



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 06:38 AM EDT

PDB ID : 1SO0  
Title : Crystal structure of human galactose mutarotase complexed with galactose  
Authors : Thoden, J.B.; Timson, D.J.; Reece, R.J.; Holden, H.M.  
Deposited on : unknown  
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

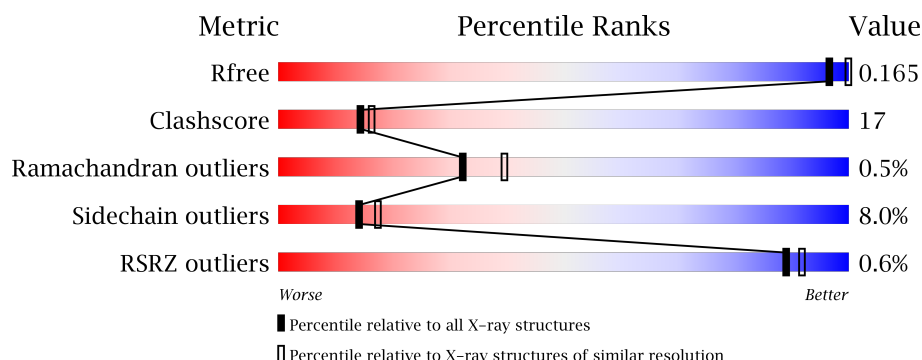
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	344	<div> <div style="width: 65%;"></div> <div style="width: 29%;"></div> <div style="width: 5%;"></div> <div>65%29%5% .</div> </div>
1	B	344	<div> <div style="width: 59%;"></div> <div style="width: 32%;"></div> <div style="width: 7%;"></div> <div>59%32%7% ..</div> </div>
1	C	344	<div> <div style="width: 58%;"></div> <div style="width: 33%;"></div> <div style="width: 8%;"></div> <div>58%33%8% .</div> </div>
1	D	344	<div> <div style="width: 59%;"></div> <div style="width: 32%;"></div> <div style="width: 8%;"></div> <div>59%32%8% .</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11200 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.

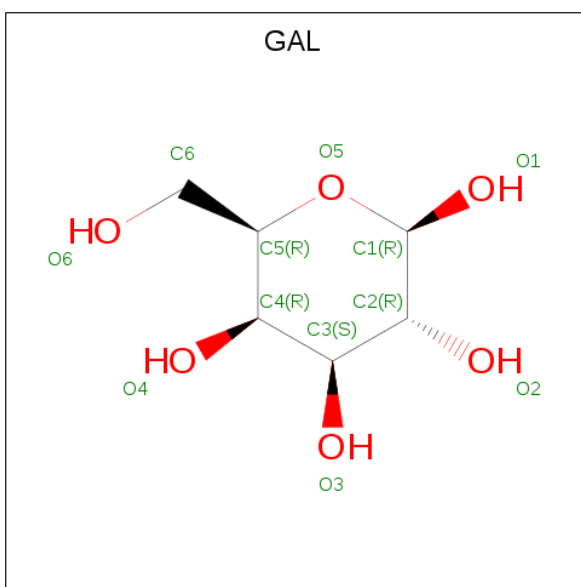
- Molecule 1 is a protein called aldose 1-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	2	0
			2698	1718	469	506	5			
1	B	342	Total	C	N	O	S	0	1	0
			2679	1707	465	502	5			
1	C	344	Total	C	N	O	S	0	0	0
			2688	1712	469	502	5			
1	D	342	Total	C	N	O	S	0	1	0
			2681	1708	468	500	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q96C23
A	0	HIS	-	CLONING ARTIFACT	UNP Q96C23
B	-1	GLY	-	CLONING ARTIFACT	UNP Q96C23
B	0	HIS	-	CLONING ARTIFACT	UNP Q96C23
C	-1	GLY	-	CLONING ARTIFACT	UNP Q96C23
C	0	HIS	-	CLONING ARTIFACT	UNP Q96C23
D	-1	GLY	-	CLONING ARTIFACT	UNP Q96C23
D	0	HIS	-	CLONING ARTIFACT	UNP Q96C23

- Molecule 2 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

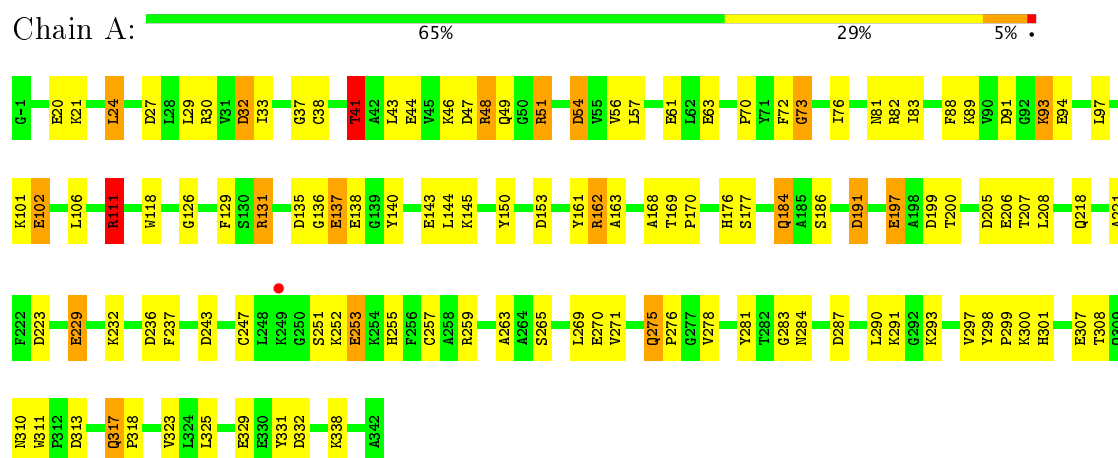
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	99	Total	O	0	0
			99	99		
3	C	113	Total	O	0	0
			113	113		
3	D	76	Total	O	0	0
			76	76		

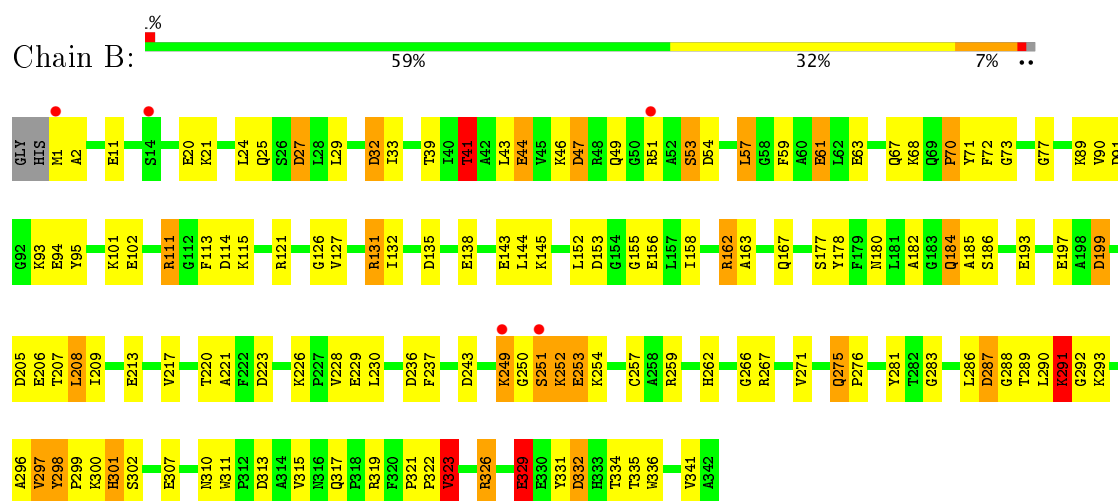
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

