ALA:O	1:B:476:GLN:HA	2.16	0.46
1:A:170:ILE:HB	2:A:1513:GOL:H12	1.97	0.46
1:B:14:PRO:HB2	1:B:16[A]:ASN:OD1	2.16	0.46
1:A:32:PRO:CD	1:A:35:ASN:ND2	2.78	0.46
1:B:390:LYS:HZ1	2:B:1507:GOL:H11	1.80	0.46
1:B:23:GLU:HG3	2:B:1510:GOL:H11	1.98	0.46
1:B:481:TYR:CD2	2:B:1531:GOL:H2	2.49	0.46
1:B:244:ARG:NH1	7:B:2223:HOH:O	2.47	0.46
1:B:147:GLN:O	1:B:148:ALA:C	2.54	0.46
1:B:479:TRP:HD1	1:B:480:GLY:HA3	1.81	0.45
1:A:12:PHE:HZ	2:A:1529:GOL:H2	1.80	0.45
1:B:463:ALA:HB3	1:B:481:TYR:CD1	2.51	0.45
1:B:188:GLY:N	2:B:1502:GOL:H31	2.17	0.45
1:B:467:LEU:HD23	1:B:476:GLN:HB2	1.97	0.45
1:A:288:GLY:HA2	1:A:401:MET:O	2.16	0.45
1:A:220:TRP:O	2:B:1531:GOL:O3	2.33	0.45
1:B:393:LYS:HD3	2:B:1525:GOL:H12	1.99	0.45
1:B:284:LYS:HZ1	2:B:1508:GOL:H31	1.82	0.45
1:B:489:ASP:O	2:B:1522:GOL:H32	2.17	0.45
1:B:101:ASN:HA	1:B:144:GLU:O	2.17	0.45
1:A:50:SER:HA	1:A:51:PHE:HA	1.68	0.44
1:A:294:ARG:NH2	2:A:1505:GOL:H11	2.32	0.44
1:B:344:GLN:HG3	1:B:348[B]:MET:HE2	1.99	0.44
1:A:347:GLN:NE2	7:A:2261:HOH:O	2.44	0.44
2:B:1512:GOL:H12	7:B:2419:HOH:O	2.16	0.44
1:B:481:TYR:O	1:B:482:ILE:HG23	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:HD12	2:B:1512:GOL:C1	2.47	0.44
1:B:297:LYS:HD3	1:B:324:TRP:NE1	2.32	0.44
1:B:356:GLN:HG3	7:B:2291:HOH:O	2.18	0.44
1:B:465:GLY:HA2	1:B:476:GLN:NE2	2.33	0.43
1:B:191:PHE:HE2	6:B:2503:PHJ:C5	2.31	0.43
1:A:201:GLN:HG3	7:A:2181:HOH:O	2.17	0.43
2:B:1503:GOL:C3	7:B:2343:HOH:O	2.66	0.43
1:A:89:ARG:HH12	2:A:1519:GOL:H2	1.83	0.43
1:A:67:ASN:HA	7:A:2070:HOH:O	2.17	0.43
1:A:67:ASN:ND2	1:A:70:LYS:HG3	2.28	0.43
1:B:467:LEU:CD2	1:B:476:GLN:HB2	2.49	0.43
1:B:484:SER:CB	1:B:489:ASP:OD2	2.66	0.43
1:B:371:ALA:O	1:B:372:GLN:HG3	2.18	0.43
1:A:333:ARG:NH1	3:A:1536:SO4:O1	2.52	0.43
1:B:213:THR:HB	1:B:267:VAL:HG22	2.00	0.43
1:B:435:GLY:CA	2:B:1516:GOL:H12	2.49	0.43
1:B:50:SER:HA	1:B:51:PHE:HA	1.74	0.43
1:A:13:ILE:O	1:A:13:ILE:HG23	2.18	0.43
1:B:463:ALA:H	1:B:477:THR:HG21	1.84	0.43
1:A:87:SER:HB3	7:A:2386:HOH:O	2.18	0.43
1:A:37:THR:OG1	1:A:40:LYS:HG3	2.19	0.43
1:B:370:HIS:HB3	1:B:375:LEU:HB2	2.01	0.43
1:A:170:ILE:HB	2:A:1513:GOL:C1	2.48	0.43
1:A:53:ASP:CG	1:A:54:ILE:H	2.21	0.43
1:B:489:ASP:O	2:B:1522:GOL:C3	2.67	0.43
1:A:224:THR:HG22	1:A:296:PHE:CD2	2.53	0.43
1:A:232:GLY:HA2	2:A:1502:GOL:C1	2.48	0.43
1:B:67:ASN:HD21	1:B:69:ALA:HB3	1.84	0.43
1:B:370:HIS:CE1	1:B:372:GLN:HB2	2.54	0.42
1:A:450:ILE:HG13	1:A:497:ARG:NH1	2.34	0.42
1:B:315:GLU:H	1:B:315:GLU:HG2	1.69	0.42
1:A:201:GLN:O	2:A:1512:GOL:H32	2.19	0.42
1:B:13:ILE:HA	1:B:14:PRO:HD3	1.87	0.42
1:B:178:PRO:HD2	2:B:1515:GOL:H32	2.01	0.42
1:A:101:ASN:HA	1:A:144:GLU:O	2.19	0.42
1:A:201:GLN:HA	2:A:1512:GOL:H12	2.01	0.42
