Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:43 PM EDT

PDB ID	:	1LCF
Title	:	CRYSTAL STRUCTURE OF COPPER-AND OXALATE-SUBSTITUTED HUMAN LACTOFERRIN AT 2.0 ANGSTROMS RESOLUTION
Authors	:	Smith, C.A.; Anderson, B.F.; Baker, H.M.; Baker, E.N.
Deposited on	:	1994-01-11
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

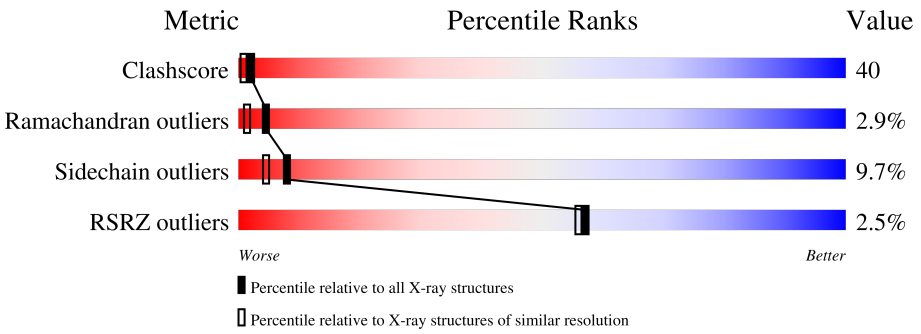
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

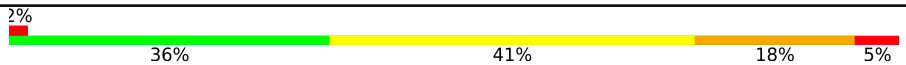
The reported resolution of this entry is 2.00 Å.

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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	691	

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
5	OXL	A	696	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5664 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.

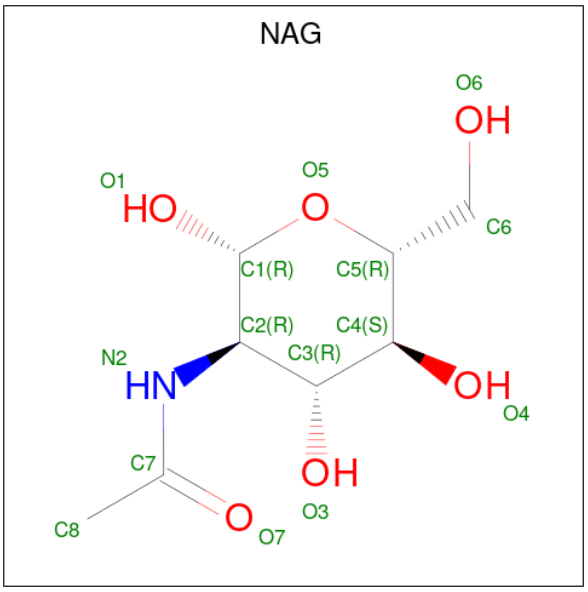
- Molecule 1 is a protein called LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	691	5313	3321	946	1009	37	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	conflict	UNP P02788
A	37	LEU	ILE	conflict	UNP P02788
A	200	LYS	ARG	conflict	UNP P02788

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

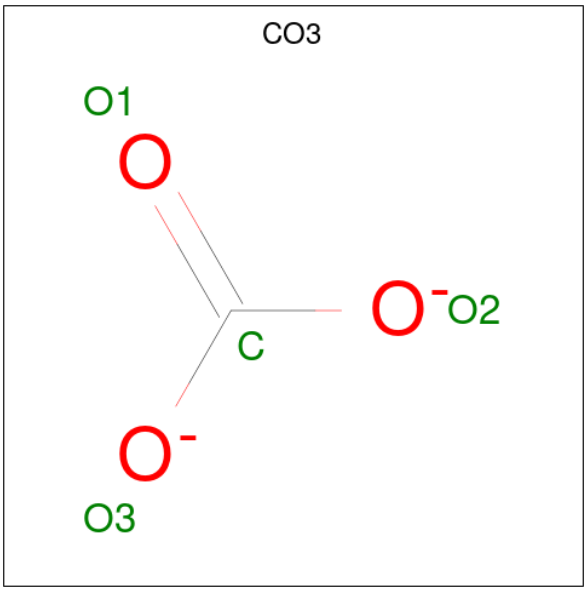


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

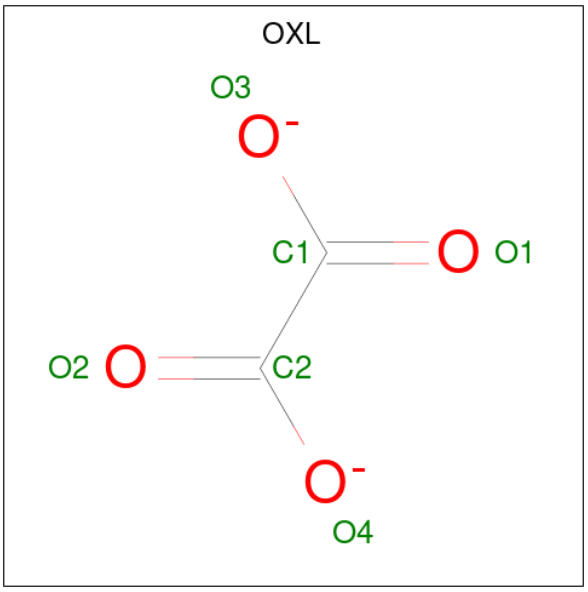
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
3	A	2	2	2	0	0

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 5 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



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

- Molecule 6 is water.

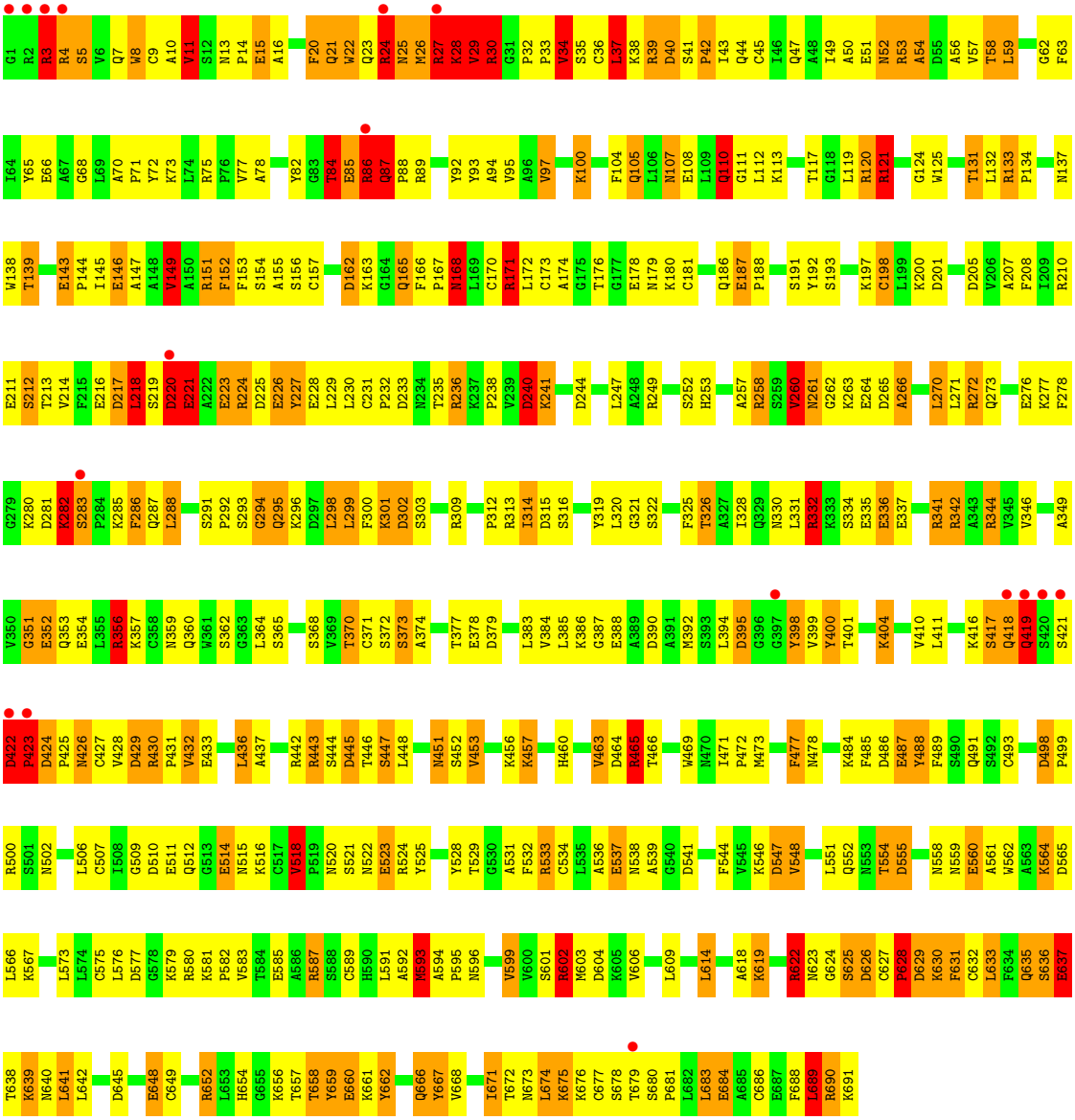
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	325	325	325	0	0

