



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:56 PM UTC

PDB ID : 2W48 / pdb_00002w48
Title : Crystal structure of the Full-length Sorbitol Operon Regulator SorC from *Klebsiella pneumoniae*
Authors : de Sanctis, D.; McVey, C.E.; Enguita, F.J.; Carrondo, M.A.
Deposited on : 2008-11-21
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

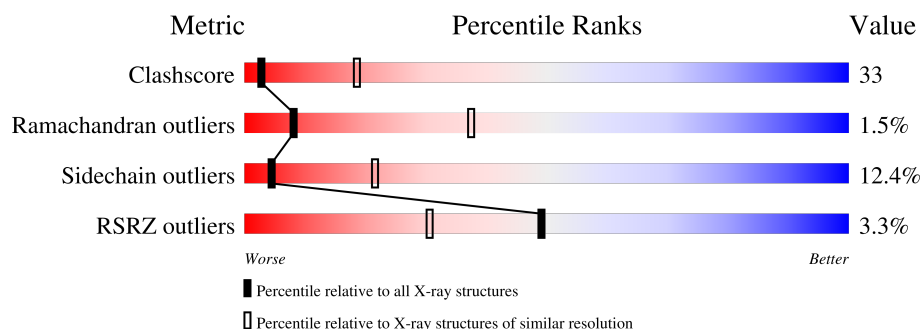
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	315	0% 47% 40% 10% ..
1	B	315	2% 51% 37% 10% ..
1	C	315	7% 49% 38% 7% 5%
1	D	315	3% 52% 33% 11% ..

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
3	MPD	A	1317	-	-	X	-

2 Entry composition [i](#)

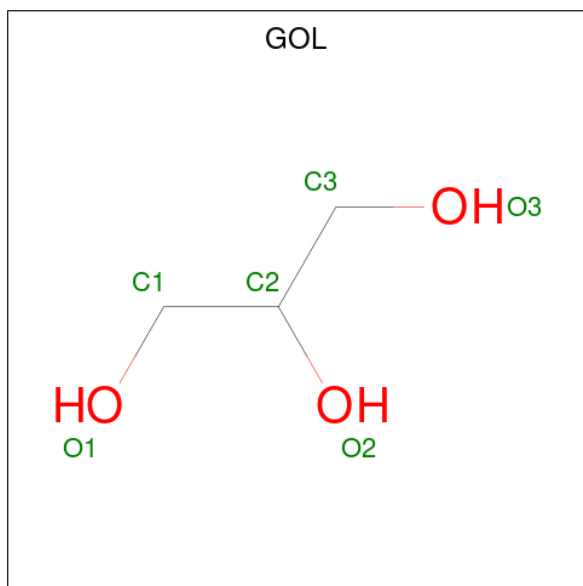
There are 6 unique types of molecules in this entry. The entry contains 9626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SORBITOL OPERON REGULATOR.

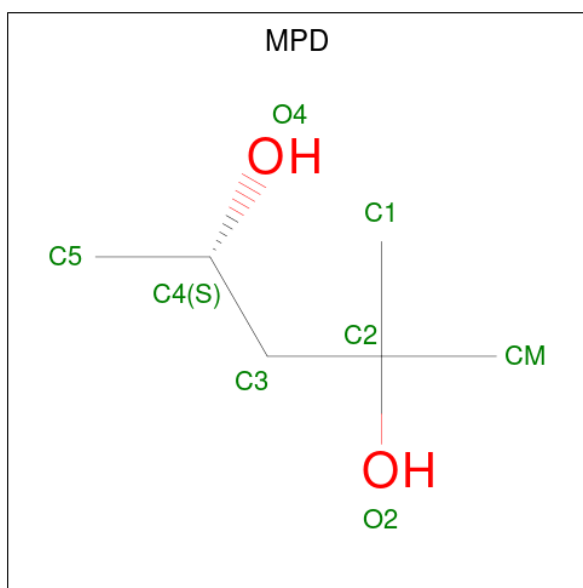
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2408	1514	429	456	9			
1	B	313	Total	C	N	O	S	0	0	0
			2443	1534	435	465	9			
1	C	299	Total	C	N	O	S	0	0	0
			2337	1472	417	439	9			
1	D	308	Total	C	N	O	S	0	0	0
			2408	1514	429	457	8			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).