1:B:479:TRP:O	1:B:480:GLY:C	2.58	0.42
1:A:373:ASN:N	1:A:373:ASN:ND2	2.60	0.42
1:A:187:GLY:N	2:A:1504:GOL:O3	2.42	0.42
2:A:1508:GOL:O1	2:A:1528:GOL:O1	2.37	0.42
1:B:244:ARG:NH1	2:B:1528:GOL:O2	2.50	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:VAL:CG1	1:A:499:ARG:H	2.26	0.42
1:B:481:TYR:HD2	2:B:1531:GOL:C3	2.32	0.42
2:A:1515:GOL:H32	2:B:1531:GOL:H11	2.02	0.42
1:B:191:PHE:CE2	6:B:2503:PHJ:C5	3.03	0.42
2:A:1505:GOL:H12	3:A:1533:SO4:S	2.60	0.42
1:B:8:ILE:O	1:B:401:MET:HA	2.20	0.42
1:A:23:GLU:OE2	1:A:77:ARG:HD3	2.20	0.41
1:B:302:GLY:H	2:B:1529:GOL:C1	2.33	0.41
1:A:37:THR:HB	2:A:1507:GOL:O3	2.20	0.41
1:A:25:ASP:HA	7:A:2026:HOH:O	2.19	0.41
1:B:481:TYR:O	1:B:482:ILE:HG22	2.20	0.41
1:B:107:HIS:HE1	7:B:2155:HOH:O	2.03	0.41
2:B:1504:GOL:H2	3:B:1534:SO4:O3	2.20	0.41
1:B:36:ILE:HD11	1:B:405:LEU:HD21	2.02	0.41
1:B:282:SER:N	2:B:1500:GOL:H31	2.29	0.41
1:A:320:SER:OG	1:A:321:THR:N	2.53	0.41
1:B:351:GLY:HA3	1:B:353:TYR:CD2	2.55	0.41
1:A:144:GLU:HA	1:A:145:TYR:CG	2.55	0.41
1:B:238:THR:HB	1:B:262:PRO:HB2	2.03	0.41
1:A:390:LYS:O	1:A:394:GLN:HG3	2.21	0.41
1:A:359:TRP:CD1	2:A:1510:GOL:H12	2.56	0.41
1:B:479:TRP:CA	7:B:2376:HOH:O	2.68	0.41
1:A:215:ASP:H	1:A:227:GLN:NE2	2.19	0.41
1:B:155:ILE:O	1:B:159[A]:GLN:HG3	2.21	0.41
1:A:450:ILE:HG13	1:A:497:ARG:CZ	2.51	0.41
1:A:53:ASP:HB2	1:A:99:TYR:CE2	2.56	0.41
1:B:427:TYR:HA	7:B:2333:HOH:O	2.20	0.41
1:A:347:GLN:NE2	2:A:1520:GOL:O3	2.54	0.40
1:B:435:GLY:HA2	2:B:1516:GOL:H12	2.04	0.40
1:B:368:LEU:HB2	1:B:377:VAL:HB	2.02	0.40
1:B:482:ILE:N	1:B:482:ILE:HD13	2.36	0.40
1:A:167:GLN:O	2:A:1513:GOL:C1	2.65	0.40
1:A:8:ILE:O	1:A:401:MET:HA	2.21	0.40
1:A:116:THR:O	1:A:120:ARG:HG3	2.22	0.40
1:A:481:TYR:HD1	2:B:1524:GOL:C1	2.35	0.40
1:A:238:THR:H	2:A:1527:GOL:C3	2.34	0.40
1:A:201:GLN:HA	2:A:1512:GOL:C1	2.52	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	497/499 (100%)	480 (97%)	14 (3%)	3 (1%)	30	14
1	B	503/499 (101%)	482 (96%)	14 (3%)	7 (1%)	14	3
All	All	1000/998 (100%)	962 (96%)	28 (3%)	10 (1%)	19	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	PRO
1	B	148	ALA
1	B	372	GLN
1	B	483	THR
1	B	463	ALA
1	B	480	GLY
1	A	320	SER
1	A	498	VAL
1	B	482	ILE
1	B	319	PRO

### 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	403/406 (99%)	396 (98%)	7 (2%)	68	57
1	B	408/406 (100%)	396 (97%)	12 (3%)	50	34
All	All	811/812 (100%)	792 (98%)	19 (2%)	60	42

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	213	THR
1	A	227	GLN
1	A	373	ASN
1	A	380	ASP
1	A	405	LEU
1	A	447	ASN
1	B	52	LEU
1	B	175	GLN
1	B	213	THR
1	B	227	GLN
1	B	308	SER
1	B	316[A]	ASP
1	B	316[B]	ASP
1	B	339	ILE
1	B	380	ASP
1	B	411	ASN
1	B	464	GLN