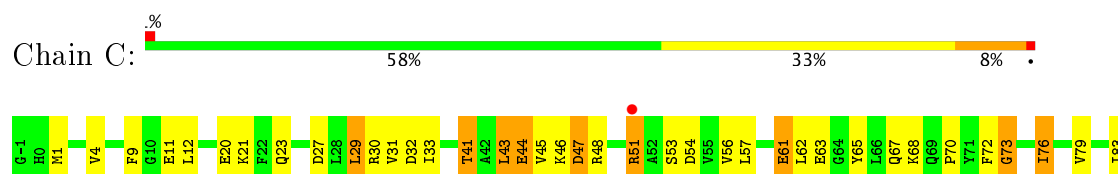
#### • Molecule 1: aldose 1-epimerase

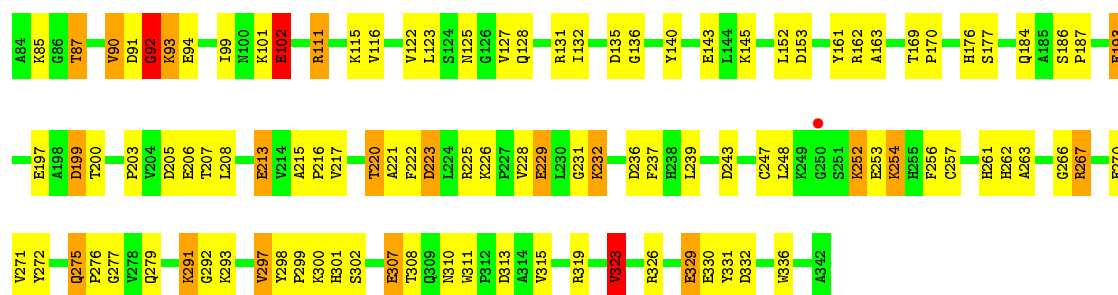


#### • Molecule 1: aldose 1-epimerase



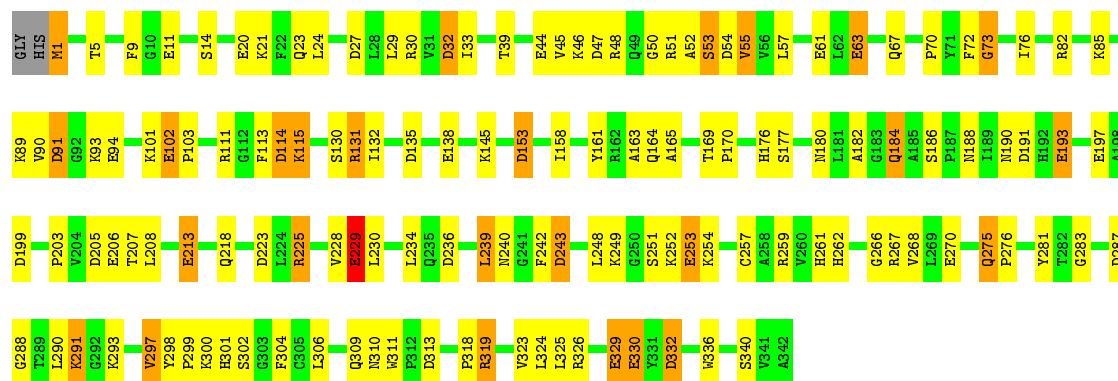
#### • Molecule 1: aldose 1-epimerase





- Molecule 1: aldose 1-epimerase

Chain D: 59% 32% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.00Å 68.70Å 98.90Å 107.70° 98.40° 102.70°	Depositor
Resolution (Å)	30.00 – 2.30 57.92 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.30) 81.1 (57.92-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.25Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.167 , 0.198 0.164 , 0.165	Depositor DCC
$R_{free}$ test set	6054 reflections (11.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 69.0	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	0.96	EDS
Total number of atoms	11200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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: GAL

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	1.01	18/2778 (0.6%)	1.48	37/3775 (1.0%)
1	B	0.99	19/2754 (0.7%)	1.44	40/3742 (1.1%)
1	C	1.02	20/2760 (0.7%)	1.43	34/3750 (0.9%)
1	D	1.00	16/2756 (0.6%)	1.42	36/3744 (1.0%)
All	All	1.01	73/11048 (0.7%)	1.44	147/15011 (1.0%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	253	GLU	CD-OE2	9.76	1.36	1.25
1	D	61	GLU	CD-OE2	9.55	1.36	1.25
1	B	61	GLU	CD-OE2	9.53	1.36	1.25
1	C	90	VAL	C-O	8.33	1.39	1.23
1	D	102	GLU	CD-OE2	8.31	1.34	1.25
1	B	253	GLU	CD-OE2	8.30	1.34	1.25
1	C	11	GLU	CD-OE2	8.24	1.34	1.25
1	D	330	GLU	CD-OE2	7.50	1.33	1.25
1	C	61	GLU	CD-OE2	7.47	1.33	1.25
1	B	63	GLU	CD-OE2	7.38	1.33	1.25
1	C	102	GLU	CD-OE2	7.16	1.33	1.25
1	A	206	GLU	CD-OE2	6.80	1.33	1.25
1	A	253	GLU	CD-OE2	6.74	1.33	1.25
1	D	213	GLU	CD-OE2	6.32	1.32	1.25
1	A	94	GLU	CD-OE2	6.30	1.32	1.25
1	A	229[A]	GLU	CD-OE2	6.28	1.32	1.25
1	A	229[B]	GLU	CD-OE2	6.28	1.32	1.25
1	C	63	GLU	CD-OE2	6.28	1.32	1.25
1	C	193	GLU	CD-OE2	6.26	1.32	1.25
1	B	143	GLU	CD-OE2	6.22	1.32	1.25
1	A	307	GLU	CD-OE2	6.21	1.32	1.25
1	C	143	GLU	CD-OE2	6.21	1.32	1.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	GLU	CD-OE2	6.18	1.32	1.25
1	B	213	GLU	CD-OE2	6.07	1.32	1.25
1	C	20	GLU	CD-OE2	6.04	1.32	1.25
1	A	20	GLU	CD-OE2	6.04	1.32	1.25
1	C	94	GLU	CD-OE2	6.03	1.32	1.25
1	D	44	GLU	CD-OE2	5.93	1.32	1.25
1	B	138	GLU	CD-OE2	5.88	1.32	1.25
1	D	94	GLU	CD-OE2	5.82	1.32	1.25
1	A	143	GLU	CD-OE2	5.82	1.32	1.25
1	B	156	GLU	CD-OE2	5.81	1.32	1.25
1	D	206	GLU	CD-OE2	5.80	1.32	1.25
1	C	330	GLU	CD-OE2	5.78	1.32	1.25
1	B	94	GLU	CD-OE2	5.75	1.31	1.25
1	D	229	GLU	CD-OE2	5.74	1.31	1.25
1	D	197	GLU	CD-OE2	5.71	1.31	1.25
1	C	253	GLU	CD-OE2	5.67	1.31	1.25
1	D	63	GLU	CD-OE2	5.66	1.31	1.25
1	B	197	GLU	CD-OE2	5.64	1.31	1.25
1	C	213	GLU	CD-OE2	5.63	1.31	1.25
1	B	307	GLU	CD-OE2	5.61	1.31	1.25
1	A	61	GLU	CD-OE2	5.57	1.31	1.25
1	B	229[A]	GLU	CD-OE2	5.57	1.31	1.25
1	B	229[B]	GLU	CD-OE2	5.57	1.31	1.25
1	B	11	GLU	CD-OE2	5.55	1.31	1.25
1	A	102[A]	GLU	CD-OE2	5.54	1.31	1.25
1	A	102[B]	GLU	CD-OE2	5.54	1.31	1.25
1	A	44	GLU	CD-OE2	5.50	1.31	1.25
1	C	197	GLU	CD-OE2	5.43	1.31	1.25
1	C	307	GLU	CD-OE2	5.42	1.31	1.25
1	B	102	GLU	CD-OE2	5.42	1.31	1.25
1	C	92	GLY	CA-C	5.41	1.60	1.51
1	A	138	GLU	CD-OE2	5.40	1.31	1.25
1	A	63	GLU	CD-OE2	5.37	1.31	1.25
1	C	329	GLU	CD-OE2	5.35	1.31	1.25
1	A	197	GLU	CD-OE2	5.33	1.31	1.25
1	D	20	GLU	CD-OE2	5.33	1.31	1.25
1	D	193	GLU	CD-OE2	5.30	1.31	1.25
1	A	329	GLU	CD-OE2	5.29	1.31	1.25
1	C	270	GLU	CD-OE2	5.26	1.31	1.25
1	C	206	GLU	CD-OE2	5.21	1.31	1.25
1	D	11	GLU	CD-OE2	5.20	1.31	1.25
1	B	329	GLU	CD-OE2	5.20	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	GLU	CD-OE2	5.20	1.31	1.25
1	D	270	GLU	CD-OE2	5.17	1.31	1.25
1	B	193	GLU	CD-OE2	5.16	1.31	1.25
1	B	44	GLU	CD-OE2	5.14	1.31	1.25
1	B	20	GLU	CD-OE2	5.13	1.31	1.25
1	C	44	GLU	CD-OE2	5.07	1.31	1.25
1	C	229	GLU	CD-OE2	5.05	1.31	1.25
1	A	253	GLU	CD-OE1	-5.05	1.20	1.25
1	A	137	GLU	CD-OE1	-5.03	1.20	1.25