3 Residue-property plots (i)

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

- Molecule 1: LACTOFERRIN

Chain A: 2% 36% 41% 18% 5%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	155.80Å 97.10Å 56.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 30.40 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 85.8 (30.40-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.00Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.193 , (Not available) 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 124.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5664	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: OXL, CU, NAG, CO3

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	0/5427	2.72	413/7343 (5.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (413) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	602	ARG	NE-CZ-NH2	-24.98	107.81	120.30
1	A	27	ARG	CD-NE-CZ	23.83	156.96	123.60
1	A	430	ARG	NE-CZ-NH2	21.81	131.20	120.30
1	A	133	ARG	NE-CZ-NH1	21.03	130.81	120.30
1	A	30	ARG	NE-CZ-NH1	20.39	130.50	120.30
1	A	86	ARG	NE-CZ-NH1	20.00	130.30	120.30
1	A	133	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	A	30	ARG	CD-NE-CZ	18.51	149.51	123.60
1	A	313	ARG	NE-CZ-NH1	17.35	128.98	120.30
1	A	309	ARG	NE-CZ-NH2	-17.27	111.67	120.30
1	A	171	ARG	NE-CZ-NH1	16.67	128.63	120.30
1	A	604	ASP	CB-CG-OD1	15.75	132.47	118.30
1	A	488	TYR	CB-CG-CD1	15.51	130.31	121.00
1	A	602	ARG	NE-CZ-NH1	15.37	127.99	120.30
1	A	486	ASP	CB-CG-OD1	15.31	132.08	118.30
1	A	430	ARG	NE-CZ-NH1	-15.18	112.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	A	236	ARG	NE-CZ-NH2	14.25	127.43	120.30
1	A	315	ASP	CB-CG-OD1	14.07	130.97	118.30
1	A	587	ARG	CD-NE-CZ	13.80	142.92	123.60
1	A	258	ARG	NE-CZ-NH2	13.77	127.18	120.30
1	A	313	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	A	264	GLU	CA-CB-CG	13.69	143.51	113.40
1	A	39	ARG	NE-CZ-NH1	-13.62	113.49	120.30
1	A	30	ARG	NE-CZ-NH2	-13.59	113.50	120.30
1	A	442	ARG	NE-CZ-NH1	-13.41	113.59	120.30
1	A	276	GLU	CA-CB-CG	13.32	142.71	113.40
1	A	442	ARG	NE-CZ-NH2	13.27	126.93	120.30
1	A	498	ASP	CB-CG-OD1	13.19	130.17	118.30
1	A	629	ASP	CB-CG-OD2	-13.01	106.59	118.30
1	A	249	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	A	533	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	660	GLU	OE1-CD-OE2	12.66	138.49	123.30
1	A	443	ARG	CD-NE-CZ	-12.65	105.88	123.60
1	A	667	TYR	CB-CG-CD2	12.23	128.34	121.00
1	A	302	ASP	CB-CG-OD1	12.20	129.28	118.30
1	A	121	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	A	465	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	A	344	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	A	236	ARG	NE-CZ-NH1	-11.39	114.61	120.30
1	A	75	ARG	CD-NE-CZ	11.37	139.52	123.60
1	A	86	ARG	NE-CZ-NH2	-11.33	114.63	120.30
1	A	487	GLU	OE1-CD-OE2	11.17	136.70	123.30
1	A	341	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	A	430	ARG	CD-NE-CZ	-10.55	108.83	123.60
1	A	3	ARG	NE-CZ-NH2	-10.35	115.13	120.30
1	A	309	ARG	CD-NE-CZ	10.24	137.94	123.60
1	A	75	ARG	NE-CZ-NH2	10.16	125.38	120.30
1	A	87	GLN	CB-CG-CD	10.06	137.76	111.60
1	A	429	ASP	CB-CG-OD1	-9.90	109.39	118.30
1	A	690	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	623	ASN	CB-CA-C	9.81	130.01	110.40
1	A	93	TYR	CB-CG-CD1	-9.79	115.12	121.00
1	A	120	ARG	CD-NE-CZ	-9.68	110.05	123.60
1	A	587	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	240	ASP	CB-CG-OD1	9.59	126.93	118.30
1	A	486	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	A	240	ASP	CB-CG-OD2	-9.48	109.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	302	ASP	CB-CG-OD2	-9.48	109.76	118.30
1	A	39	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	A	211	GLU	CG-CD-OE1	9.41	137.12	118.30
1	A	593	MET	CA-CB-CG	9.35	129.20	113.30
1	A	120	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	210	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	A	684	GLU	OE1-CD-OE2	9.14	134.27	123.30
1	A	390	ASP	CB-CG-OD1	9.13	126.52	118.30
1	A	94	ALA	CB-CA-C	9.08	123.72	110.10
1	A	143	GLU	CG-CD-OE2	9.07	136.44	118.30
1	A	319	TYR	CB-CG-CD2	8.94	126.36	121.00
1	A	560	GLU	CA-CB-CG	8.93	133.03	113.40
1	A	341	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	264	GLU	CB-CG-CD	8.80	137.95	114.20
1	A	54	ALA	N-CA-CB	8.75	122.35	110.10
1	A	228	GLU	OE1-CD-OE2	8.74	133.79	123.30
1	A	332	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	488	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	A	533	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	70	ALA	CB-CA-C	8.67	123.11	110.10
1	A	648	GLU	CG-CD-OE2	8.67	135.64	118.30
1	A	315	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	A	421	SER	N-CA-CB	8.63	123.44	110.50
1	A	93	TYR	CB-CG-CD2	8.53	126.11	121.00
1	A	27	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	217	ASP	CB-CG-OD2	8.47	125.93	118.30
1	A	648	GLU	CA-CB-CG	8.46	132.01	113.40
1	A	659	TYR	CB-CG-CD2	8.42	126.05	121.00
1	A	211	GLU	OE1-CD-OE2	-8.41	113.20	123.30
1	A	518	VAL	N-CA-CB	-8.39	93.05	111.50
1	A	87	GLN	CB-CA-C	8.36	127.12	110.40
1	A	418	GLN	C-N-CA	8.35	142.57	121.70
1	A	272	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	249	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	398	TYR	CB-CG-CD2	8.19	125.91	121.00
1	A	224	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	227	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	A	224	ARG	CD-NE-CZ	-8.12	112.23	123.60
1	A	131	THR	CA-CB-CG2	8.12	123.76	112.40
1	A	514	GLU	CA-CB-CG	8.10	131.21	113.40
1	A	3	ARG	CD-NE-CZ	8.08	134.91	123.60
1	A	224	ARG	NE-CZ-NH1	-8.05	116.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	648	GLU	OE1-CD-OE2	-8.05	113.63	123.30
1	A	152	PHE	CB-CG-CD1	-8.05	115.16	120.80
1	A	426	ASN	CA-CB-CG	-8.05	95.69	113.40
1	A	20	PHE	CB-CG-CD1	-8.03	115.18	120.80
1	A	151	ARG	NH1-CZ-NH2	8.00	128.20	119.40
1	A	200	LYS	CA-CB-CG	7.92	130.84	113.40
1	A	332	ARG	CA-CB-CG	7.92	130.82	113.40
1	A	24	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	3	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	565	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	A	171	ARG	NH1-CZ-NH2	-7.82	110.80	119.40
1	A	541	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	A	198	CYS	O-C-N	-7.81	110.20	122.70
1	A	65	TYR	CB-CG-CD1	-7.79	116.32	121.00
1	A	565	ASP	CB-CG-OD1	7.78	125.31	118.30
1	A	143	GLU	CG-CD-OE1	-7.63	103.03	118.30
1	A	34	VAL	CG1-CB-CG2	7.62	123.09	110.90
1	A	309	ARG	NH1-CZ-NH2	7.56	127.71	119.40
1	A	518	VAL	CA-CB-CG1	7.55	122.22	110.90
1	A	11	VAL	CG1-CB-CG2	7.54	122.97	110.90
1	A	384	VAL	CA-CB-CG1	7.54	122.22	110.90
1	A	262	GLY	N-CA-C	7.54	131.95	113.10
1	A	120	ARG	CA-CB-CG	-7.54	96.82	113.40
1	A	120	ARG	NH1-CZ-NH2	7.53	127.69	119.40
1	A	205	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	A	641	LEU	CB-CG-CD1	7.49	123.73	111.00
1	A	342	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	445	ASP	O-C-N	7.44	134.60	122.70
1	A	498	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	A	143	GLU	N-CA-CB	7.38	123.88	110.60
1	A	224	ARG	NH1-CZ-NH2	7.36	127.50	119.40
1	A	120	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	A	677	CYS	O-C-N	7.34	134.45	122.70
1	A	493	CYS	N-CA-CB	7.34	123.81	110.60
1	A	75	ARG	CG-CD-NE	7.30	127.13	111.80
1	A	97	VAL	O-C-N	7.30	134.38	122.70
1	A	411	LEU	CA-CB-CG	7.26	132.00	115.30
1	A	212	SER	CA-CB-OG	7.22	130.69	111.20
1	A	4	ARG	CA-C-O	7.18	135.17	120.10
1	A	524	ARG	CD-NE-CZ	7.17	133.63	123.60
1	A	264	GLU	OE1-CD-OE2	-7.14	114.73	123.30
1	A	659	TYR	CB-CG-CD1	-7.13	116.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	469	TRP	CA-C-N	7.12	132.86	117.20
1	A	618	ALA	N-CA-CB	7.12	120.06	110.10
1	A	198	CYS	CA-CB-SG	7.10	126.78	114.00
1	A	673	ASN	CB-CG-OD1	-7.08	107.45	121.60
1	A	108	GLU	CG-CD-OE2	7.07	132.44	118.30
1	A	110	GLN	N-CA-CB	7.02	123.24	110.60
1	A	625	SER	CA-CB-OG	7.00	130.11	111.20
1	A	370	THR	CA-CB-OG1	-6.99	94.32	109.00
1	A	356	ARG	N-CA-CB	6.90	123.02	110.60
1	A	10	ALA	CB-CA-C	6.86	120.39	110.10
1	A	603	MET	CB-CG-SD	-6.84	91.88	112.40
1	A	66	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	A	187	GLU	OE1-CD-OE2	6.81	131.47	123.30
1	A	558	ASN	N-CA-CB	6.80	122.84	110.60
1	A	544	PHE	CB-CG-CD1	-6.79	116.05	120.80
1	A	356	ARG	CB-CG-CD	6.76	129.19	111.60
1	A	619	LYS	CA-CB-CG	6.75	128.25	113.40
1	A	299	LEU	O-C-N	6.72	133.45	122.70
1	A	352	GLU	CG-CD-OE1	6.71	131.72	118.30
1	A	398	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	A	110	GLN	CA-CB-CG	6.68	128.09	113.40
1	A	422	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	319	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	A	422	ASP	CB-CA-C	6.67	123.74	110.40
1	A	466	THR	CA-CB-OG1	-6.66	95.01	109.00
1	A	221	GLU	CB-CG-CD	6.66	132.18	114.20
1	A	604	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	657	THR	C-N-CA	6.64	138.29	121.70
1	A	332	ARG	NH1-CZ-NH2	6.63	126.70	119.40
1	A	635	GLN	C-N-CA	6.62	138.25	121.70
1	A	216	GLU	OE1-CD-OE2	-6.61	115.37	123.30
1	A	92	TYR	CZ-CE2-CD2	-6.60	113.86	119.80
1	A	294	GLY	C-N-CA	6.57	138.12	121.70
1	A	29	VAL	CG1-CB-CG2	-6.56	100.40	110.90
1	A	386	LYS	CB-CA-C	-6.56	97.28	110.40
1	A	662	TYR	CB-CG-CD1	6.55	124.93	121.00
1	A	589	CYS	CA-CB-SG	6.55	125.79	114.00
1	A	629	ASP	OD1-CG-OD2	6.55	135.74	123.30
1	A	15	GLU	N-CA-CB	6.54	122.38	110.60
1	A	364	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	29	VAL	CA-CB-CG1	6.49	120.64	110.90
1	A	465	ARG	CG-CD-NE	-6.47	98.20	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	ASN	N-CA-CB	-6.43	99.02	110.60
1	A	466	THR	CA-CB-CG2	6.43	121.41	112.40
1	A	684	GLU	CG-CD-OE2	-6.42	105.47	118.30
1	A	56	ALA	N-CA-CB	-6.38	101.16	110.10
1	A	392	MET	CA-CB-CG	-6.36	102.48	113.30
1	A	547	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	163	LYS	N-CA-CB	6.35	122.02	110.60
1	A	548	VAL	N-CA-CB	-6.35	97.54	111.50
1	A	105	GLN	CA-CB-CG	-6.34	99.44	113.40
1	A	34	VAL	CB-CA-C	-6.33	99.37	111.40
1	A	618	ALA	O-C-N	6.32	132.82	122.70
1	A	417	SER	CA-CB-OG	6.30	128.22	111.20
1	A	22	TRP	CB-CA-C	6.30	123.00	110.40
1	A	473	MET	CA-CB-CG	6.29	123.99	113.30