1	B	482	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	159	GLN
1	A	168	GLN
1	A	210	ASN
1	A	225	ASN
1	A	227	GLN
1	A	347	GLN
1	A	373	ASN
1	A	411	ASN
1	A	447	ASN
1	B	35	ASN
1	B	67	ASN
1	B	175	GLN
1	B	210	ASN
1	B	227	GLN
1	B	247	ASN
1	B	347	GLN
1	B	350	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	372	GLN
1	B	394	GLN
1	B	407	GLN
1	B	464	GLN
1	B	476	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

79 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	GOL	A	1500	-	5,5,5	0.20	0	5,5,5	0.32	0
2	GOL	A	1501	-	5,5,5	0.31	0	5,5,5	0.30	0
2	GOL	A	1502	-	5,5,5	0.18	0	5,5,5	0.37	0
2	GOL	A	1503	-	5,5,5	0.15	0	5,5,5	0.34	0
2	GOL	A	1504	-	5,5,5	0.28	0	5,5,5	0.19	0
2	GOL	A	1505	-	5,5,5	0.18	0	5,5,5	0.14	0
2	GOL	A	1506	-	5,5,5	0.57	0	5,5,5	0.14	0
2	GOL	A	1507	-	5,5,5	0.37	0	5,5,5	0.21	0
2	GOL	A	1508	-	5,5,5	0.19	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	1509	-	5,5,5	0.28	0	5,5,5	0.34	0
2	GOL	A	1510	-	5,5,5	0.31	0	5,5,5	0.16	0
2	GOL	A	1511	-	5,5,5	0.26	0	5,5,5	0.33	0
2	GOL	A	1512	-	5,5,5	0.37	0	5,5,5	0.27	0
2	GOL	A	1513	-	5,5,5	0.15	0	5,5,5	0.28	0
2	GOL	A	1514	-	5,5,5	0.22	0	5,5,5	0.20	0
2	GOL	A	1515	-	5,5,5	0.24	0	5,5,5	0.23	0
2	GOL	A	1516	-	5,5,5	0.48	0	5,5,5	0.14	0
2	GOL	A	1517	-	5,5,5	0.28	0	5,5,5	0.19	0
2	GOL	A	1518	-	5,5,5	0.22	0	5,5,5	0.23	0
2	GOL	A	1519	-	5,5,5	0.28	0	5,5,5	0.28	0
2	GOL	A	1520	-	5,5,5	0.23	0	5,5,5	0.27	0
2	GOL	A	1521	-	5,5,5	0.22	0	5,5,5	0.28	0
2	GOL	A	1522	-	5,5,5	0.22	0	5,5,5	0.29	0
2	GOL	A	1523	-	5,5,5	0.28	0	5,5,5	0.16	0
2	GOL	A	1524	-	5,5,5	0.18	0	5,5,5	0.30	0
2	GOL	A	1525	-	5,5,5	0.20	0	5,5,5	0.21	0
2	GOL	A	1526	-	5,5,5	0.29	0	5,5,5	0.24	0
2	GOL	A	1527	-	5,5,5	0.22	0	5,5,5	0.19	0
2	GOL	A	1528	-	5,5,5	0.19	0	5,5,5	0.28	0
2	GOL	A	1529	-	5,5,5	0.28	0	5,5,5	0.28	0
3	SO4	A	1532	-	4,4,4	0.21	0	6,6,6	0.19	0
3	SO4	A	1533	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	A	1534	-	4,4,4	0.34	0	6,6,6	0.15	0
3	SO4	A	1535	-	4,4,4	0.18	0	6,6,6	0.13	0
3	SO4	A	1536	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	A	1537	-	4,4,4	0.25	0	6,6,6	0.09	0
2	GOL	A	1538	-	5,5,5	0.21	0	5,5,5	0.31	0
4	NAG	A	2501	5	14,14,15	0.89	0	15,19,21	0.65	0
5	GDL	A	2502	4,6	14,14,15	1.39	2 (14%)	15,19,21	1.31	1 (6%)
6	PHJ	A	2503	5	10,11,11	1.76	2 (20%)	11,13,13	0.58	0
2	GOL	B	1500	-	5,5,5	0.17	0	5,5,5	0.22	0
2	GOL	B	1501	-	5,5,5	0.32	0	5,5,5	0.18	0
2	GOL	B	1502	-	5,5,5	0.14	0	5,5,5	0.39	0
2	GOL	B	1503	-	5,5,5	0.19	0	5,5,5	0.16	0
2	GOL	B	1504	-	5,5,5	0.26	0	5,5,5	0.23	0
2	GOL	B	1505	-	5,5,5	0.38	0	5,5,5	0.22	0
2	GOL	B	1506	-	5,5,5	0.32	0	5,5,5	0.30	0
2	GOL	B	1507	-	5,5,5	0.24	0	5,5,5	0.28	0
2	GOL	B	1508	-	5,5,5	0.37	0	5,5,5	0.19	0
