



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 1SO0 / pdb_00001so0
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 : 2004-03-12
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

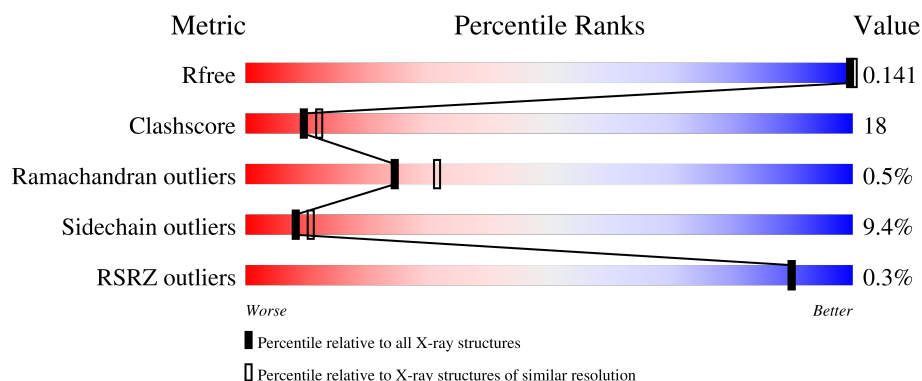
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	 68% 26% 6%
1	B	344	 61% 29% 8% ..
1	C	344	 58% 33% 6% .
1	D	344	 59% 31% 9% .

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-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



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		

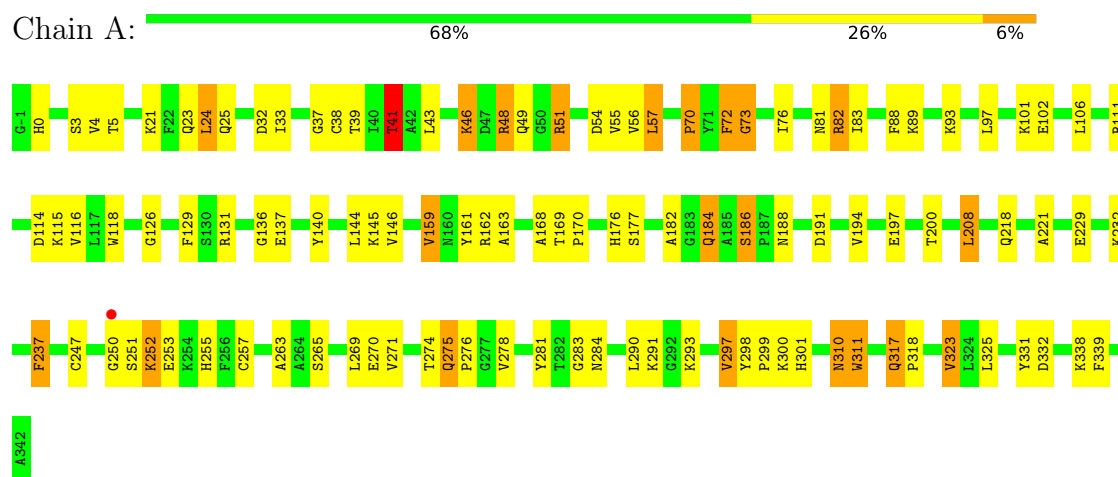
- Molecule 3 is water.

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		

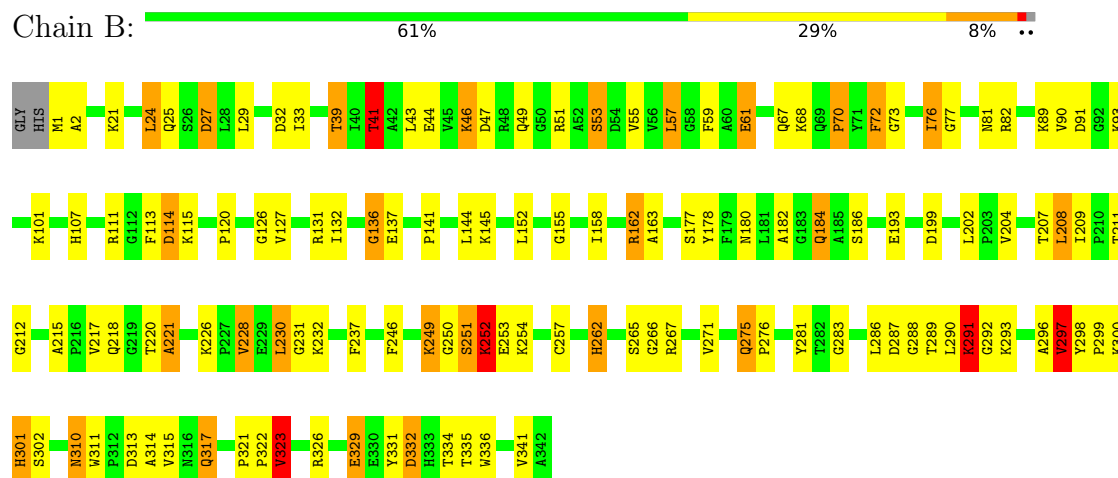
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: aldose 1-epimerase