1	A	216	GLU	CG-CD-OE2	6.28	130.87	118.30
1	A	178	GLU	CB-CA-C	6.28	122.96	110.40
1	A	85	GLU	O-C-N	6.28	132.75	122.70
1	A	86	ARG	N-CA-CB	6.28	121.90	110.60
1	A	27	ARG	CA-CB-CG	6.27	127.20	113.40
1	A	200	LYS	CD-CE-NZ	6.27	126.12	111.70
1	A	226	GLU	CB-CG-CD	6.25	131.08	114.20
1	A	52	ASN	CA-C-O	-6.24	106.99	120.10
1	A	298	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	8	TRP	O-C-N	6.22	132.66	122.70
1	A	625	SER	CA-C-N	6.18	130.80	117.20
1	A	493	CYS	O-C-N	6.18	132.59	122.70
1	A	533	ARG	CD-NE-CZ	6.17	132.25	123.60
1	A	40	ASP	O-C-N	6.16	132.56	122.70
1	A	220	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	332	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	11	VAL	N-CA-CB	-6.13	98.01	111.50
1	A	163	LYS	CA-CB-CG	6.13	126.88	113.40
1	A	100	LYS	CD-CE-NZ	6.11	125.75	111.70
1	A	424	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	637	GLU	CG-CD-OE1	6.09	130.47	118.30
1	A	622	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	157	CYS	CA-CB-SG	-6.07	103.08	114.00
1	A	683	LEU	N-CA-CB	6.07	122.53	110.40
1	A	469	TRP	CA-C-O	-6.05	107.39	120.10
1	A	502	ASN	O-C-N	6.05	132.38	122.70
1	A	484	LYS	O-C-N	6.03	132.34	122.70
1	A	532	PHE	CB-CG-CD1	-6.01	116.59	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	A	260	VAL	CG1-CB-CG2	6.01	120.51	110.90
1	A	628	PRO	O-C-N	6.00	132.31	122.70
1	A	400	TYR	CB-CG-CD2	5.99	124.59	121.00
1	A	89	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	276	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	A	5	SER	N-CA-CB	-5.98	101.54	110.50
1	A	395	ASP	CA-C-N	5.97	128.13	116.20
1	A	478	ASN	CA-CB-CG	5.96	126.52	113.40
1	A	657	THR	N-CA-CB	-5.94	99.02	110.30
1	A	342	ARG	CA-CB-CG	5.93	126.45	113.40
1	A	378	GLU	CG-CD-OE2	-5.93	106.44	118.30
1	A	28	LYS	N-CA-CB	-5.92	99.94	110.60
1	A	104	PHE	O-C-N	5.92	132.17	122.70
1	A	53	ARG	C-N-CA	5.90	136.46	121.70
1	A	491	GLN	N-CA-CB	5.90	121.23	110.60
1	A	21	GLN	CA-CB-CG	5.89	126.35	113.40
1	A	385	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	A	674	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	A	53	ARG	CB-CG-CD	5.85	126.81	111.60
1	A	662	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	A	165	GLN	O-C-N	5.84	132.05	122.70
1	A	37	LEU	O-C-N	5.84	132.04	122.70
1	A	144	PRO	O-C-N	5.83	132.02	122.70
1	A	121	ARG	NH1-CZ-NH2	5.81	125.80	119.40
1	A	368	SER	N-CA-CB	5.81	119.22	110.50
1	A	619	LYS	N-CA-CB	-5.81	100.15	110.60
1	A	428	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	A	524	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	432	VAL	CB-CA-C	5.79	122.41	111.40
1	A	266	ALA	N-CA-CB	-5.79	102.00	110.10
1	A	20	PHE	O-C-N	5.79	131.96	122.70
1	A	351	GLY	CA-C-O	5.78	131.01	120.60
1	A	244	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	657	THR	CA-CB-OG1	-5.76	96.91	109.00
1	A	652	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	156	SER	CB-CA-C	-5.74	99.20	110.10
1	A	633	LEU	N-CA-CB	-5.74	98.93	110.40
1	A	11	VAL	CB-CA-C	5.73	122.29	111.40
1	A	447	SER	CB-CA-C	-5.73	99.21	110.10
1	A	675	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	A	260	VAL	CB-CA-C	-5.68	100.61	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	GLN	CA-CB-CG	-5.67	100.92	113.40
1	A	108	GLU	CG-CD-OE1	-5.67	106.96	118.30
1	A	249	ARG	CB-CA-C	5.66	121.73	110.40
1	A	149	VAL	CA-CB-CG1	5.66	119.39	110.90
1	A	684	GLU	CB-CG-CD	-5.65	98.94	114.20
1	A	230	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	372	SER	CA-CB-OG	-5.65	95.96	111.20
1	A	332	ARG	N-CA-CB	5.64	120.76	110.60
1	A	201	ASP	CB-CA-C	-5.63	99.14	110.40
1	A	221	GLU	CG-CD-OE1	5.63	129.56	118.30
1	A	26	MET	N-CA-C	-5.63	95.80	111.00
1	A	603	MET	N-CA-CB	-5.63	100.47	110.60
1	A	288	LEU	CB-CA-C	5.62	120.89	110.20
1	A	537	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	A	265	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	384	VAL	N-CA-CB	5.59	123.81	111.50
1	A	419	GLN	CB-CA-C	5.58	121.57	110.40
1	A	676	LYS	CB-CA-C	-5.57	99.26	110.40
1	A	575	CYS	O-C-N	5.56	131.60	122.70
1	A	689	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	331	LEU	O-C-N	5.55	131.57	122.70
1	A	537	GLU	CG-CD-OE2	-5.54	107.21	118.30
1	A	390	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	639	LYS	N-CA-CB	5.52	120.54	110.60
1	A	640	ASN	O-C-N	-5.52	113.87	122.70
1	A	626	ASP	CA-CB-CG	5.51	125.53	113.40
1	A	373	SER	N-CA-CB	-5.51	102.24	110.50
1	A	50	ALA	N-CA-CB	-5.50	102.40	110.10
1	A	344	ARG	CB-CG-CD	-5.50	97.31	111.60
1	A	146	GLU	CG-CD-OE2	5.49	129.28	118.30
1	A	52	ASN	O-C-N	5.48	131.47	122.70
1	A	560	GLU	N-CA-C	-5.48	96.21	111.00
1	A	628	PRO	CA-CB-CG	-5.48	93.59	104.00
1	A	213	THR	CA-CB-OG1	-5.47	97.50	109.00
1	A	536	ALA	O-C-N	5.47	131.46	122.70
1	A	537	GLU	CA-C-O	5.47	131.59	120.10
1	A	4	ARG	CA-C-N	-5.46	105.18	117.20
1	A	84	THR	CA-C-N	-5.46	105.18	117.20
1	A	171	ARG	N-CA-CB	5.45	120.41	110.60
1	A	546	LYS	CD-CE-NZ	-5.45	99.17	111.70
1	A	460	HIS	O-C-N	5.44	131.40	122.70
1	A	220	ASP	O-C-N	5.43	131.39	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	A	236	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	A	493	CYS	N-CA-C	-5.41	96.38	111.00
1	A	564	LYS	CG-CD-CE	5.41	128.14	111.90
1	A	157	CYS	C-N-CA	5.41	135.23	121.70
1	A	29	VAL	CB-CA-C	5.41	121.68	111.40
1	A	336	GLU	CB-CA-C	-5.41	99.58	110.40
1	A	360	GLN	N-CA-CB	5.41	120.33	110.60
1	A	75	ARG	CB-CA-C	-5.40	99.61	110.40
1	A	42	PRO	O-C-N	-5.40	114.07	122.70
1	A	162	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	423	PRO	N-CA-C	-5.38	98.11	112.10
1	A	354	GLU	CG-CD-OE2	-5.38	107.55	118.30
1	A	444	SER	CA-CB-OG	5.37	125.69	111.20
1	A	614	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	A	689	LEU	CB-CG-CD1	5.37	120.12	111.00
1	A	656	LYS	CB-CA-C	-5.36	99.67	110.40
1	A	548	VAL	CB-CA-C	5.36	121.59	111.40
1	A	315	ASP	CB-CA-C	5.36	121.12	110.40
1	A	619	LYS	CB-CG-CD	-5.36	97.67	111.60
1	A	623	ASN	CA-C-O	5.36	131.35	120.10
1	A	105	GLN	N-CA-CB	-5.35	100.97	110.60
1	A	599	VAL	CA-CB-CG1	5.35	118.92	110.90
1	A	77	VAL	CA-CB-CG1	5.34	118.91	110.90
1	A	642	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	A	489	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	A	359	ASN	CB-CA-C	5.33	121.06	110.40
1	A	301	LYS	CD-CE-NZ	-5.33	99.45	111.70
1	A	637	GLU	C-N-CA	5.33	135.01	121.70
1	A	554	THR	CA-CB-OG1	-5.32	97.82	109.00
1	A	640	ASN	C-N-CA	5.32	135.01	121.70
1	A	573	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	A	286	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	A	491	GLN	CB-CA-C	-5.31	99.78	110.40
1	A	261	ASN	C-N-CA	5.30	133.44	122.30
1	A	666	GLN	O-C-N	5.29	131.17	122.70
1	A	418	GLN	CA-C-N	-5.29	105.57	117.20
1	A	249	ARG	CA-CB-CG	5.28	125.02	113.40
1	A	119	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	A	187	GLU	CG-CD-OE1	-5.28	107.75	118.30
1	A	39	ARG	CB-CA-C	5.27	120.95	110.40
1	A	104	PHE	N-CA-CB	5.26	120.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	TRP	CB-CG-CD2	-5.25	119.77	126.60
1	A	28	LYS	CA-CB-CG	5.25	124.95	113.40
1	A	386	LYS	CD-CE-NZ	-5.25	99.63	111.70
1	A	218	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	421	SER	C-N-CA	5.24	134.80	121.70
1	A	386	LYS	O-C-N	5.24	132.10	123.20
1	A	453	VAL	CA-CB-CG1	5.23	118.75	110.90
1	A	314	ILE	CA-CB-CG1	-5.22	101.07	111.00
1	A	335	GLU	N-CA-CB	-5.22	101.19	110.60
1	A	528	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	630	LYS	N-CA-CB	-5.20	101.25	110.60
1	A	356	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	A	477	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	A	637	GLU	CG-CD-OE2	-5.18	107.93	118.30
1	A	378	GLU	C-N-CA	5.16	134.60	121.70
1	A	276	GLU	CG-CD-OE2	5.16	128.62	118.30
1	A	400	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	A	356	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	132	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	A	523	GLU	N-CA-CB	-5.13	101.36	110.60
1	A	95	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	A	287	GLN	O-C-N	5.13	130.91	122.70
1	A	404	LYS	CD-CE-NZ	-5.13	99.91	111.70
1	A	541	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	631	PHE	CG-CD1-CE1	5.12	126.44	120.80
1	A	192	TYR	CG-CD1-CE1	-5.10	117.22	121.30
1	A	538	ASN	O-C-N	5.10	130.86	122.70
1	A	636	SER	CA-C-N	-5.10	105.97	117.20
1	A	388	GLU	CB-CG-CD	-5.09	100.45	114.20
1	A	388	GLU	N-CA-CB	-5.09	101.44	110.60
1	A	356	ARG	CA-CB-CG	5.09	124.59	113.40
1	A	299	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	A	637	GLU	CB-CG-CD	5.08	127.93	114.20
1	A	78	ALA	N-CA-CB	-5.08	102.98	110.10
1	A	671	ILE	CA-CB-CG1	-5.08	101.34	111.00
1	A	555	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	89	ARG	CD-NE-CZ	-5.08	116.50	123.60
1	A	629	ASP	O-C-N	5.07	130.81	122.70
1	A	26	MET	N-CA-CB	5.07	119.72	110.60
1	A	227	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	457	LYS	CB-CG-CD	-5.07	98.43	111.60
1	A	528	TYR	CZ-CE2-CD2	-5.06	115.24	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	ASN	OD1-CG-ND2	5.06	133.54	121.90
1	A	399	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	A	244	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	A	258	ARG	CG-CD-NE	-5.05	101.20	111.80
1	A	354	GLU	CA-CB-CG	5.05	124.50	113.40
1	A	587	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	8	TRP	CB-CG-CD1	5.04	133.56	127.00
1	A	640	ASN	N-CA-CB	-5.04	101.52	110.60
1	A	295	GLN	N-CA-C	5.04	124.62	111.00
1	A	641	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	371	CYS	CA-CB-SG	-5.04	104.93	114.00
1	A	401	THR	CA-CB-CG2	5.04	119.45	112.40
1	A	626	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	326	THR	N-CA-CB	-5.02	100.77	110.30
1	A	337	GLU	O-C-N	-5.02	114.67	122.70
1	A	544	PHE	CB-CG-CD2	5.01	124.31	120.80
1	A	249	ARG	N-CA-CB	-5.01	101.58	110.60
1	A	4	ARG	CA-CB-CG	5.00	124.41	113.40
1	A	288	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ARG	Sidechain
1	A	602	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5313	0	5156	423	0
2	A	14	0	12	0	0
3	A	2	0	0	0	0
4	A	4	0	0	0	0
5	A	6	0	0	2	0
6	A	325	0	0	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5664	0	5168	425	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 40.