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	VAL	O-C-N	10.92	140.17	122.70
1	A	54	ASP	CB-CG-OD2	-10.68	108.69	118.30
1	C	313	ASP	CB-CG-OD2	-10.39	108.95	118.30
1	A	236	ASP	CB-CG-OD2	-9.39	109.85	118.30
1	A	47	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	A	54	ASP	CB-CG-OD1	9.08	126.47	118.30
1	B	135	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	B	243	ASP	CB-CG-OD1	8.76	126.18	118.30
1	B	326	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	A	243	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	C	199	ASP	CB-CG-OD2	-8.52	110.64	118.30
1	A	47	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	135	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	A	32	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	243	ASP	CB-CG-OD1	8.26	125.73	118.30
1	D	199	ASP	CB-CG-OD1	8.23	125.70	118.30
1	A	259	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	71	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	C	313	ASP	CB-CG-OD1	8.05	125.55	118.30
1	D	223	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	205	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	135	ASP	CB-CG-OD1	7.89	125.40	118.30
1	C	199	ASP	CB-CG-OD1	7.81	125.33	118.30
1	B	32	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	199	ASP	CB-CG-OD1	7.69	125.22	118.30
1	C	92	GLY	O-C-N	-7.64	110.47	122.70
1	B	111	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	32	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	C	326	ARG	NE-CZ-NH2	-7.51	116.54	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	223	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	135	ASP	CB-CG-OD1	7.45	125.00	118.30
1	D	91	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	C	223	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	D	223	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	D	199	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	C	243	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	D	135	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	D	114	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	D	243	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	D	313	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	191	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	C	205	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	95	TYR	CB-CG-CD2	7.15	125.29	121.00
1	B	71	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	131	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	32	ASP	CB-CG-OD1	6.95	124.55	118.30
1	D	287	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	B	54	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	D	54	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	D	236	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	223	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	121	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	287	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	C	243	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	259	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	153	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	D	27	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	C	51	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	135	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	D	135	ASP	CB-CG-OD1	6.58	124.23	118.30
1	C	323	VAL	CG1-CB-CG2	6.57	121.41	110.90
1	B	131	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	135	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	205	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	C	326	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	111	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	131	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	236	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	323	VAL	CB-CA-C	-6.42	99.19	111.40
1	C	47	ASP	CB-CG-OD2	-6.39	112.55	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	251	SER	N-CA-C	-6.34	93.87	111.00
1	D	32	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	287	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	C	54	ASP	CB-CG-OD1	6.27	123.94	118.30
1	D	332	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	323	VAL	CB-CA-C	-6.25	99.52	111.40
1	B	205	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	332	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	225	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	199	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	191	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	313	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	C	51	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	27	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	D	259	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	205	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	223	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	191	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	90	VAL	CB-CA-C	-5.98	100.04	111.40
1	D	131	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	243	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	205	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	27	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	30	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	C	236	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	27	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	223	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	D	153	ASP	CB-CG-OD1	5.84	123.55	118.30
1	D	191	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	27	ASP	CB-CG-OD2	-5.82	113.07	118.30
1	B	259	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	236	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	54	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	153	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	114	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	313	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	48[A]	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	48[B]	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	47	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	91	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	B	41	THR	N-CA-CB	-5.60	99.65	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	313	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	47	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	308	THR	CA-CB-CG2	-5.54	104.65	112.40
1	B	250	GLY	CA-C-N	-5.48	105.15	117.20
1	B	199	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	291	LYS	N-CA-CB	-5.44	100.81	110.60
1	D	113	PHE	CB-CG-CD2	-5.42	117.00	120.80
1	D	332	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	32	ASP	CB-CG-OD1	5.42	123.17	118.30
1	D	287	ASP	CB-CG-OD1	5.33	123.09	118.30
1	C	92	GLY	N-CA-C	5.33	126.41	113.10
1	B	95	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	C	267	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	B	199	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	297	VAL	C-N-CA	-5.25	108.57	121.70
1	B	319	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	205	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	332	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	236	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	308	THR	CA-CB-CG2	-5.18	105.15	112.40
1	A	41	THR	N-CA-CB	-5.16	100.49	110.30
1	A	153	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	207	THR	CA-CB-CG2	-5.16	105.18	112.40
1	C	41	THR	N-CA-CB	-5.14	100.54	110.30
1	C	161	TYR	CB-CA-C	-5.13	100.14	110.40
1	A	223	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	150	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	47	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	29	LEU	CB-CA-C	-5.03	100.65	110.20
1	B	298	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	54	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	330	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	B	251	SER	N-CA-C	-5.01	97.48	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	2698	0	2614	75	0
1	B	2679	0	2602	90	0
1	C	2688	0	2610	110	0
1	D	2681	0	2609	98	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	118	0	0	3	0
3	B	99	0	0	2	0
3	C	113	0	0	7	0
3	D	76	0	0	5	0
All	All	11200	0	10483	368	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 17.