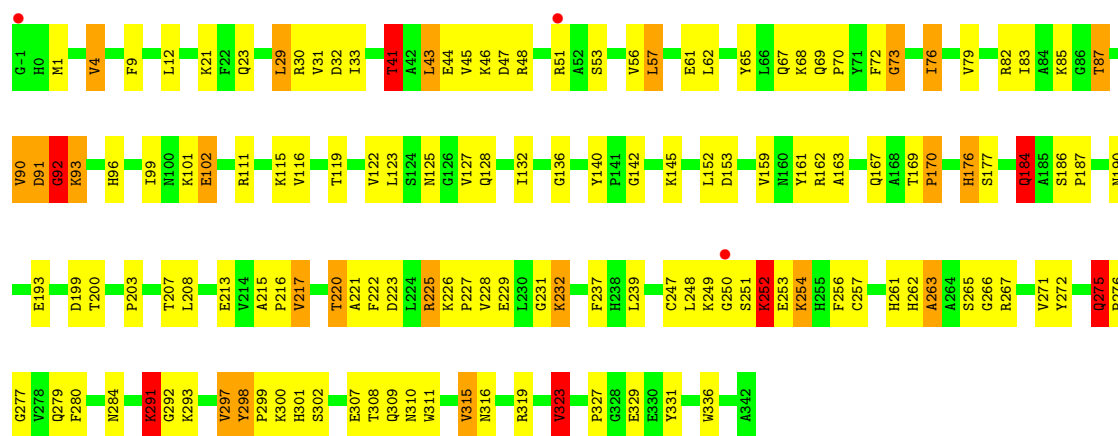


- Molecule 1: aldose 1-epimerase



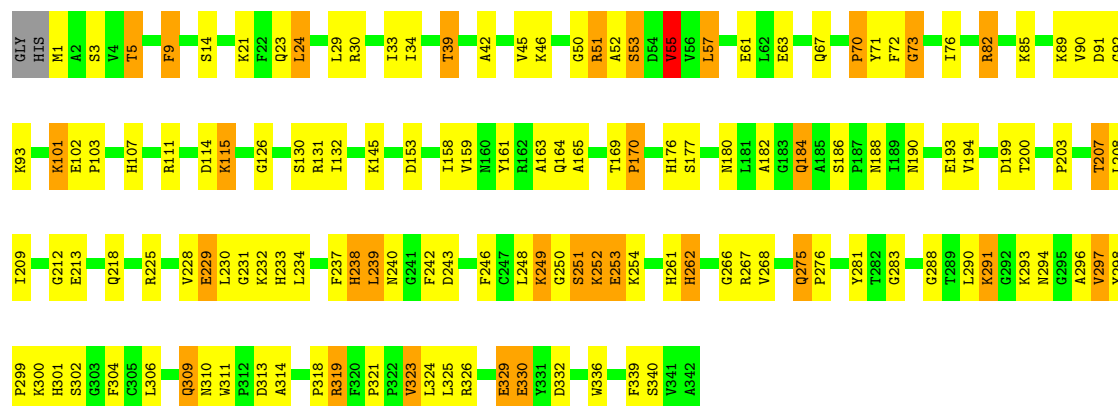
- Molecule 1: aldose 1-epimerase





● Molecule 1: aldose 1-epimerase

Chain D: 59% 31% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.00Å 68.70Å 98.90Å 107.70° 98.40° 102.70°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.30) 93.5 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.25Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.167 , 0.198 (Not available) , 0.141	Depositor DCC
R_{free} test set	6136 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11200	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.20	3/2778 (0.1%)	1.69	35/3775 (0.9%)
1	B	1.15	1/2754 (0.0%)	1.72	34/3742 (0.9%)
1	C	1.20	3/2760 (0.1%)	1.72	42/3750 (1.1%)
1	D	1.15	4/2756 (0.1%)	1.68	35/3744 (0.9%)
All	All	1.18	11/11048 (0.1%)	1.70	146/15011 (1.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	VAL	C-O	14.68	1.39	1.24
1	C	92	GLY	CA-C	6.12	1.60	1.51
1	D	253	GLU	CD-OE2	5.81	1.36	1.25
1	D	61	GLU	CD-OE2	5.69	1.36	1.25
1	D	5	THR	CB-OG1	5.68	1.52	1.43
1	B	61	GLU	CD-OE2	5.67	1.36	1.25
1	A	5	THR	CB-OG1	5.48	1.52	1.43
1	C	90	VAL	C-N	5.39	1.40	1.33
1	A	339	PHE	C-O	-5.14	1.17	1.23
1	A	25	GLN	CA-C	-5.14	1.46	1.52
1	D	330	GLU	N-CA	-5.11	1.40	1.46