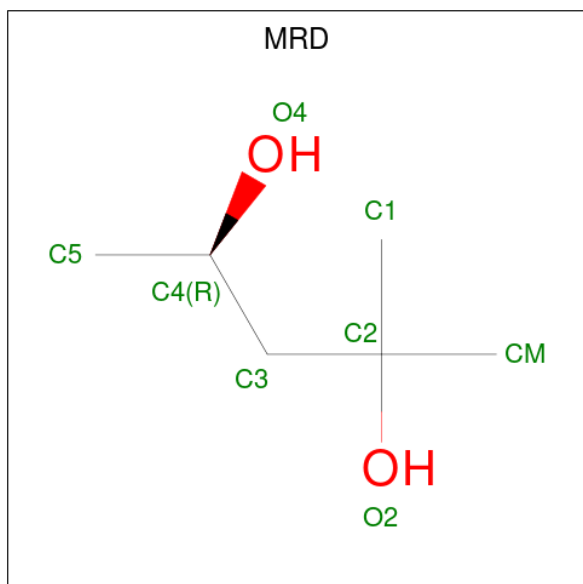


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

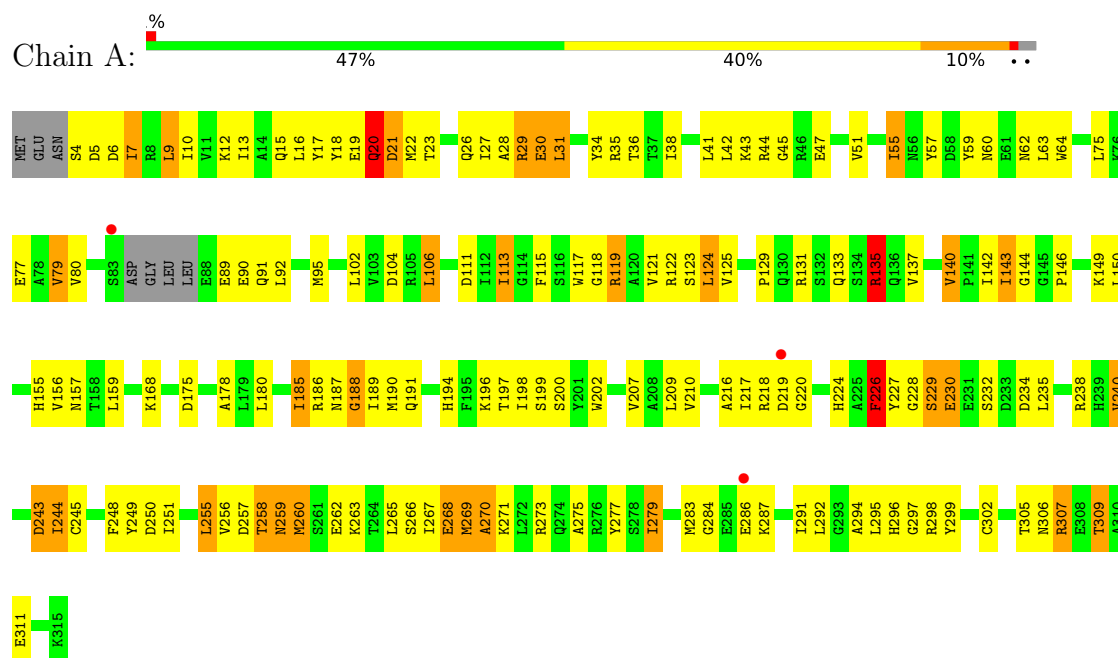
- Molecule 6 is water.