All (368) 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:76:ILE:HD11	1:A:176:HIS:HB2	1.19	1.14
1:C:1:MET:HE2	1:C:125:ASN:HD22	1.11	1.08
1:D:240:ASN:HD21	1:D:300:LYS:NZ	1.50	1.07
1:C:90:VAL:C	3:C:791:HOH:O	1.91	1.07
1:B:184:GLN:HE22	1:B:293:LYS:HB2	1.24	1.02
1:B:32:ASP:HB2	1:B:41:THR:HG22	1.50	0.90
1:D:76:ILE:HD11	1:D:176:HIS:HB2	1.54	0.87
1:C:67:GLN:HE22	1:C:291:LYS:HD2	1.40	0.85
1:C:76:ILE:CD1	1:C:176:HIS:HB2	2.06	0.85
1:A:76:ILE:CD1	1:A:176:HIS:HB2	2.05	0.84
1:C:315:VAL:HG12	1:C:323:VAL:HG21	1.61	0.83
1:C:1:MET:HE2	1:C:125:ASN:ND2	1.94	0.82
1:D:240:ASN:HD21	1:D:300:LYS:HZ3	1.25	0.81
1:D:240:ASN:HD21	1:D:300:LYS:HZ1	1.26	0.81
1:D:240:ASN:ND2	1:D:300:LYS:NZ	2.29	0.80
1:C:275:GLN:HE21	1:C:276:PRO:HD2	1.47	0.80
1:D:76:ILE:CD1	1:D:176:HIS:HB2	2.11	0.80
1:D:23:GLN:OE1	1:D:30:ARG:HD2	1.84	0.77
1:A:184:GLN:OE1	1:A:293:LYS:HB2	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:OE1	1:A:293:LYS:HE3	1.85	0.76
1:A:24:LEU:HD13	1:A:126:GLY:HA2	1.68	0.75
1:C:220:THR:HG23	1:C:222:PHE:HD1	1.50	0.74
1:D:29:LEU:CD2	1:D:45:VAL:HG22	2.17	0.74
1:B:32:ASP:CB	1:B:41:THR:HG22	2.18	0.74
1:C:220:THR:CG2	1:C:222:PHE:H	1.99	0.74
1:D:326:ARG:O	1:D:329:GLU:HG3	1.88	0.73
1:D:309:GLN:HG3	1:D:310:ASN:O	1.88	0.73
1:C:275:GLN:HE21	1:C:276:PRO:CD	2.02	0.73
1:C:297:VAL:O	1:C:299:PRO:HD3	1.89	0.72
1:C:73:GLY:HA2	1:C:177:SER:HA	1.70	0.72
1:D:5:THR:HG23	3:D:802:HOH:O	1.91	0.71
1:B:162:ARG:HA	1:B:331:TYR:O	1.90	0.70
1:C:91:ASP:C	3:C:791:HOH:O	2.30	0.70
1:D:240:ASN:ND2	1:D:300:LYS:HZ3	1.85	0.70
1:C:51:ARG:NH1	1:D:288:GLY:HA3	2.06	0.69
1:C:252:LYS:HD2	1:C:252:LYS:H	1.57	0.69
1:C:85:LYS:O	1:C:87:THR:HG22	1.92	0.69
1:C:220:THR:HG23	1:C:222:PHE:H	1.58	0.68
1:D:46:LYS:HA	1:D:51:ARG:O	1.94	0.68
1:A:76:ILE:HD11	1:A:176:HIS:CB	2.11	0.68
1:B:1:MET:HG3	1:B:2:ALA:H	1.57	0.68
1:D:57:LEU:HD13	1:D:298:TYR:CD2	2.29	0.68
1:B:59:PHE:CE1	1:B:72:PHE:HD1	2.12	0.67
1:D:53:SER:HB2	1:D:267:ARG:NH2	2.09	0.67
1:B:21:LYS:NZ	1:B:41:THR:HG21	2.10	0.66
1:A:88:PHE:HE2	1:A:97:LEU:HD11	1.61	0.66
1:A:197:GLU:HG3	3:A:565:HOH:O	1.96	0.66
1:B:252:LYS:HD2	1:B:252:LYS:H	1.60	0.66
1:D:9:PHE:CD1	1:D:21:LYS:HE3	2.30	0.66
1:B:310:ASN:ND2	1:B:323:VAL:HG13	2.10	0.65
1:A:221:ALA:HB2	1:A:237:PHE:CD2	2.31	0.65
1:D:275:GLN:HE21	1:D:276:PRO:HD2	1.61	0.64
1:D:165:ALA:HB2	1:D:325:LEU:HD23	1.78	0.64
1:A:21:LYS:CE	1:A:41:THR:HG21	2.26	0.64
1:C:91:ASP:N	3:C:791:HOH:O	2.22	0.64
1:D:53:SER:HB2	1:D:267:ARG:HH22	1.63	0.64
1:C:21:LYS:NZ	1:C:41:THR:HG21	2.13	0.63
1:B:208:LEU:N	1:B:208:LEU:HD23	2.12	0.63
1:C:299:PRO:HD2	1:C:302:SER:HB3	1.80	0.63
1:B:57:LEU:N	1:B:57:LEU:HD23	2.14	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLN:HE21	1:A:276:PRO:CD	2.11	0.62
1:B:326:ARG:O	1:B:329:GLU:HG3	1.99	0.62
1:D:158:ILE:HG12	1:D:336:TRP:CD1	2.35	0.62
1:B:49:GLN:NE2	1:B:51:ARG:NH1	2.48	0.61
1:C:132:ILE:HG12	1:C:145:LYS:HG2	1.83	0.61
1:C:220:THR:HG23	1:C:222:PHE:CD1	2.34	0.61
1:A:276:PRO:HG2	1:A:310:ASN:HA	1.80	0.61
1:D:164:GLN:NE2	1:D:330:GLU:OE1	2.33	0.61
1:D:29:LEU:HD21	1:D:45:VAL:HG22	1.81	0.60
1:A:24:LEU:CD1	1:A:126:GLY:HA2	2.30	0.60
1:B:57:LEU:HD13	1:B:298:TYR:CD2	2.36	0.60
1:C:51:ARG:HH12	1:D:288:GLY:HA3	1.65	0.60
1:B:70:PRO:HB2	1:B:178:TYR:OH	2.01	0.60
1:A:145:LYS:O	1:A:163:ALA:HA	2.01	0.60
1:C:276:PRO:HG2	1:C:310:ASN:HA	1.84	0.59
1:D:184:GLN:OE1	1:D:293:LYS:HB2	2.02	0.59
1:C:257:CYS:HB3	1:C:271:VAL:O	2.02	0.59
1:A:48:ARG:NH1	1:A:263:ALA:O	2.30	0.59
1:C:1:MET:CE	1:C:153:ASP:HB2	2.33	0.58
1:D:73:GLY:HA2	1:D:177:SER:HA	1.84	0.58
1:D:300:LYS:HE2	1:D:301:HIS:CE1	2.37	0.58
1:D:169:THR:OG1	1:D:170:PRO:HD2	2.03	0.58
1:D:299:PRO:HD2	1:D:302:SER:HB3	1.85	0.58
1:A:73:GLY:HA2	1:A:177:SER:HA	1.85	0.58
1:A:57:LEU:HB3	1:A:72:PHE:HE2	1.69	0.58
1:C:31:VAL:HG22	1:C:43:LEU:HG	1.85	0.58
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.69	0.58
1:A:21:LYS:HE2	1:A:41:THR:HG21	1.86	0.57
1:A:21:LYS:NZ	1:A:41:THR:HG21	2.20	0.57
1:C:275:GLN:NE2	1:C:276:PRO:HD2	2.19	0.57
1:C:1:MET:HE3	1:C:153:ASP:CB	2.35	0.57
1:C:57:LEU:HD13	1:C:298:TYR:CD2	2.40	0.57
1:A:88:PHE:CE2	1:A:97:LEU:HD11	2.40	0.57
1:B:77:GLY:HA3	1:B:113:PHE:CD2	2.39	0.57
1:B:217:VAL:O	1:B:220:THR:HG23	2.05	0.57
1:C:92:GLY:N	3:C:791:HOH:O	2.36	0.57
1:A:275:GLN:HE21	1:A:276:PRO:HD2	1.69	0.57
1:D:299:PRO:HD2	1:D:302:SER:CB	2.34	0.57
1:C:29:LEU:HD12	1:C:152:LEU:HD11	1.86	0.57
1:A:57:LEU:CB	1:A:72:PHE:HE2	2.16	0.56
1:B:49:GLN:HE21	1:B:51:ARG:HH11	1.52	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:HA2	1:B:177:SER:HA	1.87	0.56
1:B:180:ASN:HD21	1:B:186:SER:HB2	1.71	0.56
1:B:287:ASP:O	1:B:289:THR:HG23	2.06	0.56
1:C:184:GLN:OE1	1:C:293:LYS:HB2	2.05	0.56
1:A:57:LEU:HD23	1:A:57:LEU:N	2.20	0.56
1:D:319:ARG:N	1:D:319:ARG:HD3	2.20	0.56
1:C:315:VAL:HG12	1:C:323:VAL:CG2	2.34	0.55
1:C:315:VAL:CG1	1:C:323:VAL:HG21	2.33	0.55
1:C:51:ARG:CZ	1:D:299:PRO:HB3	2.36	0.55
1:A:24:LEU:HD23	1:A:24:LEU:N	2.21	0.55
1:A:43:LEU:O	1:A:54:ASP:HA	2.06	0.55
1:B:252:LYS:HD2	1:B:252:LYS:N	2.20	0.55
1:C:199:ASP:O	1:C:217:VAL:HG13	2.07	0.55
1:C:48:ARG:NH2	1:C:263:ALA:O	2.35	0.55
1:A:318:PRO:HD2	3:A:589:HOH:O	2.05	0.55
1:C:252:LYS:CD	1:C:252:LYS:H	2.19	0.55
1:A:82:ARG:NH2	1:A:208:LEU:HD12	2.22	0.55
1:D:33:ILE:HA	1:D:39:THR:O	2.07	0.55
1:D:131:ARG:HG2	1:D:132:ILE:N	2.22	0.54
1:B:49:GLN:NE2	1:B:51:ARG:HH11	2.05	0.54
1:C:1:MET:CE	1:C:125:ASN:HD22	2.01	0.54
1:C:221:ALA:HB2	1:C:237:PHE:CD2	2.42	0.54
1:D:281:TYR:CE2	1:D:283:GLY:HA2	2.42	0.54