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	VAL	O-C-N	16.64	140.17	123.03
1	A	251	SER	N-CA-C	-11.05	93.87	108.34
1	C	323	VAL	CB-CA-C	-10.67	99.19	110.93
1	B	323	VAL	CB-CA-C	-10.28	99.52	110.62
1	C	249	LYS	CA-C-N	-10.08	113.85	121.61
1	C	249	LYS	C-N-CA	-10.08	113.85	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	GLY	O-C-N	-9.41	110.47	122.70
1	B	297	VAL	CA-C-N	-9.11	108.57	122.42
1	B	297	VAL	C-N-CA	-9.11	108.57	122.42
1	D	92	GLY	CA-C-N	-8.54	110.54	122.93
1	D	92	GLY	C-N-CA	-8.54	110.54	122.93
1	B	251	SER	N-CA-C	-8.15	97.48	109.63
1	C	91	ASP	CA-CB-CG	-8.15	104.45	112.60
1	C	90	VAL	CA-C-O	-8.11	112.22	120.25
1	A	39	THR	N-CA-C	8.08	121.47	109.59
1	A	250	GLY	N-CA-C	7.94	124.10	111.64
1	D	252	LYS	N-CA-C	-7.91	102.70	113.30
1	D	39	THR	N-CA-C	7.68	121.48	109.96
1	D	55	VAL	N-CA-C	7.60	121.54	112.80
1	D	249	LYS	CA-C-N	-7.60	113.43	121.48
1	D	249	LYS	C-N-CA	-7.60	113.43	121.48
1	C	90	VAL	CB-CA-C	-7.41	100.04	110.12
1	B	41	THR	N-CA-CB	-7.41	99.65	110.47
1	C	251	SER	N-CA-C	-7.34	98.42	109.94
1	A	237	PHE	CA-CB-CG	-7.24	106.56	113.80
1	B	252	LYS	N-CA-C	-7.08	104.25	113.17
1	A	70	PRO	N-CA-CB	6.88	107.24	102.35
1	C	82	ARG	N-CA-C	6.87	121.25	110.32
1	A	41	THR	N-CA-CB	-6.84	100.49	110.47
1	C	316	ASN	CA-CB-CG	6.79	119.39	112.60
1	B	291	LYS	N-CA-CB	-6.79	100.81	110.58
1	B	246	PHE	CA-CB-CG	-6.65	107.15	113.80
1	D	238	HIS	CA-CB-CG	-6.64	107.16	113.80
1	C	41	THR	N-CA-CB	-6.53	100.54	110.33
1	B	82	ARG	N-CA-C	6.43	120.52	110.17
1	A	182	ALA	N-CA-C	-6.34	105.29	113.16
1	B	212	GLY	N-CA-C	-6.29	106.99	114.48
1	B	221	ALA	N-CA-C	-6.29	105.57	113.18
1	D	250	GLY	N-CA-C	6.24	120.20	111.10
1	B	215	ALA	N-CA-C	6.14	117.81	110.07
1	B	250	GLY	N-CA-C	6.14	122.51	111.03
1	C	119	THR	CA-C-O	6.12	123.85	119.32
1	D	70	PRO	N-CA-CB	6.11	106.82	102.79
1	B	107	HIS	CA-C-N	-6.05	112.33	122.25
1	B	107	HIS	C-N-CA	-6.05	112.33	122.25
1	C	161	TYR	CB-CA-C	-6.04	100.14	110.16
1	B	262	HIS	CA-CB-CG	-6.01	107.79	113.80
1	A	250	GLY	CA-C-N	5.96	132.17	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLY	C-N-CA	5.96	132.17	122.39
1	D	9	PHE	N-CA-C	-5.96	106.55	113.88
1	B	211	THR	CA-C-N	-5.96	116.41	123.08
1	B	211	THR	C-N-CA	-5.96	116.41	123.08
1	D	82	ARG	N-CA-C	5.96	119.79	110.32
1	A	82	ARG	N-CA-C	5.93	119.71	110.17
1	A	339	PHE	CA-C-N	-5.90	111.94	122.32
1	A	339	PHE	C-N-CA	-5.90	111.94	122.32
1	C	69	GLN	CB-CA-C	5.89	117.99	109.45
1	C	263	ALA	N-CA-C	5.89	117.70	111.28
1	D	251	SER	N-CA-C	-5.89	98.25	110.80
1	D	107	HIS	N-CA-C	5.88	119.29	111.30
1	D	194	VAL	N-CA-C	5.85	116.91	108.48
1	B	136	GLY	CA-C-O	5.80	125.56	119.07
1	C	142	GLY	N-CA-C	5.80	119.49	112.48
1	B	120	PRO	CB-CA-C	-5.76	101.81	110.17
1	D	262	HIS	CA-CB-CG	-5.67	108.14	113.80
1	D	321	PRO	N-CA-CB	5.66	106.36	103.19
1	A	114	ASP	CA-CB-CG	-5.66	106.94	112.60
1	C	250	GLY	N-CA-C	5.64	120.58	111.38
1	A	72	PHE	N-CA-C	5.63	118.52	110.24
1	B	204	VAL	N-CA-CB	-5.62	104.65	112.52
1	C	159	VAL	CB-CA-C	-5.60	102.82	110.77
1	A	25	GLN	O-C-N	5.59	130.09	123.33
1	C	92	GLY	N-CA-C	5.58	126.41	113.18