2	GOL	B	1509	-	5,5,5	0.20	0	5,5,5	0.24	0
2	GOL	B	1510	-	5,5,5	0.27	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	1511	-	5,5,5	0.25	0	5,5,5	0.23	0
2	GOL	B	1512	-	5,5,5	0.39	0	5,5,5	0.27	0
2	GOL	B	1513	-	5,5,5	0.25	0	5,5,5	0.28	0
2	GOL	B	1514	-	5,5,5	0.24	0	5,5,5	0.22	0
2	GOL	B	1515	-	5,5,5	0.32	0	5,5,5	0.26	0
2	GOL	B	1516	-	5,5,5	0.22	0	5,5,5	0.28	0
2	GOL	B	1517	-	5,5,5	0.45	0	5,5,5	0.40	0
2	GOL	B	1518	-	5,5,5	0.38	0	5,5,5	0.15	0
2	GOL	B	1519	-	5,5,5	0.22	0	5,5,5	0.28	0
2	GOL	B	1520	-	5,5,5	0.22	0	5,5,5	0.28	0
2	GOL	B	1521	-	5,5,5	0.24	0	5,5,5	0.27	0
2	GOL	B	1522	-	5,5,5	0.24	0	5,5,5	0.34	0
2	GOL	B	1523	-	5,5,5	0.36	0	5,5,5	0.14	0
2	GOL	B	1524	-	5,5,5	0.17	0	5,5,5	0.29	0
2	GOL	B	1525	-	5,5,5	0.21	0	5,5,5	0.25	0
2	GOL	B	1526	-	5,5,5	0.36	0	5,5,5	0.18	0
2	GOL	B	1527	-	5,5,5	0.27	0	5,5,5	0.20	0
2	GOL	B	1528	-	5,5,5	0.35	0	5,5,5	0.18	0
2	GOL	B	1529	-	5,5,5	0.36	0	5,5,5	0.22	0
2	GOL	B	1530	-	5,5,5	0.32	0	5,5,5	0.26	0
2	GOL	B	1531	-	5,5,5	0.17	0	5,5,5	0.26	0
3	SO4	B	1534	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	B	1535	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	B	1536	-	4,4,4	0.23	0	6,6,6	0.08	0
2	GOL	B	1537	-	5,5,5	0.10	0	5,5,5	0.28	0
4	NAG	B	2501	5	14,14,15	1.08	1 (7%)	15,19,21	0.57	0
5	GDL	B	2502	4,6	14,14,15	1.39	3 (21%)	15,19,21	1.27	1 (6%)
6	PHJ	B	2503	5	10,11,11	1.75	2 (20%)	11,13,13	0.75	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	GOL	A	1500	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1501	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1503	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1504	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1505	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1506	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1507	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1508	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1509	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1510	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1511	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1512	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1513	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1514	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1515	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1516	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1517	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1518	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1519	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1520	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1521	