1:C:217:VAL:O	1:C:220:THR:HB	2.06	0.54
1:C:220:THR:HG22	1:C:222:PHE:H	1.70	0.54
1:B:162:ARG:NH1	1:B:162:ARG:HG2	2.23	0.54
1:A:32:ASP:CB	1:A:41:THR:HG22	2.37	0.54
1:A:275:GLN:HE21	1:A:275:GLN:HA	1.73	0.54
1:C:1:MET:HE3	1:C:153:ASP:HB2	1.90	0.54
1:A:269:LEU:HD12	1:A:270:GLU:N	2.23	0.54
1:D:281:TYR:CZ	1:D:283:GLY:HA2	2.43	0.54
1:C:47:ASP:OD2	1:C:51:ARG:HB2	2.08	0.54
1:A:70:PRO:HD2	1:A:72:PHE:CE1	2.42	0.53
1:B:1:MET:CG	1:B:2:ALA:H	2.18	0.53
1:C:254:LYS:HG3	1:C:336:TRP:CZ3	2.42	0.53
1:D:251:SER:OG	1:D:253:GLU:HB2	2.08	0.53
1:C:111:ARG:HB3	3:C:737:HOH:O	2.09	0.53
1:A:32:ASP:HB3	1:A:41:THR:HG22	1.90	0.53
1:C:200:THR:OG1	1:C:247:CYS:HB2	2.09	0.53
1:A:118:TRP:HB3	1:A:129:PHE:HB3	1.89	0.53
1:B:221:ALA:HB2	1:B:237:PHE:CD2	2.43	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:SER:HB3	1:C:187:PRO:HD2	1.90	0.53
1:D:290:LEU:O	1:D:297:VAL:HA	2.08	0.53
1:C:46:LYS:HA	1:C:51:ARG:O	2.09	0.53
1:B:21:LYS:HE2	1:B:41:THR:HG21	1.91	0.52
1:D:188:ASN:OD1	1:D:190:ASN:HB2	2.10	0.52
1:A:297:VAL:O	1:A:299:PRO:HD3	2.10	0.52
1:B:21:LYS:CE	1:B:41:THR:HG21	2.40	0.52
1:C:57:LEU:HD23	1:C:57:LEU:N	2.25	0.52
1:B:290:LEU:O	1:B:297:VAL:HG22	2.10	0.52
1:D:323:VAL:HG22	1:D:323:VAL:O	2.09	0.52
1:C:169:THR:OG1	1:C:170:PRO:HD2	2.10	0.52
1:D:114:ASP:OD2	1:D:115:LYS:HE3	2.10	0.51
1:B:24:LEU:HD13	1:B:126:GLY:HA2	1.91	0.51
1:B:275:GLN:HE21	1:B:275:GLN:HA	1.76	0.51
1:B:300:LYS:HE2	1:B:301:HIS:CE1	2.45	0.51
1:C:67:GLN:NE2	1:C:291:LYS:HD2	2.18	0.51
1:D:57:LEU:N	1:D:57:LEU:HD23	2.26	0.51
1:C:299:PRO:HD2	1:C:302:SER:CB	2.41	0.51
1:A:162:ARG:HA	1:A:331:TYR:O	2.11	0.51
1:D:103:PRO:CG	1:D:207:THR:HG21	2.41	0.51
1:B:199:ASP:CG	1:B:249:LYS:HE2	2.31	0.51
1:C:162:ARG:HA	1:C:331:TYR:O	2.11	0.51
1:C:93:LYS:N	3:C:791:HOH:O	2.33	0.51
1:D:161:TYR:O	1:D:332:ASP:HA	2.10	0.50
1:B:184:GLN:NE2	1:B:293:LYS:HB2	2.09	0.50
1:C:70:PRO:HD2	1:C:72:PHE:CE1	2.46	0.50
1:B:266:GLY:O	1:B:341:VAL:HA	2.11	0.50
1:A:70:PRO:HD2	1:A:72:PHE:HE1	1.77	0.50
1:D:240:ASN:ND2	1:D:300:LYS:HZ1	2.00	0.50
1:C:79:VAL:HG11	1:C:83:ILE:HD11	1.93	0.50
1:C:231:GLY:O	1:C:232:LYS:C	2.49	0.50
1:C:220:THR:CG2	1:C:222:PHE:HD1	2.20	0.50
1:C:275:GLN:HB3	1:C:276:PRO:HD2	1.93	0.50
1:B:251:SER:OG	1:B:253:GLU:HB2	2.11	0.49
1:B:257:CYS:HB3	1:B:271:VAL:O	2.12	0.49
1:D:188:ASN:OD1	1:D:190:ASN:N	2.42	0.49
1:D:311:TRP:N	1:D:311:TRP:CD1	2.77	0.49
1:A:144:LEU:HD11	1:A:163:ALA:HB1	1.94	0.49
1:C:220:THR:CG2	1:C:222:PHE:HB2	2.43	0.49
1:C:184:GLN:OE1	1:C:298:TYR:OH	2.31	0.49
1:B:290:LEU:O	1:B:297:VAL:HA	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:THR:O	1:C:208:LEU:HB2	2.13	0.49
1:C:292:GLY:HA3	1:C:298:TYR:CE1	2.47	0.49
1:D:24:LEU:HD23	1:D:24:LEU:N	2.28	0.49
1:B:311:TRP:N	1:B:311:TRP:CD1	2.80	0.49
1:D:23:GLN:C	1:D:24:LEU:HD23	2.34	0.48
1:B:180:ASN:ND2	1:B:186:SER:HB2	2.28	0.48
1:B:162:ARG:HD2	1:B:332:ASP:CG	2.34	0.48
1:C:226:LYS:O	1:C:228:VAL:HG13	2.13	0.48
1:D:115:LYS:NZ	3:D:869:HOH:O	2.46	0.48
1:C:279:GLN:HB3	1:C:307:GLU:HB2	1.95	0.48
1:A:323:VAL:HG22	1:A:323:VAL:O	2.12	0.48
1:B:2:ALA:HA	1:B:25:GLN:O	2.14	0.48
1:B:72:PHE:HD2	1:B:178:TYR:CD1	2.32	0.48
1:D:203:PRO:HD2	1:D:213:GLU:O	2.14	0.48
1:B:53:SER:HB2	1:B:267:ARG:NH2	2.29	0.48
1:D:262:HIS:O	1:D:266:GLY:N	2.47	0.48
1:A:253:GLU:OE1	1:B:1:MET:HB2	2.12	0.48
1:D:23:GLN:CD	1:D:30:ARG:HD2	2.34	0.48
1:D:55:VAL:HG22	1:D:180:ASN:O	2.14	0.48
1:C:311:TRP:N	1:C:311:TRP:CD1	2.80	0.47
1:D:275:GLN:HE21	1:D:276:PRO:CD	2.27	0.47
1:A:48:ARG:HG3	1:A:265:SER:O	2.14	0.47
1:C:184:GLN:OE1	1:C:293:LYS:HE3	2.14	0.47
1:D:182:ALA:HB2	1:D:262:HIS:CE1	2.50	0.47
1:A:253:GLU:O	1:A:255:HIS:ND1	2.48	0.47
1:B:131:ARG:HG2	1:B:132:ILE:N	2.30	0.47
1:B:182:ALA:HB2	1:B:262:HIS:CE1	2.50	0.47
1:B:184:GLN:NE2	1:B:293:LYS:CE	2.78	0.47
1:B:61:GLU:HB2	3:B:612:HOH:O	2.14	0.47
1:C:319:ARG:HB2	3:C:772:HOH:O	2.13	0.47
1:D:290:LEU:HA	1:D:290:LEU:HD23	1.74	0.47
1:A:184:GLN:HG2	1:A:184:GLN:O	2.10	0.47
1:A:275:GLN:HE21	1:A:275:GLN:CA	2.24	0.47
1:C:57:LEU:HB2	1:C:72:PHE:CE2	2.49	0.47
1:D:326:ARG:HD3	3:D:840:HOH:O	2.15	0.47
1:D:45:VAL:O	1:D:52:ALA:HA	2.15	0.47
1:D:70:PRO:HD2	1:D:72:PHE:CE1	2.50	0.47
1:D:9:PHE:HB2	1:D:21:LYS:HB2	1.97	0.46
1:A:191:ASP:HA	1:A:229[B]:GLU:OE2	2.14	0.46
1:D:145:LYS:O	1:D:163:ALA:HA	2.14	0.46
1:A:275:GLN:NE2	1:A:276:PRO:HD2	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.49	0.46
1:C:73:GLY:HA2	1:C:177:SER:CA	2.42	0.46
1:A:82:ARG:CZ	1:A:208:LEU:HD12	2.45	0.46
1:D:261:HIS:CD2	1:D:268:VAL:HG22	2.50	0.46
1:D:248:LEU:HA	1:D:248:LEU:HD23	1.54	0.46
1:B:59:PHE:CE1	1:B:72:PHE:CD1	3.00	0.46
1:D:261:HIS:HD2	1:D:268:VAL:HG22	1.81	0.46
1:B:27:ASP:N	1:B:27:ASP:OD1	2.49	0.46
1:B:334:THR:HG22	1:B:335:THR:N	2.30	0.46
1:A:136:GLY:N	1:A:140:TYR:O	2.50	0.45
1:A:57:LEU:HA	1:A:184:GLN:HG3	1.98	0.45
1:C:51:ARG:NH2	1:D:299:PRO:HB3	2.31	0.45
1:C:215:ALA:HA	1:C:216:PRO:HD3	1.72	0.45
1:A:311:TRP:CD1	1:A:311:TRP:N	2.80	0.45
1:D:76:ILE:HD11	1:D:176:HIS:CB	2.38	0.45
1:C:223:ASP:OD2	1:C:225:ARG:NH2	2.48	0.45
1:B:47:ASP:OD2	1:B:51:ARG:HD3	2.16	0.45
1:B:44:GLU:HA	1:B:53:SER:O	2.17	0.45
1:B:89:LYS:HA	1:B:93:LYS:O	2.16	0.45
1:D:230:LEU:HA	1:D:230:LEU:HD12	1.73	0.45
1:C:252:LYS:N	1:C:252:LYS:CD	2.80	0.45
1:A:290:LEU:O	1:A:297:VAL:HA	2.17	0.45
1:A:32:ASP:C	1:A:33:ILE:HG13	2.37	0.45
1:C:76:ILE:HD11	1:C:176:HIS:HB2	1.93	0.45
1:C:291:LYS:HG2	1:C:291:LYS:H	1.25	0.45
1:D:184:GLN:OE1	1:D:293:LYS:HE3	2.17	0.45
1:C:145:LYS:O	1:C:163:ALA:HA	2.16	0.45