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

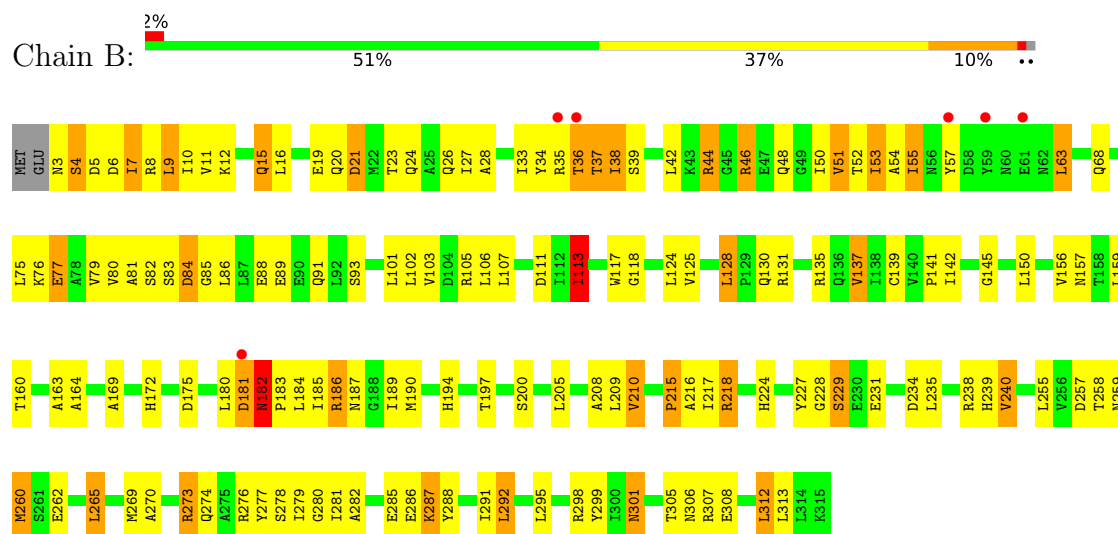
3 Residue-property plots

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.