1	C	4	VAL	N-CA-C	5.56	115.90	108.11
1	A	194	VAL	N-CA-C	5.55	116.48	108.48
1	B	72	PHE	N-CA-C	5.55	118.62	110.30
1	A	274	THR	N-CA-C	-5.53	106.58	113.38
1	D	170	PRO	CB-CA-C	-5.53	103.05	110.85
1	C	291	LYS	N-CA-CB	-5.52	102.63	110.58
1	A	186	SER	CA-C-N	5.50	125.03	119.19
1	A	186	SER	C-N-CA	5.50	125.03	119.19
1	A	310	ASN	N-CA-C	-5.50	102.38	110.52
1	C	327	PRO	N-CA-C	-5.50	102.47	111.21
1	D	3	SER	CA-C-N	-5.49	115.36	122.99
1	D	3	SER	C-N-CA	-5.49	115.36	122.99
1	B	250	GLY	O-C-N	5.48	128.58	123.54
1	A	297	VAL	CA-C-N	-5.46	112.52	122.35
1	A	297	VAL	C-N-CA	-5.46	112.52	122.35
1	B	55	VAL	N-CA-C	5.46	117.36	112.17
1	C	184	GLN	CB-CG-CD	5.46	121.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	PRO	N-CA-CB	5.44	108.04	103.25
1	C	309	GLN	N-CA-CB	-5.44	101.92	111.49
1	C	91	ASP	N-CA-C	-5.43	104.56	110.91
1	D	323	VAL	CA-C-N	-5.42	113.67	121.42
1	D	323	VAL	C-N-CA	-5.42	113.67	121.42
1	D	42	ALA	O-C-N	5.40	129.53	123.48
1	A	311	TRP	N-CA-C	5.40	116.50	109.64
1	B	39	THR	N-CA-C	5.38	117.49	109.25
1	C	250	GLY	O-C-N	5.38	128.10	123.37
1	C	265	SER	N-CA-C	-5.36	106.91	113.50
1	B	27	ASP	CA-CB-CG	-5.35	107.25	112.60
1	C	252	LYS	N-CA-C	-5.34	106.26	112.89
1	A	159	VAL	CB-CA-C	-5.34	103.19	110.77
1	B	332	ASP	CB-CA-C	-5.30	104.47	111.42
1	B	202	LEU	CB-CA-C	-5.28	104.31	110.17
1	D	199	ASP	N-CA-C	-5.28	107.01	113.50
1	D	339	PHE	CA-CB-CG	-5.28	108.52	113.80
1	C	176	HIS	CA-CB-CG	5.27	119.07	113.80
1	D	246	PHE	CA-CB-CG	-5.26	108.54	113.80
1	D	200	THR	CA-CB-OG1	-5.26	101.72	109.60
1	D	207	THR	N-CA-CB	5.24	118.21	110.56
1	C	167	GLN	CB-CG-CD	-5.22	103.72	112.60
1	D	51	ARG	N-CA-CB	5.21	117.93	110.06
1	C	284	ASN	CA-CB-CG	-5.20	107.40	112.60
1	C	308	THR	N-CA-C	-5.20	102.17	109.96
1	D	233	HIS	CA-CB-CG	-5.19	108.61	113.80
1	C	90	VAL	CA-C-N	5.18	130.76	122.93
1	C	90	VAL	C-N-CA	5.18	130.76	122.93
1	B	114	ASP	N-CA-C	-5.18	106.47	112.89
1	D	309	GLN	N-CA-CB	-5.18	101.73	110.49
1	A	55	VAL	CA-C-N	-5.17	115.81	122.99
1	A	55	VAL	C-N-CA	-5.17	115.81	122.99
1	C	96	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	39	THR	CA-CB-OG1	-5.15	101.87	109.60
1	C	170	PRO	CB-CA-C	-5.15	104.23	110.98
1	B	141	PRO	CB-CA-C	-5.15	103.27	110.63
1	A	252	LYS	N-CA-C	-5.14	106.86	112.72
1	A	323	VAL	CA-C-O	5.14	123.86	119.38
1	D	212	GLY	CA-C-O	5.14	124.89	119.03
1	A	146	VAL	N-CA-C	5.14	115.88	108.48
1	A	3	SER	N-CA-C	-5.13	101.80	109.95
1	C	275	GLN	CA-C-N	5.13	125.58	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	GLN	C-N-CA	5.13	125.58	120.04
1	D	250	GLY	CA-C-N	5.13	131.33	121.54
1	D	250	GLY	C-N-CA	5.13	131.33	121.54
1	A	188	ASN	CA-CB-CG	-5.12	107.48	112.60
1	A	0	HIS	N-CA-C	5.11	118.08	110.52
1	B	310	ASN	N-CA-C	-5.11	102.20	110.32
1	C	280	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	208	LEU	CD1-CG-CD2	-5.05	99.68	110.80
1	A	4	VAL	N-CA-C	5.03	115.16	108.11
1	C	298	TYR	N-CA-C	5.03	118.46	108.59
1	B	41	THR	OG1-CB-CG2	5.03	119.36	109.30
1	B	76	ILE	N-CA-CB	-5.03	105.12	111.46
1	D	126	GLY	CA-C-O	5.02	124.37	120.91
1	B	317	GLN	CB-CA-C	5.00	118.88	110.97