All (425) 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:260:VAL:CG1	1:A:261:ASN:H	1.11	1.48
1:A:436:LEU:CD1	1:A:593:MET:CE	1.99	1.39
1:A:436:LEU:CD1	1:A:593:MET:HE3	1.53	1.34
1:A:296:LYS:HE3	6:A:1153:HOH:O	1.37	1.24
1:A:176:THR:HA	6:A:1148:HOH:O	1.10	1.22
1:A:220:ASP:OD2	1:A:223:GLU:N	1.75	1.20
1:A:107:ASN:H	1:A:107:ASN:ND2	1.35	1.19
1:A:107:ASN:HD22	1:A:107:ASN:N	1.37	1.16
1:A:296:LYS:CE	6:A:1153:HOH:O	1.88	1.16
1:A:432:VAL:HG13	6:A:1087:HOH:O	1.44	1.16
1:A:37:LEU:N	1:A:37:LEU:HD22	1.50	1.16
1:A:260:VAL:HG13	1:A:261:ASN:N	1.06	1.15
1:A:36:CYS:C	1:A:37:LEU:HD22	1.67	1.12
1:A:680:SER:HB2	6:A:1170:HOH:O	1.49	1.11
1:A:436:LEU:HD13	1:A:593:MET:HE1	1.18	1.10
1:A:436:LEU:HD13	1:A:593:MET:CE	1.73	1.09
1:A:87:GLN:H	1:A:88:PRO:HD3	1.04	1.08
1:A:25:ASN:N	1:A:25:ASN:HD22	1.48	1.05
1:A:87:GLN:H	1:A:88:PRO:CD	1.57	1.05
1:A:87:GLN:N	1:A:88:PRO:CD	2.18	1.04
1:A:220:ASP:OD2	1:A:223:GLU:HB2	1.57	1.04
1:A:577:ASP:OD1	1:A:579:LYS:HG2	1.58	1.03
1:A:87:GLN:N	1:A:88:PRO:HD3	1.75	1.02
1:A:37:LEU:N	1:A:37:LEU:CD2	2.21	1.02
1:A:86:ARG:O	1:A:87:GLN:HB2	1.56	1.02
1:A:436:LEU:CD1	1:A:593:MET:HE1	1.75	1.01
1:A:680:SER:CB	6:A:1170:HOH:O	2.07	1.00
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.26	0.99
1:A:8:TRP:O	1:A:37:LEU:HD23	1.62	0.98
1:A:436:LEU:HD12	1:A:593:MET:CE	1.75	0.96
1:A:622:ARG:HD3	1:A:622:ARG:C	1.85	0.95
1:A:24:ARG:O	1:A:27:ARG:HG2	1.67	0.94
1:A:30:ARG:HH11	1:A:30:ARG:HA	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:CYS:O	1:A:180:LYS:HD2	1.69	0.93
1:A:672:THR:OG1	6:A:1226:HOH:O	1.85	0.92
1:A:430:ARG:HH21	1:A:648:GLU:CD	1.72	0.92
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.35	0.91
1:A:43:ILE:CG2	6:A:1130:HOH:O	2.19	0.91
1:A:417:SER:C	1:A:419:GLN:H	1.64	0.90
1:A:260:VAL:HG12	1:A:261:ASN:H	1.32	0.90
1:A:425:PRO:C	1:A:426:ASN:HD22	1.73	0.89
1:A:138:TRP:HE1	1:A:143:GLU:HG3	1.36	0.88
1:A:3:ARG:HB3	1:A:3:ARG:HH11	1.37	0.88
1:A:3:ARG:HE	1:A:7:GLN:CG	1.85	0.88
1:A:113:LYS:HE3	1:A:172:LEU:HD21	1.56	0.88
1:A:436:LEU:HD12	1:A:593:MET:HE3	0.90	0.88
1:A:686:CYS:O	1:A:690:ARG:HG2	1.73	0.88
1:A:25:ASN:HD22	1:A:25:ASN:H	1.20	0.87
1:A:241:LYS:HD2	1:A:241:LYS:N	1.87	0.86
1:A:138:TRP:NE1	1:A:143:GLU:O	2.09	0.86
1:A:260:VAL:CG1	1:A:261:ASN:N	1.81	0.86
1:A:283:SER:OG	1:A:285:LYS:HG2	1.75	0.86
1:A:667:TYR:CE2	1:A:671:ILE:HD11	2.11	0.85
1:A:658:THR:HG22	1:A:660:GLU:H	1.39	0.85
1:A:430:ARG:NH2	1:A:648:GLU:CD	2.31	0.84
1:A:638:THR:HA	6:A:1188:HOH:O	1.76	0.84
1:A:3:ARG:HE	1:A:7:GLN:HG2	1.43	0.84
1:A:425:PRO:O	1:A:426:ASN:ND2	2.10	0.83
1:A:357:LYS:NZ	1:A:633:LEU:O	2.10	0.83
1:A:654:HIS:HD2	6:A:1264:HOH:O	1.60	0.83
1:A:425:PRO:C	1:A:426:ASN:ND2	2.32	0.83
1:A:559:ASN:HB2	1:A:564:LYS:NZ	1.94	0.82
1:A:139:THR:HG22	6:A:1302:HOH:O	1.79	0.82
1:A:295:GLN:HG3	1:A:298:LEU:HD11	1.59	0.82
1:A:422:ASP:HB2	1:A:423:PRO:CD	2.10	0.82
1:A:43:ILE:HG23	6:A:1130:HOH:O	1.75	0.81
1:A:238:PRO:HD2	1:A:241:LYS:HD3	1.60	0.81
1:A:658:THR:HG22	1:A:660:GLU:N	1.96	0.80
1:A:626:ASP:O	1:A:630:LYS:N	2.13	0.80
5:A:696:OXL:O4	6:A:1205:HOH:O	1.98	0.80
1:A:220:ASP:OD2	1:A:223:GLU:CB	2.29	0.79
1:A:658:THR:CG2	1:A:660:GLU:H	1.94	0.79
1:A:138:TRP:NE1	1:A:143:GLU:HG3	1.96	0.79
1:A:22:TRP:HB2	1:A:286:PHE:CZ	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASN:OD1	6:A:1289:HOH:O	2.00	0.78
1:A:422:ASP:O	1:A:424:ASP:N	2.16	0.78
1:A:422:ASP:HB2	1:A:423:PRO:HD3	1.65	0.77
1:A:485:PHE:CZ	1:A:674:LEU:HD22	2.20	0.77
1:A:7:GLN:HB3	1:A:37:LEU:HD21	1.66	0.76
1:A:430:ARG:NH2	1:A:648:GLU:OE2	2.15	0.76
1:A:509:GLY:HA3	1:A:514:GLU:O	1.86	0.76
1:A:658:THR:HG22	1:A:661:LYS:H	1.51	0.75
1:A:465:ARG:NH2	6:A:1204:HOH:O	2.21	0.74
1:A:452:SER:O	1:A:456:LYS:CE	2.36	0.74
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.03	0.74
1:A:430:ARG:NH2	1:A:648:GLU:OE1	2.21	0.74
1:A:100:LYS:NZ	1:A:225:ASP:O	2.17	0.73
1:A:238:PRO:HB2	1:A:240:ASP:OD1	1.89	0.73
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.00	0.73
1:A:113:LYS:CE	1:A:172:LEU:HD21	2.18	0.73
1:A:231:CYS:HB3	1:A:232:PRO:HD2	1.71	0.73
1:A:25:ASN:N	1:A:25:ASN:ND2	2.28	0.72
1:A:296:LYS:HE2	6:A:1153:HOH:O	1.72	0.72
1:A:260:VAL:HG13	1:A:261:ASN:CA	2.16	0.71
1:A:11:VAL:HG23	1:A:45:CYS:SG	2.31	0.71
1:A:686:CYS:O	1:A:690:ARG:CG	2.37	0.71
1:A:667:TYR:HB2	6:A:1202:HOH:O	1.91	0.71
1:A:146:GLU:OE1	1:A:146:GLU:N	2.24	0.70
1:A:452:SER:O	1:A:456:LYS:NZ	2.24	0.70
1:A:577:ASP:CG	1:A:579:LYS:HG2	2.12	0.70
1:A:86:ARG:C	1:A:86:ARG:HD3	2.11	0.70
1:A:688:PHE:HD1	1:A:689:LEU:HD13	1.57	0.70
1:A:233:ASP:OD2	1:A:235:THR:HB	1.93	0.69
1:A:121:ARG:NH1	6:A:1128:HOH:O	2.12	0.69
1:A:658:THR:HB	1:A:661:LYS:HG3	1.73	0.69
1:A:7:GLN:HG2	1:A:35:SER:OG	1.93	0.68
1:A:9:CYS:HB2	1:A:54:ALA:CB	2.24	0.68
1:A:24:ARG:HE	1:A:24:ARG:CA	2.05	0.67
1:A:342:ARG:HH11	1:A:342:ARG:HG2	1.58	0.67
1:A:457:LYS:HB3	1:A:506:LEU:HD11	1.76	0.67
1:A:282:LYS:O	1:A:283:SER:HB2	1.93	0.67
1:A:36:CYS:CA	1:A:37:LEU:HD22	2.24	0.67
1:A:147:ALA:O	1:A:151:ARG:HG3	1.93	0.67
1:A:24:ARG:HE	1:A:24:ARG:HA	1.59	0.67
1:A:533:ARG:O	1:A:537:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:C	1:A:167:PRO:HD3	2.16	0.66
1:A:322:SER:O	1:A:326:THR:HB	1.95	0.66
1:A:223:GLU:OE1	1:A:223:GLU:HA	1.94	0.66
1:A:212:SER:OG	6:A:1151:HOH:O	2.13	0.66
1:A:221:GLU:O	1:A:224:ARG:HB2	1.95	0.66
1:A:424:ASP:OD1	1:A:424:ASP:C	2.34	0.66
1:A:679:THR:CG2	1:A:683:LEU:HB2	2.25	0.66
1:A:622:ARG:HD3	1:A:622:ARG:O	1.96	0.66
1:A:577:ASP:OD1	1:A:579:LYS:CG	2.42	0.66
1:A:105:GLN:CA	1:A:105:GLN:HE21	2.09	0.65
1:A:559:ASN:CB	1:A:564:LYS:NZ	2.59	0.65
1:A:86:ARG:O	1:A:87:GLN:CB	2.38	0.65
1:A:445:ASP:O	1:A:580:ARG:NH1	2.30	0.65
1:A:627:CYS:HB2	1:A:631:PHE:O	1.97	0.65
1:A:344:ARG:HD3	1:A:370:THR:HG22	1.78	0.65
1:A:220:ASP:OD2	1:A:223:GLU:CA	2.45	0.64
1:A:105:GLN:NE2	1:A:105:GLN:CA	2.59	0.64
1:A:684:GLU:OE1	6:A:1254:HOH:O	2.15	0.64
1:A:14:PRO:O	1:A:298:LEU:HD13	1.98	0.63
1:A:283:SER:OG	1:A:285:LYS:CG	2.46	0.63
1:A:13:ASN:HB3	1:A:14:PRO:HD3	1.80	0.63
1:A:561:ALA:HB3	6:A:1177:HOH:O	1.97	0.63
1:A:30:ARG:HA	1:A:30:ARG:NH1	2.09	0.63
1:A:430:ARG:HD2	6:A:1174:HOH:O	1.99	0.63
1:A:652:ARG:HB3	6:A:1266:HOH:O	1.99	0.63
1:A:362:SER:O	1:A:365:SER:OG	2.16	0.63
1:A:666:GLN:H	1:A:666:GLN:NE2	1.96	0.63
1:A:353:GLN:HE22	1:A:639:LYS:CD	2.12	0.62
1:A:424:ASP:HB3	1:A:648:GLU:OE2	1.99	0.62
1:A:559:ASN:HB2	1:A:564:LYS:CE	2.30	0.62