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1522	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1523	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1524	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1525	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1526	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1527	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1528	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1529	-	-	0/4/4/4	0/0/0/0
3	SO4	A	1532	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1533	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1534	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1535	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1536	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1537	-	-	0/0/0/0	0/0/0/0
2	GOL	A	1538	-	-	0/4/4/4	0/0/0/0
4	NAG	A	2501	5	-	0/6/23/26	0/1/1/1
5	GDL	A	2502	4,6	-	0/6/23/26	0/1/1/1
6	PHJ	A	2503	5	-	0/4/6/6	0/1/1/1
2	GOL	B	1500	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1502	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1504	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1505	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1506	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1507	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1508	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1509	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1510	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1511	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1512	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1513	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1514	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1515	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1516	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1517	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1518	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1519	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1520	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1521	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1522	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1523	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1524	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1525	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1526	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1527	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1528	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1529	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1530	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1531	-	-	0/4/4/4	0/0/0/0
3	SO4	B	1534	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1535	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1536	-	-	0/0/0/0	0/0/0/0
2	GOL	B	1537	-	-	0/4/4/4	0/0/0/0
4	NAG	B	2501	5	-	0/6/23/26	0/1/1/1
5	GDL	B	2502	4,6	-	0/6/23/26	0/1/1/1
6	PHJ	B	2503	5	-	0/4/6/6	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2503	PHJ	C1-N	-3.47	1.35	1.41
5	A	2502	GDL	O5-C1	-3.47	1.37	1.43
6	B	2503	PHJ	C1-N	-3.42	1.35	1.41
5	B	2502	GDL	O5-C1	-2.87	1.38	1.43
5	B	2502	GDL	C2-N1	2.04	1.49	1.46
5	A	2502	GDL	C2-N1	2.13	1.50	1.46
6	B	2503	PHJ	OXT-C	2.24	1.26	1.21
6	A	2503	PHJ	OXT-C	2.25	1.26	1.21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2502	GDL	C1-C2	2.38	1.55	1.52
4	B	2501	NAG	C1-C2	2.63	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2502	GDL	C1-O5-C5	3.63	116.85	112.25
5	B	2502	GDL	C1-O5-C5	3.73	116.99	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

67 monomers are involved in 219 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	GOL	6	0
2	A	1501	GOL	2	0
2	A	1502	GOL	7	0
2	A	1503	GOL	2	0
2	A	1504	GOL	2	0
2	A	1505	GOL	4	0
2	A	1506	GOL	3	0
2	A	1507	GOL	7	0
2	A	1508	GOL	1	0
2	A	1509	GOL	4	0
2	A	1510	GOL	3	0
2	A	1512	GOL	12	0
2	A	1513	GOL	8	0
2	A	1515	GOL	1	0
2	A	1516	GOL	1	0
2	A	1517	GOL	5	0
2	A	1518	GOL	2	0
2	A	1519	GOL	1	0
2	A	1520	GOL	2	0
2	A	1521	GOL	4	0
2	A	1523	GOL	1	0
2	A	1524	GOL	3	0
2	A	1525	GOL	5	0
2	A	1526	GOL	3	0
2	A	1527	GOL	5	0
2	A	1528	GOL	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1529	GOL	2	0
3	A	1533	SO4	2	0
3	A	1536	SO4	1	0
3	A	1537	SO4	1	0
2	A	1538	GOL	1	0
5	A	2502	GDL	1	0
6	A	2503	PHJ	5	0
2	B	1500	GOL	6	0
2	B	1501	GOL	1	0
2	B	1502	GOL	2	0
2	B	1503	GOL	5	0
2	B	1504	GOL	1	0
2	B	1505	GOL	4	0
2	B	1506	GOL	3	0
2	B	1507	GOL	1	0
2	B	1508	GOL	8	0
2	B	1509	GOL	3	0
2	B	1510	GOL	3	0
2	B	1511	GOL	11	0
2	B	1512	GOL	3	0
2	B	1514	GOL	5	0
2	B	1515	GOL	6	0
2	B	1516	GOL	4	0
2	B	1517	GOL	1	0
2	B	1518	GOL	3	0
2	B	1519	GOL	1	0
2	B	1521	GOL	4	0
2	B	1522	GOL	4	0
2	B	1523	GOL	2	0
2	B	1524	GOL	3	0
2	B	1525	GOL	3	0
2	B	1526	GOL	1	0
2	B	1527	GOL	4	0
2	B	1528	GOL	3	0
2	B	1529	GOL	4	0
2	B	1530	GOL	2	0
2	B	1531	GOL	6	0
3	B	1534	SO4	1	0
3	B	1536	SO4	1	0
2	B	1537	GOL	2	0
6	B	2503	PHJ	7	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	497/499 (99%)	0.43	46 (9%) 11 8	16, 32, 52, 63	0
1	B	498/499 (99%)	0.35	40 (8%) 15 12	20, 30, 51, 73	0
All	All	995/998 (99%)	0.39	86 (8%) 13 10	16, 30, 52, 73	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	VAL	7.7
1	B	481	TYR	6.2
1	A	472	GLY	5.7
1	B	483	THR	5.3
1	B	463	ALA	5.2
1	B	461	THR	5.0
1	B	319	PRO	5.0