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	77	0
1	B	2679	0	2602	93	0
1	C	2688	0	2610	110	0
1	D	2681	0	2609	103	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	3	0
All	All	11200	0	10483	378	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 18.

All (378) 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:90:VAL:C	3:C:791:HOH:O	1.91	1.11
1:C:1:MET:HE2	1:C:125:ASN:HD22	1.07	1.09
1:D:240:ASN:HD21	1:D:300:LYS:NZ	1.50	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:C:1:MET:HE2	1:C:125:ASN:ND2	1.86	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:D:240:ASN:HD21	1:D:300:LYS:HZ1	1.25	0.82
1:D:240:ASN:HD21	1:D:300:LYS:HZ3	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
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:C:91:ASP:C	3:C:791:HOH:O	2.30	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:51:ARG:NH1	1:D:288:GLY:HA3	2.06	0.69
1:D:240:ASN:ND2	1:D:300:LYS:HZ3	1.86	0.69
1:C:85:LYS:O	1:C:87:THR:HG22	1.92	0.69
1:C:252:LYS:H	1:C:252:LYS:HD2	1.57	0.69
1:C:220:THR:HG23	1:C:222:PHE:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:252:LYS:HD2	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
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:1:MET:HE1	1:C:153:ASP:HB2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HD3	1:D:319:ARG:N	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:N	1:A:24:LEU:HD23	2.21	0.55
1:A:43:LEU:O	1:A:54:ASP:HA	2.06	0.55
1:B:199:ASP:CG	1:B:249:LYS:HE2	2.31	0.55
1:B:252:LYS:HD2	1:B:252:LYS:N	2.20	0.55
1:C:48:ARG:NH2	1:C:263:ALA:O	2.35	0.55
1:C:199:ASP:O	1:C:217:VAL:HG13	2.07	0.55
1:A:318:PRO:HD2	3:A:589:HOH:O	2.05	0.55
1:C:252:LYS:H	1:C:252:LYS:CD	2.19	0.55
1:D:240:ASN:ND2	1:D:300:LYS:HZ1	1.99	0.55
1:A:82:ARG:NH2	1:A:208:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLY:O	1:C:232:LYS:C	2.49	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: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:HG2	1:B:162:ARG:NH1	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: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:D:23:GLN:C	1:D:24:LEU:HD23	2.34	0.53
1:B:1:MET:CG	1:B:2:ALA:H	2.18	0.53
1:B:162:ARG:HD2	1:B:332:ASP:CG	2.34	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
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:D:23:GLN:CD	1:D:30:ARG:HD2	2.34	0.52
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:O	1:D:323:VAL:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:93:LYS:N	3:C:791:HOH:O	2.33	0.51
1:C:162:ARG:HA	1:C:331:TYR:O	2.11	0.51
1:B:262:HIS:ND1	1:B:265:SER:OG	2.31	0.50
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:C:79:VAL:HG11	1:C:83:ILE:HD11	1.93	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:A:32:ASP:C	1:A:33:ILE:HG13	2.37	0.49
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:229:GLU:O	1:D:230:LEU:C	2.55	0.49
1:A:136:GLY:O	1:A:137:GLU:C	2.54	0.49
1:D:188:ASN:OD1	1:D:190:ASN:N	2.42	0.49
1:D:311:TRP:CD1	1:D:311:TRP:N	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:B:290:LEU:O	1:B:297:VAL:HA	2.12	0.49
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:D:90:VAL:O	1:D:91:ASP:C	2.55	0.49
1:B:311:TRP:CD1	1:B:311:TRP:N	2.80	0.49
1:C:23:GLN:CD	1:C:30:ARG:HD2	2.38	0.48
1:B:180:ASN:ND2	1:B:186:SER:HB2	2.28	0.48
1:B:288:GLY:HA2	1:B:298:TYR:C	2.38	0.48
1:C:226:LYS:O	1:C:228:VAL:HG13	2.13	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:D:318:PRO:C	1:D:319:ARG:HD3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:55:VAL:HG22	1:D:180:ASN:O	2.14	0.48
1:C:199:ASP:C	1:C:217:VAL:HG13	2.39	0.47
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:61:GLU:HB2	3:B:612:HOH:O	2.14	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:C:319:ARG:HB2	3:C:772:HOH:O	2.13	0.47
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.74	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: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:326:ARG:HD3	3:D:840:HOH:O	2.15	0.47
1:C:32:ASP:C	1:C:33:ILE:HG13	2.40	0.46
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
1:D:239:LEU:HA	1:D:239:LEU:HD23	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:B:90:VAL:O	1:B:91:ASP:C	2.59	0.46
1:D:248:LEU:HD23	1:D:248:LEU:HA	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:OD1	1:B:27:ASP:N	2.49	0.46
1:B:334:THR:HG22	1:B:335:THR:N	2.30	0.46