1:A:559:ASN:HB2	1:A:564:LYS:HZ3	1.63	0.62
1:A:622:ARG:C	1:A:622:ARG:CD	2.65	0.62
1:A:84:THR:O	1:A:88:PRO:N	2.33	0.62
1:A:374:ALA:HB1	1:A:379:ASP:HB3	1.80	0.62
1:A:394:LEU:HD22	1:A:398:TYR:HB3	1.81	0.62
1:A:7:GLN:CG	1:A:35:SER:OG	2.48	0.62
1:A:352:GLU:H	1:A:352:GLU:CD	2.01	0.62
1:A:437:ALA:CB	1:A:471:ILE:HD13	2.30	0.62
1:A:465:ARG:NH2	6:A:1205:HOH:O	2.32	0.62
1:A:485:PHE:CZ	1:A:674:LEU:CD2	2.82	0.62
1:A:231:CYS:HB2	1:A:235:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLY:CA	1:A:514:GLU:O	2.48	0.61
1:A:559:ASN:HB2	1:A:564:LYS:HD3	1.82	0.61
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.82	0.61
1:A:652:ARG:HH11	1:A:652:ARG:HG2	1.65	0.61
1:A:426:ASN:ND2	1:A:426:ASN:N	2.33	0.61
1:A:510:ASP:OD2	1:A:515:ASN:ND2	2.33	0.61
1:A:635:GLN:NE2	6:A:1273:HOH:O	2.34	0.61
1:A:24:ARG:NH2	1:A:28:LYS:HE3	2.16	0.61
1:A:639:LYS:HD3	6:A:1080:HOH:O	1.99	0.60
1:A:341:ARG:O	1:A:341:ARG:HG3	2.01	0.60
1:A:8:TRP:O	1:A:37:LEU:CD2	2.46	0.60
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.35	0.60
1:A:291:SER:HB3	1:A:295:GLN:HB2	1.82	0.60
1:A:395:ASP:OD2	1:A:465:ARG:HA	2.02	0.60
1:A:25:ASN:H	1:A:25:ASN:ND2	1.94	0.60
1:A:107:ASN:ND2	1:A:107:ASN:N	2.10	0.60
1:A:477:PHE:HA	1:A:488:TYR:OH	2.00	0.60
1:A:431:PRO:HA	6:A:1264:HOH:O	2.00	0.60
1:A:25:ASN:HB3	1:A:278:PHE:CZ	2.37	0.60
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.01	0.60
1:A:437:ALA:CB	1:A:471:ILE:CD1	2.79	0.59
1:A:38:LYS:O	1:A:39:ARG:HG2	2.01	0.59
1:A:559:ASN:HB2	1:A:564:LYS:CD	2.33	0.59
1:A:3:ARG:HB3	1:A:3:ARG:NH1	2.15	0.59
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.65	0.59
1:A:25:ASN:OD1	1:A:286:PHE:HB2	2.03	0.59
1:A:33:PRO:HD2	6:A:1124:HOH:O	2.02	0.58
1:A:100:LYS:HG3	1:A:226:GLU:O	2.03	0.58
1:A:121:ARG:HD3	6:A:1128:HOH:O	2.03	0.58
1:A:258:ARG:NH1	1:A:261:ASN:O	2.36	0.58
1:A:688:PHE:CD1	1:A:689:LEU:HD13	2.38	0.58
1:A:582:PRO:HG2	1:A:585:GLU:HG3	1.86	0.58
1:A:667:TYR:O	1:A:671:ILE:HG13	2.03	0.57
1:A:342:ARG:HG2	1:A:342:ARG:NH1	2.20	0.57
1:A:671:ILE:O	1:A:675:LYS:HG2	2.04	0.57
1:A:295:GLN:O	6:A:1154:HOH:O	2.18	0.57
1:A:143:GLU:HG3	1:A:143:GLU:O	2.04	0.56
1:A:145:ILE:O	1:A:149:VAL:HG12	2.05	0.56
1:A:138:TRP:CD1	1:A:143:GLU:HG3	2.39	0.56
1:A:485:PHE:HZ	1:A:674:LEU:HD22	1.69	0.56
1:A:485:PHE:HZ	1:A:674:LEU:CD2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:HB3	1:A:165:GLN:HG3	1.86	0.56
1:A:282:LYS:O	1:A:283:SER:CB	2.52	0.56
1:A:283:SER:OG	1:A:285:LYS:HD3	2.05	0.56
1:A:667:TYR:CZ	1:A:671:ILE:HD11	2.41	0.56
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.41	0.56
1:A:374:ALA:HB1	1:A:379:ASP:CB	2.35	0.56
1:A:3:ARG:HD2	1:A:7:GLN:OE1	2.06	0.56
1:A:166:PHE:N	1:A:167:PRO:HD3	2.19	0.56
1:A:353:GLN:HE22	1:A:639:LYS:NZ	2.04	0.56
1:A:146:GLU:HA	1:A:149:VAL:HG13	1.88	0.56
1:A:436:LEU:HD11	1:A:593:MET:CE	2.25	0.55
1:A:559:ASN:CB	1:A:564:LYS:HZ3	2.16	0.55
1:A:452:SER:O	1:A:456:LYS:HE2	2.06	0.55
1:A:547:ASP:OD1	1:A:547:ASP:N	2.37	0.55
1:A:24:ARG:HG2	1:A:27:ARG:HH21	1.71	0.55
1:A:529:THR:OG1	6:A:1069:HOH:O	2.18	0.55
1:A:32:PRO:CD	1:A:273:GLN:HG3	2.37	0.54
1:A:328:ILE:O	1:A:332:ARG:NH1	2.40	0.54
1:A:278:PHE:CE1	1:A:285:LYS:NZ	2.76	0.54
1:A:38:LYS:C	1:A:39:ARG:HG2	2.27	0.54
1:A:520:ASN:OD1	1:A:522:ASN:HB2	2.08	0.54
1:A:7:GLN:HB3	1:A:37:LEU:CD2	2.36	0.54
1:A:162:ASP:CG	1:A:165:GLN:HG2	2.27	0.54
1:A:353:GLN:HE22	1:A:639:LYS:HD3	1.71	0.54
1:A:24:ARG:NH2	1:A:28:LYS:HB2	2.23	0.53
1:A:487:GLU:O	6:A:1045:HOH:O	2.18	0.53
1:A:637:GLU:HA	6:A:1190:HOH:O	2.08	0.53
1:A:11:VAL:HG22	1:A:41:SER:C	2.29	0.53
1:A:231:CYS:HB3	1:A:232:PRO:CD	2.39	0.53
1:A:38:LYS:O	1:A:39:ARG:NH1	2.36	0.53
1:A:437:ALA:HB2	1:A:471:ILE:CD1	2.38	0.53
1:A:292:PRO:C	1:A:294:GLY:N	2.62	0.53
1:A:25:ASN:HB3	1:A:285:LYS:HZ3	1.73	0.53
1:A:47:GLN:NE2	6:A:1244:HOH:O	2.41	0.53
1:A:534:CYS:O	1:A:539:ALA:HB3	2.08	0.53
1:A:628:PRO:HA	1:A:632:CYS:SG	2.49	0.53
1:A:47:GLN:HG2	1:A:72:TYR:HE1	1.73	0.53
1:A:131:THR:HG21	1:A:247:LEU:HD13	1.91	0.53
1:A:554:THR:O	1:A:555:ASP:HB2	2.09	0.53
1:A:283:SER:OG	1:A:285:LYS:CD	2.56	0.52
1:A:498:ASP:OD1	1:A:500:ARG:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLU:CD	1:A:562:TRP:HE1	2.12	0.52
1:A:601:SER:HB2	1:A:609:LEU:CD2	2.39	0.52
1:A:652:ARG:HG2	1:A:652:ARG:NH1	2.24	0.52
1:A:379:ASP:O	1:A:383:LEU:HG	2.09	0.52
1:A:427:CYS:SG	1:A:427:CYS:O	2.68	0.52
1:A:353:GLN:NE2	1:A:639:LYS:NZ	2.57	0.52
1:A:43:ILE:HG21	6:A:1130:HOH:O	2.00	0.52
1:A:548:VAL:O	1:A:552:GLN:HG3	2.10	0.52
1:A:555:ASP:OD1	1:A:567:LYS:HD3	2.10	0.52
1:A:404:LYS:HE2	1:A:404:LYS:HA	1.92	0.52
1:A:498:ASP:OD1	1:A:500:ARG:N	2.38	0.52
1:A:277:LYS:O	1:A:282:LYS:O	2.27	0.52
1:A:97:VAL:O	1:A:207:ALA:N	2.35	0.51
1:A:666:GLN:H	1:A:666:GLN:CD	2.12	0.51
1:A:349:ALA:O	1:A:373:SER:HA	2.10	0.51
1:A:133:ARG:NE	6:A:1210:HOH:O	2.35	0.51
1:A:170:CYS:O	1:A:171:ARG:C	2.48	0.51
1:A:58:THR:HG23	6:A:1020:HOH:O	2.10	0.51
5:A:696:OXL:C2	6:A:1205:HOH:O	2.56	0.51
1:A:691:LYS:O	6:A:1220:HOH:O	2.19	0.50
1:A:312:PRO:HB3	6:A:1160:HOH:O	2.12	0.50
1:A:522:ASN:OD1	6:A:1231:HOH:O	2.19	0.50
1:A:579:LYS:N	1:A:579:LYS:HD3	2.25	0.50
1:A:110:GLN:HB3	1:A:152:PHE:CE1	2.47	0.50
1:A:186:GLN:NE2	1:A:186:GLN:HA	2.25	0.50
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.94	0.50
1:A:105:GLN:CB	1:A:107:ASN:HD21	2.15	0.50
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.41	0.50
1:A:7:GLN:CB	1:A:37:LEU:HD21	2.40	0.49
1:A:9:CYS:HB2	1:A:54:ALA:HB1	1.94	0.49
1:A:32:PRO:CG	1:A:273:GLN:HG3	2.42	0.49
1:A:139:THR:CG2	6:A:1302:HOH:O	2.49	0.49
1:A:84:THR:HG22	1:A:85:GLU:OE2	2.12	0.49
1:A:100:LYS:HG3	1:A:226:GLU:C	2.32	0.49
1:A:316:SER:O	1:A:320:LEU:HG	2.12	0.49
1:A:591:LEU:O	1:A:592:ALA:HB2	2.12	0.49
1:A:8:TRP:HZ2	1:A:58:THR:HG22	1.77	0.49
1:A:437:ALA:HB3	1:A:471:ILE:HD13	1.93	0.49
1:A:3:ARG:NE	1:A:7:GLN:CG	2.67	0.49
1:A:332:ARG:HD3	6:A:1312:HOH:O	2.12	0.49
1:A:624:GLY:O	1:A:626:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:N	1:A:226:GLU:O	2.32	0.49
1:A:231:CYS:CB	1:A:232:PRO:CD	2.90	0.49
1:A:214:VAL:O	1:A:218:LEU:HB2	2.12	0.48
1:A:342:ARG:NH1	1:A:342:ARG:CG	2.76	0.48
1:A:427:CYS:O	1:A:649:CYS:SG	2.71	0.48
1:A:73:LYS:HE3	1:A:73:LYS:HB3	1.56	0.48
1:A:684:GLU:HG3	6:A:1256:HOH:O	2.13	0.48
1:A:432:VAL:CG1	6:A:1087:HOH:O	2.27	0.48
1:A:125:TRP:CH2	1:A:149:VAL:HG11	2.49	0.48