1	A	452	THR	5.0
1	A	450	ILE	4.8
1	B	464	GLN	4.4
1	A	316	ASP	4.2
1	B	316[A]	ASP	4.1
1	B	465	GLY	3.9
1	A	471	GLN	3.9
1	A	470	TYR	3.9
1	B	484	SER	3.8
1	B	480	GLY	3.6
1	B	460	THR	3.5
1	A	302	GLY	3.4
1	A	321	THR	3.4
1	A	461	THR	3.4
1	B	354	GLY	3.4
1	B	459	GLY	3.4
1	B	317	PRO	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	3.4
1	A	453	ALA	3.4
1	B	462	TYR	3.2
1	A	467	LEU	3.2
1	A	466	ALA	3.2
1	A	496	GLY	3.2
1	B	301	GLY	3.2
1	A	468	VAL	3.1
1	B	482	ILE	3.1
1	A	300	SER	3.1
1	A	319	PRO	3.0
1	B	302	GLY	2.9
1	A	451	MET	2.9
1	B	479	TRP	2.9
1	A	98	TYR	2.9
1	A	462	TYR	2.9
1	A	301	GLY	2.8
1	B	456	TYR	2.8
1	A	16	ASN	2.8
1	B	371	ALA	2.8
1	A	473	TYR	2.8
1	B	369	TYR	2.7
1	A	488	SER	2.7
1	B	315	GLU	2.7
1	A	456	TYR	2.7
1	B	457	VAL	2.7
1	A	469	SER	2.7
1	B	488	SER	2.6
1	A	329	GLU	2.6
1	B	352	ASN	2.5
1	B	234	ALA	2.5
1	A	65	ALA	2.5
1	B	441	THR	2.5
1	A	499	ARG	2.5
1	B	372	GLN	2.5
1	A	335	LYS	2.4
1	B	216	LEU	2.4
1	A	26	THR	2.4
1	A	323	TYR	2.4
1	B	148	ALA	2.4
1	B	229	ALA	2.4
1	A	458	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	470	TYR	2.3
1	A	377	VAL	2.3
1	A	497	ARG	2.3
1	A	54	ILE	2.3
1	A	449	PRO	2.2
1	B	351	GLY	2.2
1	B	228	ALA	2.1
1	A	454	PRO	2.1
1	A	24	THR	2.1
1	A	47	ILE	2.1
1	B	240	TYR	2.1
1	A	474	VAL	2.1
1	B	377	VAL	2.1
1	B	485	ALA	2.1
1	A	484	SER	2.1
1	A	116	THR	2.1
1	A	317	PRO	2.1
1	A	108	ALA	2.0
1	B	300	SER	2.0
1	B	47	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 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
2	GOL	B	1525	6/6	0.86	0.25	17.93	80,80,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	1500	6/6	0.82	0.27	17.07	42,46,49,52	0
2	GOL	A	1528	6/6	0.74	0.50	14.65	74,75,77,77	0
2	GOL	B	1512	6/6	0.54	0.35	10.90	44,51,52,55	0
2	GOL	A	1506	6/6	0.81	0.22	10.19	40,44,46,46	0
2	GOL	B	1509	6/6	0.87	0.26	9.99	49,49,50,50	0
2	GOL	A	1512	6/6	0.69	0.43	9.55	58,60,61,62	0
2	GOL	B	1528	6/6	0.60	0.44	9.29	69,70,71,71	0
2	GOL	B	1523	6/6	0.82	0.30	8.84	51,53,53,53	0
2	GOL	A	1538	6/6	0.68	0.31	8.80	66,67,68,70	0
2	GOL	B	1520	6/6	0.83	0.21	8.68	65,66,66,67	0
2	GOL	A	1525	6/6	0.81	0.40	8.44	35,39,42,46	0
2	GOL	B	1505	6/6	0.69	0.23	8.44	47,55,56,59	0
2	GOL	A	1511	6/6	0.55	0.40	7.96	78,79,79,79	0
2	GOL	A	1524	6/6	0.87	0.31	7.55	56,57,58,61	0
2	GOL	B	1511	6/6	0.72	0.30	7.36	52,53,54,55	0
2	GOL	B	1516	6/6	0.84	0.34	7.20	62,64,64,65	0
2	GOL	B	1526	6/6	0.70	0.18	6.54	58,59,60,62	0
2	GOL	B	1501	6/6	0.85	0.32	6.50	53,55,58,58	0
2	GOL	A	1503	6/6	0.88	0.25	6.23	37,39,45,48	0
2	GOL	A	1502	6/6	0.90	0.23	6.15	36,42,42,45	0
2	GOL	A	1504	6/6	0.83	0.22	5.78	39,42,43,47	0
2	GOL	A	1519	6/6	0.75	0.18	5.31	57,60,61,64	0
2	GOL	A	1526	6/6	0.83	0.35	5.08	49,52,52,53	0