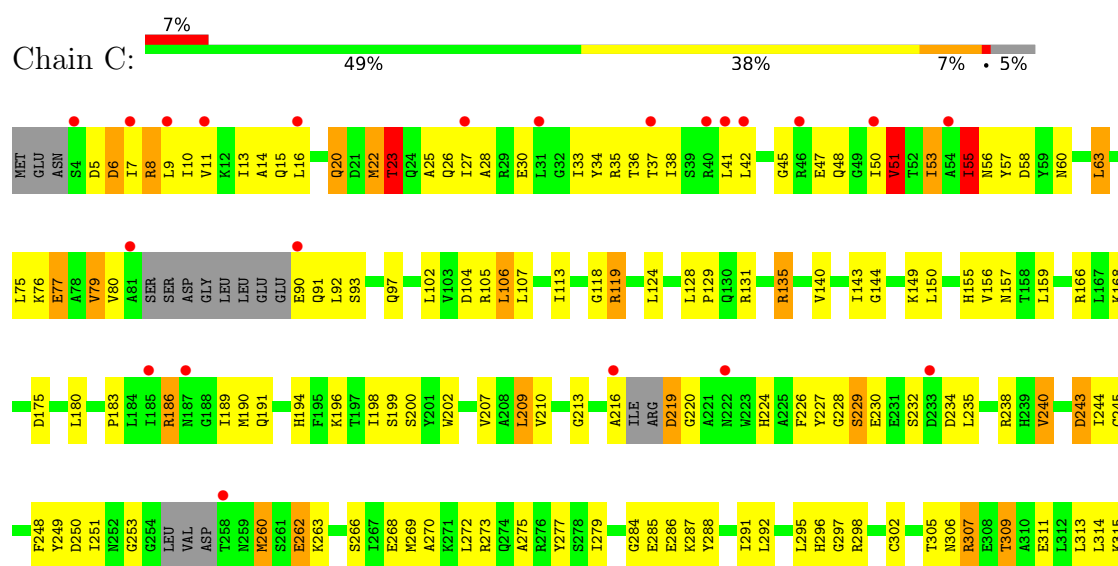
• Molecule 1: SORBITOL OPERON REGULATOR



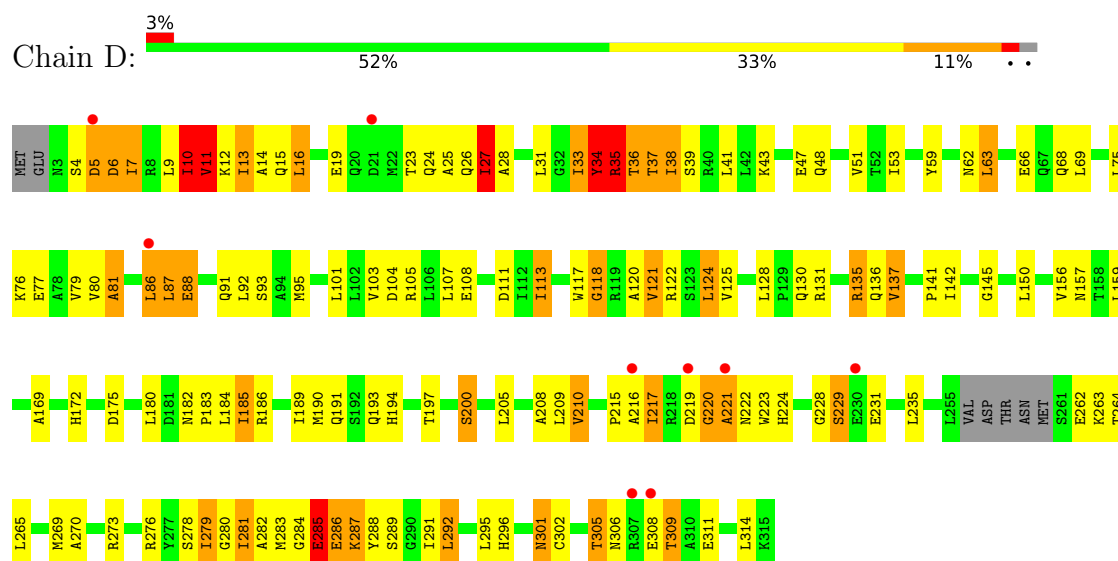
• Molecule 1: SORBITOL OPERON REGULATOR



• Molecule 1: SORBITOL OPERON REGULATOR



• Molecule 1: SORBITOL OPERON REGULATOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.67Å 113.33Å 184.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.67 – 3.20 38.67 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.67-3.20) 99.9 (38.67-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.244 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9626	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, CL, MPD, GOL

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	1.02	1/2447 (0.0%)	1.14	24/3303 (0.7%)
1	B	0.97	6/2483 (0.2%)	1.10	19/3353 (0.6%)
1	C	0.68	2/2374 (0.1%)	0.98	8/3202 (0.2%)
1	D	1.00	3/2447 (0.1%)	1.18	23/3303 (0.7%)
All	All	0.93	12/9751 (0.1%)	1.10	74/13161 (0.6%)