1:A:638:THR:HG22	6:A:1189:HOH:O	2.13	0.48
1:A:417:SER:C	1:A:419:GLN:N	2.48	0.47
1:A:417:SER:HA	1:A:433:GLU:OE1	2.14	0.47
1:A:3:ARG:NE	1:A:35:SER:OG	2.47	0.47
1:A:220:ASP:HB3	1:A:223:GLU:HB2	1.97	0.47
1:A:298:LEU:O	1:A:299:LEU:HB2	2.14	0.47
1:A:28:LYS:O	1:A:29:VAL:HG23	2.15	0.47
1:A:668:VAL:HG12	6:A:1226:HOH:O	2.14	0.47
1:A:218:LEU:HD23	1:A:224:ARG:HA	1.97	0.47
1:A:278:PHE:CZ	1:A:285:LYS:NZ	2.83	0.47
1:A:666:GLN:CD	1:A:666:GLN:N	2.68	0.47
1:A:68:GLY:O	1:A:73:LYS:HA	2.15	0.47
1:A:263:LYS:O	1:A:266:ALA:HB3	2.15	0.47
1:A:223:GLU:OE1	1:A:223:GLU:CA	2.60	0.47
1:A:515:ASN:O	1:A:518:VAL:HB	2.15	0.47
1:A:3:ARG:HH11	1:A:3:ARG:CB	2.18	0.47
1:A:227:TYR:CD1	1:A:227:TYR:N	2.82	0.46
1:A:516:LYS:HE3	1:A:516:LYS:HB2	1.54	0.46
1:A:551:LEU:HD11	1:A:583:VAL:HG12	1.97	0.46
1:A:636:SER:O	1:A:637:GLU:O	2.33	0.46
1:A:679:THR:HG23	1:A:683:LEU:HB2	1.96	0.46
1:A:576:LEU:HD21	1:A:591:LEU:HD22	1.97	0.46
1:A:13:ASN:O	1:A:16:ALA:N	2.49	0.46
1:A:679:THR:HG23	1:A:683:LEU:HD23	1.97	0.46
1:A:559:ASN:C	1:A:559:ASN:OD1	2.53	0.46
1:A:133:ARG:CG	6:A:1210:HOH:O	2.63	0.46
1:A:231:CYS:CB	1:A:232:PRO:HD2	2.45	0.46
1:A:278:PHE:HE1	1:A:285:LYS:HZ2	1.61	0.46
1:A:443:ARG:HH11	1:A:443:ARG:HD3	1.31	0.46
1:A:321:GLY:O	1:A:325:PHE:CB	2.64	0.45
1:A:628:PRO:HG2	1:A:629:ASP:N	2.29	0.45
1:A:400:TYR:O	1:A:404:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LYS:HB3	1:A:582:PRO:HD2	1.97	0.45
1:A:197:LYS:O	1:A:198:CYS:C	2.54	0.45
1:A:330:ASN:N	1:A:330:ASN:HD22	2.12	0.45
1:A:351:GLY:HA2	1:A:352:GLU:OE1	2.16	0.45
1:A:679:THR:HG22	1:A:680:SER:N	2.31	0.45
1:A:133:ARG:N	1:A:134:PRO:CD	2.79	0.45
1:A:26:MET:SD	1:A:278:PHE:HE2	2.40	0.45
1:A:37:LEU:CD2	1:A:37:LEU:H	2.17	0.45
1:A:270:LEU:C	1:A:270:LEU:CD2	2.84	0.45
1:A:110:GLN:HE21	1:A:110:GLN:HB2	1.45	0.45
1:A:257:ALA:HB1	6:A:1279:HOH:O	2.17	0.45
1:A:334:SER:HB2	1:A:336:GLU:OE1	2.17	0.45
1:A:525:TYR:N	1:A:525:TYR:CD1	2.78	0.45
1:A:187:GLU:HA	1:A:188:PRO:HD2	1.80	0.45
1:A:554:THR:HG22	1:A:566:LEU:HB3	1.98	0.45
1:A:58:THR:HG21	1:A:300:PHE:CD1	2.52	0.45
1:A:551:LEU:HD11	1:A:583:VAL:CG1	2.47	0.45
1:A:636:SER:OG	1:A:645:ASP:OD1	2.34	0.45
1:A:404:LYS:HE3	1:A:659:TYR:OH	2.16	0.44
1:A:430:ARG:HD2	1:A:430:ARG:HH11	1.19	0.44
1:A:596:ASN:O	1:A:662:TYR:OH	2.22	0.44
1:A:13:ASN:C	1:A:15:GLU:N	2.68	0.44
1:A:344:ARG:CD	1:A:370:THR:HG22	2.45	0.44
1:A:26:MET:HB3	1:A:32:PRO:O	2.17	0.44
1:A:498:ASP:HA	1:A:499:PRO:HD3	1.84	0.44
1:A:7:GLN:HG3	1:A:35:SER:HG	1.82	0.44
1:A:84:THR:O	1:A:88:PRO:CD	2.65	0.44
1:A:133:ARG:NH1	1:A:330:ASN:O	2.49	0.44
1:A:622:ARG:HG2	6:A:1078:HOH:O	2.16	0.44
1:A:679:THR:CG2	1:A:680:SER:N	2.81	0.44
1:A:214:VAL:HG23	1:A:218:LEU:HD22	1.99	0.44
1:A:387:GLY:HA2	1:A:602:ARG:NH1	2.32	0.44
1:A:510:ASP:O	1:A:512:GLN:N	2.50	0.44
1:A:429:ASP:O	1:A:654:HIS:NE2	2.51	0.44
1:A:59:LEU:HG	1:A:63:PHE:CB	2.48	0.44
1:A:105:GLN:HB2	1:A:107:ASN:ND2	2.17	0.44
1:A:357:LYS:CE	1:A:633:LEU:O	2.66	0.44
1:A:34:VAL:HG13	1:A:270:LEU:HD11	1.99	0.43
1:A:314:ILE:HD13	1:A:689:LEU:HD13	2.00	0.43
1:A:49:ILE:CD1	1:A:57:VAL:HG12	2.48	0.43
1:A:51:GLU:O	1:A:52:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLY:O	1:A:154:SER:OG	2.35	0.43
1:A:416:LYS:HB2	6:A:1085:HOH:O	2.19	0.43
1:A:155:ALA:HB1	1:A:171:ARG:HB3	1.99	0.43
1:A:601:SER:HB2	1:A:609:LEU:HD22	2.00	0.43
1:A:437:ALA:HB2	1:A:471:ILE:HD12	2.00	0.43
1:A:619:LYS:HD3	1:A:626:ASP:OD1	2.19	0.43
1:A:117:THR:HG23	1:A:208:PHE:O	2.19	0.43
1:A:168:ASN:HD22	1:A:168:ASN:HA	1.23	0.43
1:A:191:SER:HB3	6:A:1156:HOH:O	2.19	0.43
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.46	0.43
1:A:658:THR:HG23	1:A:660:GLU:H	1.80	0.43
1:A:680:SER:HB2	1:A:681:PRO:HD2	2.00	0.43
1:A:13:ASN:HB3	1:A:14:PRO:CD	2.48	0.43
1:A:224:ARG:HH11	1:A:224:ARG:HD2	1.52	0.43
1:A:236:ARG:HH11	1:A:236:ARG:HD3	1.49	0.43
1:A:342:ARG:NH1	6:A:1213:HOH:O	2.48	0.43
1:A:510:ASP:C	1:A:512:GLN:H	2.22	0.43
1:A:220:ASP:CB	1:A:223:GLU:HB2	2.49	0.43
1:A:288:LEU:HD11	1:A:300:PHE:CE2	2.54	0.43
1:A:22:TRP:HB2	1:A:286:PHE:CE2	2.54	0.42
1:A:41:SER:HB2	1:A:42:PRO:HD2	2.00	0.42
1:A:292:PRO:O	1:A:294:GLY:N	2.52	0.42
1:A:437:ALA:CB	1:A:471:ILE:HD12	2.49	0.42
1:A:453:VAL:O	1:A:456:LYS:HB2	2.19	0.42
1:A:564:LYS:HD2	1:A:564:LYS:HA	1.81	0.42
1:A:24:ARG:CZ	1:A:28:LYS:HE3	2.48	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG2	2.34	0.42
1:A:278:PHE:HE1	1:A:285:LYS:NZ	2.15	0.42
1:A:531:ALA:O	1:A:534:CYS:HB3	2.18	0.42
1:A:138:TRP:CE2	1:A:143:GLU:O	2.72	0.42
1:A:7:GLN:CG	1:A:35:SER:HG	2.32	0.42
1:A:59:LEU:HG	1:A:63:PHE:HB2	2.02	0.42
1:A:193:SER:OG	1:A:217:ASP:OD2	2.30	0.42
1:A:253:HIS:CD2	1:A:253:HIS:N	2.85	0.42
1:A:138:TRP:CD1	1:A:143:GLU:CG	3.03	0.42
1:A:353:GLN:NE2	1:A:639:LYS:HZ2	2.18	0.42
1:A:463:VAL:O	1:A:464:ASP:HB2	2.19	0.42
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.19	0.42
1:A:679:THR:CG2	1:A:680:SER:H	2.33	0.42
1:A:20:PHE:O	1:A:23:GLN:HB3	2.20	0.42
1:A:36:CYS:HA	1:A:37:LEU:HD22	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:HA3	1:A:120:ARG:O	2.19	0.41
1:A:111:GLY:C	1:A:154:SER:OG	2.59	0.41
1:A:179:ASN:ND2	1:A:186:GLN:HB3	2.34	0.41
1:A:330:ASN:OD1	6:A:1031:HOH:O	2.22	0.41
1:A:377:THR:CG2	1:A:394:LEU:CD2	2.97	0.41
1:A:684:GLU:CG	6:A:1256:HOH:O	2.67	0.41
1:A:321:GLY:O	1:A:325:PHE:HB2	2.21	0.41
1:A:465:ARG:H	1:A:465:ARG:HG2	1.46	0.41
1:A:112:LEU:O	1:A:153:PHE:HB3	2.20	0.41
1:A:352:GLU:CD	1:A:522:ASN:HD21	2.23	0.41
1:A:426:ASN:HD22	1:A:426:ASN:HA	1.21	0.41
1:A:471:ILE:HB	1:A:472:PRO:CD	2.50	0.41
1:A:594:ALA:HA	1:A:595:PRO:HD3	1.94	0.41
1:A:218:LEU:O	1:A:224:ARG:NE	2.52	0.41
1:A:21:GLN:HE21	1:A:21:GLN:HB3	1.75	0.41
1:A:40:ASP:N	1:A:44:GLN:OE1	2.35	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.91	0.41
1:A:424:ASP:OD1	1:A:425:PRO:N	2.53	0.41
1:A:302:ASP:O	1:A:303:SER:HB2	2.20	0.41
1:A:410:VAL:HG21	1:A:609:LEU:HD23	2.02	0.41
1:A:174:ALA:HB3	1:A:188:PRO:CG	2.49	0.40
1:A:658:THR:HG21	1:A:660:GLU:OE1	2.21	0.40
1:A:176:THR:HG21	6:A:1143:HOH:O	2.22	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	689/691 (100%)	611 (89%)	58 (8%)	20 (3%)	4 1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	283	SER
1	A	422	ASP
1	A	625	SER
1	A	637	GLU
1	A	29	VAL
1	A	282	LYS
1	A	678	SER
1	A	28	LYS
1	A	419	GLN
1	A	511	GLU
1	A	521	SER
1	A	293	SER
1	A	4	ARG
1	A	219	SER
1	A	423	PRO
1	A	280	LYS
1	A	418	GLN
1	A	606	VAL
1	A	260	VAL