1:D:229:GLU:O	1:D:230:LEU:C	2.55	0.45
1:A:136:GLY:O	1:A:137:GLU:C	2.54	0.45
1:B:184:GLN:NE2	1:B:293:LYS:HE2	2.31	0.45
1:B:46:LYS:HA	1:B:51:ARG:O	2.17	0.45
1:D:300:LYS:CE	1:D:301:HIS:CE1	3.00	0.45
1:A:46:LYS:HA	1:A:51:ARG:O	2.16	0.45
1:A:57:LEU:CB	1:A:72:PHE:CE2	3.00	0.45
1:A:278:VAL:HG13	1:A:278:VAL:O	2.17	0.44
1:B:145:LYS:O	1:B:163:ALA:HA	2.16	0.44
1:B:184:GLN:HG2	1:B:185:ALA:N	2.18	0.44
1:C:267:ARG:HD2	1:C:267:ARG:HH11	1.57	0.44
1:A:169:THR:OG1	1:A:170:PRO:HD2	2.17	0.44
1:A:170:PRO:HA	1:A:323:VAL:O	2.17	0.44
1:B:29:LEU:HD12	1:B:152:LEU:HD11	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:HD22	1:B:323:VAL:HG13	1.80	0.44
1:B:72:PHE:HE1	1:B:290:LEU:HD13	1.82	0.44
1:C:262:HIS:O	1:C:266:GLY:N	2.50	0.44
1:B:207:THR:O	1:B:208:LEU:HB2	2.17	0.44
1:C:193:GLU:O	1:C:261:HIS:N	2.42	0.44
1:C:53:SER:CB	1:C:267:ARG:NH2	2.80	0.44
1:D:207:THR:O	1:D:208:LEU:HB2	2.18	0.44
1:D:254:LYS:HG3	1:D:336:TRP:CZ3	2.52	0.44
1:A:89:LYS:HA	1:A:93:LYS:O	2.17	0.44
1:C:256:PHE:HA	1:C:272:TYR:CD2	2.52	0.44
1:D:90:VAL:O	1:D:91:ASP:C	2.55	0.44
1:B:21:LYS:NZ	1:B:41:THR:CG2	2.80	0.44
1:C:125:ASN:OD1	1:C:125:ASN:N	2.50	0.44
1:A:49:GLN:HB2	1:A:51:ARG:HG3	1.98	0.44
1:C:23:GLN:CD	1:C:30:ARG:HD2	2.38	0.44
1:C:53:SER:HB2	1:C:267:ARG:NH2	2.32	0.44
1:D:89:LYS:HA	1:D:93:LYS:O	2.17	0.44
1:A:57:LEU:HB2	1:A:72:PHE:CE2	2.53	0.44
1:B:288:GLY:HA2	1:B:298:TYR:C	2.38	0.44
1:B:321:PRO:HA	1:B:322:PRO:HD3	1.82	0.44
1:C:99:ILE:CG2	1:C:102:GLU:HA	2.48	0.44
1:C:21:LYS:CE	1:C:41:THR:HG21	2.48	0.44
1:B:254:LYS:HG3	1:B:336:TRP:CZ3	2.53	0.43
1:D:218:GLN:HG2	1:D:225:ARG:HH22	1.83	0.43
1:B:281:TYR:CE2	1:B:283:GLY:HA2	2.53	0.43
1:B:334:THR:CG2	1:B:335:THR:N	2.81	0.43
1:C:111:ARG:NH1	1:C:116:VAL:HG12	2.33	0.43
1:D:234:LEU:HD23	1:D:239:LEU:HB3	2.00	0.43
1:B:291:LYS:HG2	1:B:291:LYS:H	1.15	0.43
1:B:323:VAL:HG12	3:B:649:HOH:O	2.17	0.43
1:C:136:GLY:N	1:C:140:TYR:O	2.50	0.43
1:C:225:ARG:HE	1:C:225:ARG:HB2	1.67	0.43
1:D:304:PHE:HE1	1:D:306:LEU:HD12	1.82	0.43
1:D:318:PRO:C	1:D:319:ARG:HD3	2.39	0.43
1:B:29:LEU:HG	1:B:155:GLY:HA2	1.99	0.43
1:C:199:ASP:C	1:C:217:VAL:HG13	2.39	0.43
1:D:300:LYS:HE2	1:D:301:HIS:NE2	2.32	0.43
1:A:111:ARG:HB3	3:A:537:HOH:O	2.19	0.43
1:B:252:LYS:CD	1:B:252:LYS:N	2.82	0.43
1:D:324:LEU:HA	1:D:324:LEU:HD23	1.85	0.43
1:B:114:ASP:OD1	1:B:114:ASP:N	2.46	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLY:N	1:B:296:ALA:O	2.47	0.43
1:B:299:PRO:HD2	1:B:302:SER:HB3	2.01	0.43
1:D:268:VAL:HB	1:D:340:SER:OG	2.19	0.42
1:B:275:GLN:HE21	1:B:276:PRO:HD2	1.84	0.42
1:A:161:TYR:O	1:A:332:ASP:HA	2.19	0.42
1:A:317:GLN:HA	1:A:318:PRO:HD3	1.88	0.42
1:C:4:VAL:HG11	1:C:122:VAL:HG13	2.01	0.42
1:C:300:LYS:O	1:C:301:HIS:HB2	2.18	0.42
1:B:226:LYS:O	1:B:228:VAL:HG13	2.19	0.42
1:B:70:PRO:HB2	1:B:178:TYR:HH	1.84	0.42
1:D:153:ASP:HA	3:D:835:HOH:O	2.19	0.42
1:B:33:ILE:HA	1:B:39:THR:O	2.19	0.42
1:C:254:LYS:HB2	1:C:336:TRP:CH2	2.54	0.42
1:C:62:LEU:O	1:C:65:TYR:N	2.49	0.42
1:B:144:LEU:HD11	1:B:163:ALA:HB1	2.00	0.42
1:B:249:LYS:H	1:B:249:LYS:HG2	1.60	0.42
1:C:45:VAL:HG12	1:C:46:LYS:N	2.35	0.42
1:A:281:TYR:CE2	1:A:283:GLY:HA2	2.54	0.42
1:D:1:MET:HE3	3:D:835:HOH:O	2.19	0.42
1:C:203:PRO:HD2	1:C:213:GLU:O	2.19	0.42
1:C:32:ASP:C	1:C:33:ILE:HG13	2.40	0.42
1:D:242:PHE:O	1:D:281:TYR:HA	2.20	0.42
1:B:297:VAL:O	1:B:299:PRO:HD3	2.20	0.42
1:D:275:GLN:HA	1:D:276:PRO:HD3	1.80	0.42
1:D:67:GLN:HE22	1:D:291:LYS:HG3	1.85	0.42
1:B:49:GLN:HB2	1:B:51:ARG:CD	2.50	0.41
1:A:317:GLN:HB2	1:A:317:GLN:HE21	1.55	0.41
1:C:293:LYS:HB2	1:C:293:LYS:HE3	1.65	0.41
1:A:200:THR:OG1	1:A:247:CYS:HB2	2.20	0.41
1:D:180:ASN:ND2	1:D:186:SER:HB2	2.35	0.41
1:D:102:GLU:HA	1:D:103:PRO:HA	1.78	0.41
1:D:297:VAL:O	1:D:299:PRO:HD3	2.21	0.41
1:A:284:ASN:OD1	1:A:301:HIS:HE1	2.02	0.41
1:B:90:VAL:O	1:B:91:ASP:C	2.59	0.41
1:C:127:VAL:HG22	1:C:128:GLN:N	2.36	0.41
1:C:44:GLU:HA	1:C:53:SER:O	2.21	0.41
1:C:9:PHE:HB2	1:C:21:LYS:HB2	2.03	0.41
1:D:82:ARG:NH2	1:D:208:LEU:HD12	2.35	0.41
1:A:257:CYS:HB3	1:A:271:VAL:O	2.20	0.41
1:C:70:PRO:HD2	1:C:72:PHE:CD1	2.55	0.41
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.95	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:HG12	1:B:336:TRP:CD1	2.56	0.41
1:D:234:LEU:CD2	1:D:239:LEU:HB3	2.50	0.41
1:B:286:LEU:HB2	1:B:300:LYS:HA	2.01	0.41
1:C:12:LEU:HA	1:C:12:LEU:HD23	1.86	0.41
1:D:300:LYS:O	1:D:301:HIS:HB2	2.20	0.41
1:A:168:ALA:HA	1:A:325:LEU:O	2.21	0.41
1:A:325:LEU:HD22	1:A:331:TYR:HB2	2.03	0.41
1:B:208:LEU:HA	1:B:208:LEU:HD22	1.92	0.41
1:C:76:ILE:HD13	1:C:176:HIS:HB2	1.97	0.41
1:C:239:LEU:HD23	1:C:239:LEU:HA	1.87	0.41
1:D:103:PRO:CD	1:D:207:THR:HG21	2.51	0.41
1:D:170:PRO:HA	1:D:323:VAL:O	2.21	0.41
1:A:101:LYS:HG3	1:A:106:LEU:HD22	2.02	0.40
1:C:248:LEU:HG	1:C:277:GLY:HA2	2.02	0.40
1:C:67:GLN:HE22	1:C:291:LYS:CD	2.20	0.40
1:D:85:LYS:HA	1:D:103:PRO:O	2.20	0.40
1:A:57:LEU:HD13	1:A:298:TYR:CD2	2.56	0.40
1:A:300:LYS:O	1:A:301:HIS:HB2	2.21	0.40
1:A:37:GLY:O	1:A:38:CYS:C	2.59	0.40
1:A:32:ASP:HB2	1:A:41:THR:HG22	2.02	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	344/344 (100%)	323 (94%)	19 (6%)	2 (1%)	28	34
1	B	341/344 (99%)	318 (93%)	22 (6%)	1 (0%)	44	55
1	C	342/344 (99%)	319 (93%)	21 (6%)	2 (1%)	28	34
1	D	341/344 (99%)	315 (92%)	24 (7%)	2 (1%)	28	34
All	All	1368/1376 (99%)	1275 (93%)	86 (6%)	7 (0%)	32	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	73	GLY
1	D	73	GLY
1	A	81	ASN
1	D	243	ASP
1	B	70	PRO
1	A	73	GLY
1	C	92	GLY