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	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	VAL	CA-CB	-7.61	1.46	1.54
1	B	278	SER	CA-C	-7.24	1.44	1.52
1	C	55	ILE	CA-CB	-6.75	1.46	1.54
1	C	51	VAL	N-CA	6.47	1.54	1.46
1	B	282	ALA	CA-CB	-5.92	1.44	1.53
1	A	244	ILE	CA-CB	-5.75	1.46	1.54
1	B	270	ALA	CA-CB	-5.68	1.44	1.53
1	B	279	ILE	CA-C	-5.46	1.45	1.52
1	D	121	VAL	CA-CB	-5.29	1.47	1.54
1	D	282	ALA	CA-CB	-5.24	1.45	1.53
1	B	186	ARG	C-O	-5.19	1.18	1.24
1	D	81	ALA	CA-CB	-5.16	1.45	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ALA	N-CA-C	-15.05	94.87	111.28
1	A	89	GLU	N-CA-C	-13.50	97.74	114.75
1	D	220	GLY	N-CA-C	-12.44	97.81	112.73
1	D	286	GLU	N-CA-C	-12.06	97.33	112.88
1	D	10	ILE	CB-CA-C	-11.63	96.44	112.14
1	A	260	MET	N-CA-C	-10.60	99.89	112.92
1	D	36	THR	N-CA-C	-10.42	99.72	111.71
1	D	88	GLU	N-CA-C	9.67	121.82	111.28
1	A	268	GLU	N-CA-C	-9.01	98.91	110.53
1	D	27	ILE	CB-CA-C	-8.70	100.40	112.14
1	D	118	GLY	N-CA-C	8.46	119.98	111.95
1	D	278	SER	N-CA-C	-8.43	94.66	108.41
1	B	118	GLY	N-CA-C	8.18	120.38	112.04
1	B	279	ILE	N-CA-C	8.13	119.59	107.80
1	B	15	GLN	CA-C-N	-7.82	110.28	120.44
1	B	15	GLN	C-N-CA	-7.82	110.28	120.44
1	C	135	ARG	NE-CZ-NH2	7.71	126.14	119.20
1	B	105	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	D	4	SER	N-CA-C	7.57	121.88	110.14
1	C	135	ARG	NE-CZ-NH1	-7.41	114.09	121.50
1	B	105	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	C	119	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	B	273	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	D	35	ARG	N-CA-C	6.96	125.61	110.80
1	B	55	ILE	CB-CA-C	-6.92	100.86	110.96
1	C	119	ARG	NE-CZ-NH1	-6.91	114.59	121.50
1	D	87	LEU	N-CA-C	-6.71	99.09	109.76
1	D	38	ILE	CB-CA-C	-6.51	103.63	111.97
1	B	145	GLY	CA-C-N	6.48	126.11	119.56
1	B	145	GLY	C-N-CA	6.48	126.11	119.56
1	A	118	GLY	N-CA-C	6.37	120.04	112.33
1	D	37	THR	N-CA-C	-6.30	104.41	111.28
1	A	135	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	D	11	VAL	CB-CA-C	-6.24	103.72	112.14
1	D	279	ILE	N-CA-CB	-6.22	104.06	111.90
1	B	273	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	D	145	GLY	CA-C-N	6.07	125.69	119.56
1	D	145	GLY	C-N-CA	6.07	125.69	119.56
1	C	118	GLY	N-CA-C	6.07	119.68	112.33
1	D	191	GLN	N-CA-C	5.96	118.73	111.82
1	A	135	ARG	CD-NE-CZ	5.93	132.70	124.40
1	B	182	ASN	CA-C-N	5.92	125.46	119.19
1	B	182	ASN	C-N-CA	5.92	125.46	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	125	VAL	CB-CA-C	-5.83	104.17	112.22
1	A	135	ARG	NE-CZ-NH1	5.81	127.31	121.50
1	A	20	GLN	N-CA-C	-5.80	104.76	112.94
1	D	105	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	C	135	ARG	CD-NE-CZ	5.72	132.41	124.40
1	B	279	ILE	CB-CA-C	-5.68	102.67	110.96
1	B	105	ARG	CD-NE-CZ	5.63	132.29	124.40
1	A	90	GLU	N-CA-C	-5.63	105.67	112.54
1	A	140	VAL	CA-C-N	5.51	125.94	119.99
1	A	140	VAL	C-N-CA	5.51	125.94	119.99
1	A	90	GLU	CA-C-N	-5.48	112.44	121.92
1	A	90	GLU	C-N-CA	-5.48	112.44	121.92
1	A	119	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	A	257	ASP	N-CA-C	-5.38	102.42	110.23
1	D	273	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	226	PHE	N-CA-C	5.32	116.89	111.14
1	A	91	GLN	CB-CA-C	5.32	118.97	109.29
1	B	273	ARG	CD-NE-CZ	5.31	131.84	124.40
1	A	269	MET	CA-CB-CG	-5.29	103.53	114.10
1	A	279	ILE	N-CA-C	5.26	114.87	106.88
1	C	55	ILE	CB-CA-C	-5.25	102.86	110.63
1	B	113	ILE	CB-CA-C	-5.22	104.44	110.91
1	A	119	ARG	CD-NE-CZ	5.16	131.62	124.40
1	C	119	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	185	ILE	CB-CA-C	-5.12	105.16	112.22
1	A	188	GLY	N-CA-C	-5.10	106.58	112.50
1	B	38	ILE	CB-CA-C	-5.09	105.27	112.14
1	D	34	TYR	O-C-N	-5.06	115.85	122.59
1	D	273	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	278	SER	N-CA-C	-5.02	99.08	108.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ARG	Sidechain