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	568/574 (99%)	513 (90%)	55 (10%)	8 4

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	SER
1	A	11	VAL
1	A	24	ARG
1	A	25	ASN
1	A	27	ARG
1	A	30	ARG

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Mol	Chain	Res	Type
1	A	34	VAL
1	A	37	LEU
1	A	53	ARG
1	A	58	THR
1	A	59	LEU
1	A	71	PRO
1	A	84	THR
1	A	86	ARG
1	A	107	ASN
1	A	110	GLN
1	A	121	ARG
1	A	139	THR
1	A	149	VAL
1	A	168	ASN
1	A	171	ARG
1	A	181	CYS
1	A	218	LEU
1	A	220	ASP
1	A	221	GLU
1	A	223	GLU
1	A	240	ASP
1	A	241	LYS
1	A	270	LEU
1	A	271	LEU
1	A	281	ASP
1	A	282	LYS
1	A	301	LYS
1	A	332	ARG
1	A	356	ARG
1	A	422	ASP
1	A	436	LEU
1	A	446	THR
1	A	447	SER
1	A	448	LEU
1	A	451	ASN
1	A	463	VAL
1	A	465	ARG
1	A	518	VAL
1	A	587	ARG
1	A	593	MET
1	A	599	VAL
1	A	614	LEU