### 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	287/285 (101%)	266 (93%)	21 (7%)	16	21
1	B	285/285 (100%)	260 (91%)	25 (9%)	12	14
1	C	285/285 (100%)	262 (92%)	23 (8%)	14	17
1	D	285/285 (100%)	262 (92%)	23 (8%)	14	17
All	All	1142/1140 (100%)	1050 (92%)	92 (8%)	14	17

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	41	THR
1	A	48	ARG
1	A	51	ARG
1	A	56	VAL
1	A	83	ILE
1	A	93	LYS
1	A	102[A]	GLU
1	A	102[B]	GLU
1	A	111	ARG
1	A	131	ARG
1	A	162	ARG
1	A	184	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	186	SER
1	A	218	GLN
1	A	232	LYS
1	A	252	LYS
1	A	275	GLN
1	A	291	LYS
1	A	317	GLN
1	A	338	LYS
1	B	41	THR
1	B	43	LEU
1	B	53	SER
1	B	57	LEU
1	B	67	GLN
1	B	68	LYS
1	B	101	LYS
1	B	111	ARG
1	B	115	LYS
1	B	127	VAL
1	B	162	ARG
1	B	167	GLN
1	B	184	GLN
1	B	208	LEU
1	B	209	ILE
1	B	230	LEU
1	B	249	LYS
1	B	252	LYS
1	B	275	GLN
1	B	291	LYS
1	B	301	HIS
1	B	315	VAL
1	B	317	GLN
1	B	323	VAL
1	B	329	GLU
1	C	29	LEU
1	C	43	LEU
1	C	56	VAL
1	C	61	GLU
1	C	68	LYS
1	C	76	ILE
1	C	87	THR
1	C	93	LYS
1	C	101	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	102	GLU
1	C	111	ARG
1	C	115	LYS
1	C	123	LEU
1	C	220	THR
1	C	229	GLU
1	C	232	LYS
1	C	252	LYS
1	C	254	LYS
1	C	275	GLN
1	C	291	LYS
1	C	297	VAL
1	C	323	VAL
1	C	329	GLU
1	D	1	MET
1	D	14	SER
1	D	32	ASP
1	D	53	SER
1	D	55	VAL
1	D	63	GLU
1	D	101	LYS
1	D	111	ARG
1	D	115	LYS
1	D	130	SER
1	D	184	GLN
1	D	193	GLU
1	D	228	VAL
1	D	229	GLU
1	D	239	LEU
1	D	249	LYS
1	D	252	LYS
1	D	257	CYS
1	D	275	GLN
1	D	291	LYS
1	D	297	VAL
1	D	319	ARG
1	D	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	240	ASN
1	A	275	GLN
1	A	301	HIS
1	A	317	GLN
1	B	49	GLN
1	B	184	GLN
1	B	245	ASN
1	B	261	HIS
1	B	275	GLN
1	B	309	GLN
1	C	25	GLN
1	C	67	GLN
1	C	125	ASN
1	C	261	HIS
1	C	275	GLN
1	C	301	HIS
1	D	240	ASN
1	D	261	HIS
1	D	275	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](#)