1:A:57:LEU:HA	1:A:184:GLN:HG3	1.98	0.45
1:A:136:GLY:N	1:A:140:TYR:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:GLU:HA	1:B:53:SER:O	2.17	0.45
1:B:47:ASP:OD2	1:B:51:ARG:HD3	2.16	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:A:184:GLN:O	1:A:184:GLN:HG2	2.10	0.45
1:C:252:LYS:CD	1:C:252:LYS:N	2.80	0.45
1:A:37:GLY:O	1:A:38:CYS:C	2.59	0.45
1:A:290:LEU:O	1:A:297:VAL:HA	2.17	0.45
1:C:76:ILE:HD11	1:C:176:HIS:HB2	1.93	0.45
1:C:291:LYS:H	1:C:291:LYS:HG2	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:C:184:GLN:OE1	1:C:298:TYR:OH	2.31	0.45
1:B:46:LYS:HA	1:B:51:ARG:O	2.17	0.45
1:B:184:GLN:NE2	1:B:293:LYS:HE2	2.31	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:B:145:LYS:O	1:B:163:ALA:HA	2.16	0.44
1:C:267:ARG:HH11	1:C:267:ARG:HD2	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
1:B:72:PHE:HE1	1:B:290:LEU:HD13	1.82	0.44
1:B:310:ASN:HD22	1:B:323:VAL:HG13	1.80	0.44
1:C:21:LYS:HZ1	1:C:41:THR:HG21	1.83	0.44
1:C:262:HIS:O	1:C:266:GLY:N	2.50	0.44
1:B:136:GLY:O	1:B:137:GLU:C	2.58	0.44
1:B:207:THR:O	1:B:208:LEU:HB2	2.17	0.44
1:C:53:SER:CB	1:C:267:ARG:NH2	2.80	0.44
1:C:193:GLU:O	1:C:261:HIS:N	2.42	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:A:115:LYS:C	1:A:116:VAL:HG13	2.42	0.44
1:B:21:LYS:NZ	1:B:41:THR:CG2	2.80	0.44
1:D:71:TYR:O	1:D:72:PHE:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LYS:O	1:D:102:GLU:C	2.59	0.44
1:A:49:GLN:HB2	1:A:51:ARG:HG3	1.98	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:D:288:GLY:HA2	1:D:298:TYR:C	2.43	0.44
1:D:294:ASN:C	1:D:296:ALA:H	2.26	0.44
1:A:57:LEU:HB2	1:A:72:PHE:CE2	2.53	0.44
1:B:321:PRO:HA	1:B:322:PRO:HD3	1.82	0.44
1:C:21:LYS:CE	1:C:41:THR:HG21	2.48	0.44
1:C:99:ILE:CG2	1:C:102:GLU:HA	2.48	0.44
1:C:125:ASN:OD1	1:C:125:ASN:N	2.50	0.44
1:D:313:ASP:O	1:D:314:ALA:C	2.61	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:A:278:VAL:O	1:A:278:VAL:HG13	2.17	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:H	1:B:291:LYS:HG2	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:B:29:LEU:HG	1:B:155:GLY:HA2	1.99	0.43
1:D:300:LYS:HE2	1:D:301:HIS:NE2	2.32	0.43
1:B:231:GLY:O	1:B:232:LYS:C	2.62	0.43
1:A:111:ARG:HB3	3:A:537:HOH:O	2.19	0.43
1:B:252:LYS:N	1:B:252:LYS:CD	2.82	0.43
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.85	0.43
1:B:114:ASP:OD1	1:B:114:ASP:N	2.46	0.43
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:B:226:LYS:O	1:B:228:VAL:HG13	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:O	1:C:65:TYR:N	2.49	0.42
1:C:254:LYS:HB2	1:C:336:TRP:CH2	2.54	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:C:300:LYS:O	1:C:301:HIS:HB2	2.18	0.42
1:A:281:TYR:CE2	1:A:283:GLY:HA2	2.54	0.42
1:C:203:PRO:HD2	1:C:213:GLU:O	2.19	0.42
1:D:231:GLY:O	1:D:232:LYS:C	2.63	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:67:GLN:HE22	1:D:291:LYS:HG3	1.85	0.42
1:D:275:GLN:HA	1:D:276:PRO:HD3	1.80	0.42
1:B:49:GLN:HB2	1:B:51:ARG:CD	2.50	0.41
1:A:317:GLN:HE21	1:A:317:GLN:HB2	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:C:253:GLU:O	1:C:254:LYS:C	2.62	0.41
1:D:102:GLU:HA	1:D:103:PRO:HA	1.78	0.41
1:D:237:PHE:O	1:D:238:HIS:C	2.63	0.41
1:D:297:VAL:O	1:D:299:PRO:HD3	2.21	0.41
1:A:23:GLN:C	1:A:24:LEU:HD23	2.46	0.41
1:A:284:ASN:OD1	1:A:301:HIS:HE1	2.02	0.41
1:C:44:GLU:HA	1:C:53:SER:O	2.21	0.41
1:C:127:VAL:HG22	1:C:128:GLN:N	2.36	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:158:ILE:HG12	1:B:336:TRP:CD1	2.56	0.41
1:B:286:LEU:HB2	1:B:300:LYS:HA	2.01	0.41
1:B:290:LEU:HD23	1:B:290:LEU:HA	1.95	0.41
1:C:12:LEU:HA	1:C:12:LEU:HD23	1.86	0.41
1:D:234:LEU:CD2	1:D:239:LEU:HB3	2.50	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:HD22	1:B:208:LEU:HA	1.92	0.41
1:C:76:ILE:HD13	1:C:176:HIS:HB2	1.97	0.41
1:C:239:LEU:HA	1:C:239:LEU:HD23	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:GLN:HE22	1:C:291:LYS:CD	2.20	0.40
1:C:248:LEU:HG	1:C:277:GLY:HA2	2.02	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:32:ASP:HB2	1:A:41:THR:HG22	2.02	0.40
1:A:300:LYS:O	1:A:301:HIS:HB2	2.21	0.40
1:B:313:ASP:O	1:B:314:ALA:C	2.63	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%)	21	27
1	B	341/344 (99%)	318 (93%)	22 (6%)	1 (0%)	36	46
1	C	342/344 (99%)	319 (93%)	21 (6%)	2 (1%)	21	27
1	D	341/344 (99%)	315 (92%)	24 (7%)	2 (1%)	21	27
All	All	1368/1376 (99%)	1275 (93%)	86 (6%)	7 (0%)	24	31