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Mol	Chain	Res	Type
1	A	622	ARG
1	A	628	PRO
1	A	637	GLU
1	A	641	LEU
1	A	658	THR
1	A	689	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	25	ASN
1	A	47	GLN
1	A	105	GLN
1	A	107	ASN
1	A	110	GLN
1	A	168	ASN
1	A	186	GLN
1	A	261	ASN
1	A	330	ASN
1	A	353	GLN
1	A	360	GLN
1	A	426	ASN
1	A	502	ASN
1	A	552	GLN
1	A	644	ASN
1	A	666	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	OXL	A	696	3	5,5,5	0.68	0	6,6,6	2.84	2 (33%)
2	NAG	A	990	1	14,14,15	2.25	4 (28%)	17,19,21	5.68	9 (52%)
4	CO3	A	695	3	2,3,3	0.20	0	2,3,3	2.71	1 (50%)

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
5	OXL	A	696	3	-	0/4/4/4	-
2	NAG	A	990	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	990	NAG	O5-C5	-5.42	1.32	1.43
2	A	990	NAG	C2-N2	-3.98	1.39	1.46
2	A	990	NAG	C4-C5	2.90	1.59	1.53
2	A	990	NAG	C8-C7	-2.75	1.44	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	990	NAG	C2-N2-C7	21.15	153.02	122.90
5	A	696	OXL	O4-C2-O2	5.65	136.54	123.61
2	A	990	NAG	C1-O5-C5	5.55	119.71	112.19
2	A	990	NAG	O5-C5-C6	4.09	113.62	107.20
4	A	695	CO3	O3-C-O1	3.81	129.44	119.55
2	A	990	NAG	C3-C4-C5	3.75	116.93	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	696	OXL	O2-C2-C1	-3.27	110.29	120.78
2	A	990	NAG	O6-C6-C5	3.24	122.42	111.29
2	A	990	NAG	O3-C3-C2	2.80	115.26	109.47
2	A	990	NAG	C6-C5-C4	-2.47	107.22	113.00
2	A	990	NAG	O5-C1-C2	-2.34	107.60	111.29
2	A	990	NAG	C8-C7-N2	2.05	119.57	116.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	990	NAG	C3-C2-N2-C7
2	A	990	NAG	C8-C7-N2-C2
2	A	990	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	696	OXL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	691/691 (100%)	-0.10	17 (2%) 57 56	19, 37, 66, 96	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ARG	7.1
1	A	1	GLY	6.5
1	A	3	ARG	6.1
1	A	420	SER	5.7
1	A	421	SER	4.2
1	A	418	GLN	3.6
1	A	86	ARG	3.5
1	A	679	THR	3.3
1	A	422	ASP	3.2
1	A	423	PRO	2.9
1	A	397	GLY	2.6
1	A	4	ARG	2.6
1	A	283	SER	2.5
1	A	419	GLN	2.4
1	A	27	ARG	2.2
1	A	220	ASP	2.1
1	A	24	ARG	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 monosaccharides 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(Å^2)	Q<0.9
2	NAG	A	990	14/15	0.73	0.31	90,96,98,98	0
4	CO3	A	695	4/4	0.95	0.29	26,29,30,34	0
5	OXL	A	696	6/6	0.97	0.13	17,17,21,24	0
3	CU	A	693	1/1	0.98	0.10	34,34,34,34	0
3	CU	A	694	1/1	0.98	0.07	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.