2	GOL	A	1509	6/6	0.68	0.37	5.03	58,61,63,65	0
2	GOL	A	1520	6/6	0.76	0.34	4.77	58,60,61,63	0
2	GOL	B	1522	6/6	0.61	0.35	4.01	64,66,67,68	0
2	GOL	B	1515	6/6	0.65	0.28	3.91	57,59,60,61	0
3	SO4	B	1535	5/5	0.94	0.23	3.89	71,72,73,73	0
2	GOL	B	1503	6/6	0.82	0.22	3.60	55,56,58,62	0
2	GOL	B	1507	6/6	0.64	0.23	3.30	55,57,58,58	0
2	GOL	B	1506	6/6	0.77	0.29	3.28	49,54,55,55	0
2	GOL	B	1510	6/6	0.83	0.14	3.26	68,69,70,70	0
2	GOL	B	1537	6/6	0.86	0.21	3.22	56,57,59,59	0
2	GOL	B	1502	6/6	0.81	0.23	3.19	46,49,50,52	0
2	GOL	B	1524	6/6	0.81	0.29	2.94	72,72,73,73	0
6	PHJ	A	2503	11/11	0.91	0.14	2.62	28,34,42,43	0
2	GOL	B	1529	6/6	0.61	0.34	2.36	66,66,66,67	0
2	GOL	A	1513	6/6	0.79	0.39	2.29	68,70,70,72	0
2	GOL	A	1516	6/6	0.54	0.25	2.18	47,52,53,53	0
2	GOL	A	1514	6/6	0.74	0.23	2.09	74,74,75,75	0
2	GOL	B	1518	6/6	0.52	0.27	1.78	63,65,65,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	1523	6/6	0.70	0.21	1.66	66,69,69,71	0
2	GOL	A	1529	6/6	0.64	0.27	1.64	60,62,62,63	0
2	GOL	A	1510	6/6	0.72	0.14	1.43	63,64,65,65	0
6	PHJ	B	2503	11/11	0.93	0.12	1.27	25,34,37,38	0
2	GOL	B	1508	6/6	0.67	0.21	1.27	58,59,59,60	0
2	GOL	A	1501	6/6	0.67	0.25	1.03	64,65,66,68	0
3	SO4	A	1536	5/5	0.94	0.21	0.82	78,79,79,80	0
3	SO4	A	1532	5/5	0.98	0.12	0.66	42,44,46,46	0
4	NAG	A	2501	14/15	0.90	0.10	-0.69	26,28,32,34	0
5	GDL	A	2502	14/15	0.94	0.09	-0.72	21,23,27,27	0
5	GDL	B	2502	14/15	0.95	0.08	-1.18	20,23,25,25	0
4	NAG	B	2501	14/15	0.96	0.07	-1.87	21,24,27,28	0
2	GOL	A	1507	6/6	0.84	0.16	-	48,49,51,53	0
2	GOL	B	1514	6/6	0.63	0.38	-	71,73,73,75	0
2	GOL	B	1519	6/6	0.72	0.32	-	69,70,71,72	0
2	GOL	A	1505	6/6	0.88	0.19	-	43,50,53,55	0
2	GOL	B	1521	6/6	0.75	0.34	-	65,66,67,67	0
2	GOL	B	1530	6/6	0.82	0.31	-	60,62,62,63	0
3	SO4	A	1535	5/5	0.92	0.14	-	82,82,83,83	0
2	GOL	A	1527	6/6	0.73	0.36	-	69,70,70,71	0
2	GOL	B	1527	6/6	0.86	0.23	-	63,64,64,66	0
2	GOL	A	1521	6/6	0.84	0.21	-	58,59,61,62	0
2	GOL	B	1517	6/6	0.60	0.25	-	51,53,54,54	0
2	GOL	A	1515	6/6	0.80	0.18	-	68,69,69,70	0
3	SO4	B	1536	5/5	0.90	0.19	-	92,92,92,92	0
2	GOL	A	1518	6/6	0.85	0.27	-	82,82,83,83	0
2	GOL	B	1500	6/6	0.85	0.26	-	60,61,64,64	0
3	SO4	A	1537	5/5	0.93	0.37	-	92,93,93,93	0
3	SO4	A	1533	5/5	0.99	0.20	-	49,53,53,54	0
2	GOL	B	1513	6/6	0.84	0.16	-	65,67,67,67	0
2	GOL	A	1508	6/6	0.80	0.30	-	57,61,63,65	0
2	GOL	A	1522	6/6	0.80	0.33	-	72,73,75,75	0
3	SO4	A	1534	5/5	0.95	0.15	-	46,46,49,49	0
2	GOL	B	1531	6/6	0.84	0.32	-	69,69,70,71	0
2	GOL	A	1517	6/6	0.73	0.31	-	60,62,62,62	0
3	SO4	B	1534	5/5	0.99	0.15	-	53,54,54,56	0
2	GOL	B	1504	6/6	0.82	0.20	-	41,47,51,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.