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

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Mol	Chain	Res	Type
1	A	73	GLY
1	C	92	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/285 (101%)	266 (93%)	21 (7%)	13	18
1	B	285/285 (100%)	253 (89%)	32 (11%)	6	7
1	C	285/285 (100%)	256 (90%)	29 (10%)	7	8
1	D	285/285 (100%)	259 (91%)	26 (9%)	9	11
All	All	1142/1140 (100%)	1034 (90%)	108 (10%)	8	10

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	41	THR
1	A	46	LYS
1	A	48	ARG
1	A	51	ARG
1	A	56	VAL
1	A	57	LEU
1	A	83	ILE
1	A	102[A]	GLU
1	A	102[B]	GLU
1	A	131	ARG
1	A	159	VAL
1	A	184	GLN
1	A	186	SER
1	A	218	GLN
1	A	232	LYS
1	A	252	LYS
1	A	275	GLN
1	A	291	LYS

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Mol	Chain	Res	Type
1	A	317	GLN
1	A	338	LYS
1	B	24	LEU
1	B	41	THR
1	B	43	LEU
1	B	46	LYS
1	B	53	SER
1	B	57	LEU
1	B	67	GLN
1	B	68	LYS
1	B	76	ILE
1	B	81	ASN
1	B	101	LYS
1	B	111	ARG
1	B	115	LYS
1	B	127	VAL
1	B	162	ARG
1	B	184	GLN
1	B	193	GLU
1	B	208	LEU
1	B	209	ILE
1	B	218	GLN
1	B	228	VAL
1	B	230	LEU
1	B	249	LYS
1	B	252	LYS
1	B	275	GLN
1	B	291	LYS
1	B	297	VAL
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	41	THR
1	C	43	LEU
1	C	56	VAL
1	C	57	LEU
1	C	61	GLU
1	C	68	LYS
1	C	76	ILE