4 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	GAL	A	500	-	12,12,12	0.58	0	17,17,17	1.27	2 (11%)
2	GAL	B	600	-	12,12,12	0.49	0	17,17,17	1.40	3 (17%)
2	GAL	C	700	-	12,12,12	0.48	0	17,17,17	1.43	2 (11%)
2	GAL	D	800	-	12,12,12	0.44	0	17,17,17	1.48	2 (11%)

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	GAL	A	500	-	-	0/2/22/22	0/1/1/1
2	GAL	B	600	-	-	0/2/22/22	0/1/1/1
2	GAL	C	700	-	-	0/2/22/22	0/1/1/1
2	GAL	D	800	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	GAL	C4-C3-C2	-3.98	103.81	110.84
2	D	800	GAL	C3-C4-C5	-3.06	104.82	110.22
2	B	600	GAL	C3-C4-C5	-2.53	105.77	110.22
2	B	600	GAL	C1-C2-C3	-2.51	106.12	110.65
2	A	500	GAL	C3-C4-C5	-2.39	106.01	110.22
2	D	800	GAL	O5-C5-C4	2.02	113.37	109.66
2	A	500	GAL	O2-C2-C1	2.47	114.88	109.75
2	C	700	GAL	O2-C2-C1	2.48	114.90	109.75
2	B	600	GAL	O2-C2-C1	2.48	114.91	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	344/344 (100%)	-0.55	1 (0%) 93 96	18, 29, 54, 87	0
1	B	342/344 (99%)	-0.48	5 (1%) 74 78	20, 32, 60, 86	0
1	C	344/344 (100%)	-0.50	2 (0%) 89 92	19, 32, 60, 89	0
1	D	342/344 (99%)	-0.48	0 100 100	20, 34, 63, 88	0
All	All	1372/1376 (99%)	-0.50	8 (0%) 89 92	18, 31, 60, 89	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	SER	2.8
1	B	251	SER	2.8
1	B	249	LYS	2.5
1	B	1	MET	2.4
1	A	249	LYS	2.3
1	C	250	GLY	2.2
1	C	51	ARG	2.2
1	B	51	ARG	2.1

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

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

### 6.3 Carbohydrates ⓘ

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	GAL	B	600	12/12	0.97	0.12	1.12	17,33,49,89	0
2	GAL	D	800	12/12	0.96	0.11	0.83	18,35,71,100	0
2	GAL	A	500	12/12	0.96	0.11	-0.06	17,33,45,77	0
2	GAL	C	700	12/12	0.97	0.10	-0.56	21,38,51,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.