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Mol	Chain	Res	Type
1	C	87	THR
1	C	93	LYS
1	C	101	LYS
1	C	102	GLU
1	C	115	LYS
1	C	123	LEU
1	C	184	GLN
1	C	190	ASN
1	C	217	VAL
1	C	220	THR
1	C	225	ARG
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	315	VAL
1	C	323	VAL
1	C	329	GLU
1	D	1	MET
1	D	14	SER
1	D	24	LEU
1	D	34	ILE
1	D	53	SER
1	D	55	VAL
1	D	57	LEU
1	D	63	GLU
1	D	101	LYS
1	D	111	ARG
1	D	115	LYS
1	D	130	SER
1	D	159	VAL
1	D	184	GLN
1	D	193	GLU
1	D	209	ILE
1	D	228	VAL
1	D	229	GLU
1	D	239	LEU
1	D	249	LYS
1	D	252	LYS

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Mol	Chain	Res	Type
1	D	275	GLN
1	D	291	LYS
1	D	297	VAL
1	D	319	ARG
1	D	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	96	HIS
1	A	128	GLN
1	A	160	ASN
1	A	218	GLN
1	A	240	ASN
1	A	275	GLN
1	A	284	ASN
1	A	301	HIS
1	A	317	GLN
1	B	23	GLN
1	B	49	GLN
1	B	160	ASN
1	B	184	GLN
1	B	261	HIS
1	B	275	GLN
1	C	25	GLN
1	C	67	GLN
1	C	128	GLN
1	C	167	GLN
1	C	245	ASN
1	C	261	HIS
1	C	275	GLN
1	C	279	GLN
1	C	301	HIS
1	C	309	GLN
1	D	96	HIS
1	D	128	GLN
1	D	240	ASN
1	D	245	ASN
1	D	261	HIS
1	D	275	GLN
1	D	301	HIS

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Mol	Chain	Res	Type
1	D	309	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	600	-	12,12,12	0.48	0	17,17,17	1.33	3 (17%)
2	GAL	A	500	-	12,12,12	0.56	0	17,17,17	1.23	2 (11%)
2	GAL	C	700	-	12,12,12	0.46	0	17,17,17	1.40	2 (11%)
2	GAL	D	800	-	12,12,12	0.42	0	17,17,17	1.45	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	B	600	-	-	2/2/22/22	0/1/1/1
2	GAL	A	500	-	-	1/2/22/22	0/1/1/1
2	GAL	C	700	-	-	2/2/22/22	0/1/1/1
2	GAL	D	800	-	-	2/2/22/22	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	-4.00	103.81	110.83
2	D	800	GAL	C3-C4-C5	-2.99	104.82	110.23
2	B	600	GAL	C3-C4-C5	-2.46	105.77	110.23
2	B	600	GAL	O2-C2-C1	2.45	114.91	109.25
2	C	700	GAL	O2-C2-C1	2.45	114.90	109.25
2	A	500	GAL	O2-C2-C1	2.44	114.88	109.25
2	A	500	GAL	C3-C4-C5	-2.33	106.01	110.23
2	B	600	GAL	C1-C2-C3	-2.07	106.12	110.36
2	D	800	GAL	O5-C5-C4	2.04	113.37	109.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	700	GAL	O5-C5-C6-O6
2	B	600	GAL	O5-C5-C6-O6
2	D	800	GAL	O5-C5-C6-O6
2	D	800	GAL	C4-C5-C6-O6
2	B	600	GAL	C4-C5-C6-O6
2	C	700	GAL	C4-C5-C6-O6
2	A	500	GAL	O5-C5-C6-O6

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	344/344 (100%)	-0.59	1 (0%) 90 90	18, 29, 54, 87	2 (0%)
1	B	342/344 (99%)	-0.50	0 100 100	20, 31, 60, 86	1 (0%)
1	C	344/344 (100%)	-0.48	3 (0%) 81 82	19, 32, 60, 89	0
1	D	342/344 (99%)	-0.42	0 100 100	20, 34, 63, 88	1 (0%)
All	All	1372/1376 (99%)	-0.50	4 (0%) 90 90	18, 31, 60, 89	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	GLY	2.7
1	C	250	GLY	2.5
1	C	-1	GLY	2.2
1	C	51	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	A	500	12/12	0.97	0.07	17,33,45,77	0
2	GAL	B	600	12/12	0.97	0.07	17,33,49,89	0
2	GAL	D	800	12/12	0.97	0.08	18,35,71,100	0
2	GAL	C	700	12/12	0.98	0.06	21,38,51,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.