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	2408	0	2401	167	0
1	B	2443	0	2433	160	4
1	C	2337	0	2334	179	0
1	D	2408	0	2401	159	4
2	A	6	0	8	0	0
2	D	6	0	8	3	0
3	A	8	0	14	7	0
4	A	1	0	0	0	0
5	B	8	0	14	4	0
6	A	1	0	0	0	0
All	All	9626	0	9613	634	4

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 33.

All (634) 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:B:55:ILE:HA	1:C:51:VAL:CG2	1.32	1.51
1:A:124:LEU:C	1:A:124:LEU:HD23	1.49	1.32
1:B:4:SER:CB	1:B:5:ASP:HA	1.48	1.30
1:A:227:TYR:CD2	1:A:260:MET:HE1	1.67	1.27
1:B:44:ARG:NH1	1:B:48:GLN:OE1	1.69	1.26
1:C:28:ALA:CB	1:C:35:ARG:HG2	1.67	1.23
1:D:33:ILE:CG2	1:D:38:ILE:HD11	1.69	1.21
1:D:33:ILE:HG21	1:D:38:ILE:CD1	1.69	1.20
1:C:47:GLU:HB3	1:C:48:GLN:OE1	1.31	1.20
1:B:19:GLU:OE1	1:C:57:TYR:OH	1.59	1.17
1:B:4:SER:HB3	1:B:5:ASP:CA	1.72	1.17
1:C:76:LYS:O	1:C:77:GLU:HG2	1.44	1.17
1:A:124:LEU:HD23	1:A:124:LEU:O	1.42	1.16
1:B:55:ILE:CA	1:C:51:VAL:HG23	1.75	1.16
1:C:284:GLY:H	1:C:309:THR:HG21	1.08	1.16
1:A:31:LEU:HD12	1:A:31:LEU:H	1.02	1.15
1:D:35:ARG:CA	1:D:38:ILE:HG12	1.74	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:CA	1:C:51:VAL:CG2	2.25	1.14
1:D:35:ARG:HA	1:D:38:ILE:CG1	1.77	1.12
1:A:284:GLY:H	1:A:309:THR:HG21	1.07	1.12
1:B:53:ILE:HG22	1:C:53:ILE:CB	1.82	1.10
1:B:53:ILE:HG22	1:C:53:ILE:HB	1.29	1.10
1:A:31:LEU:HD12	1:A:31:LEU:N	1.56	1.10
1:A:258:THR:O	1:A:259:ASN:HB3	1.47	1.09
1:B:53:ILE:HG22	1:C:53:ILE:CG2	1.80	1.09
1:A:31:LEU:H	1:A:31:LEU:CD1	1.62	1.08
1:C:53:ILE:HD13	1:C:53:ILE:O	1.53	1.08
1:D:33:ILE:HG22	1:D:35:ARG:H	1.19	1.08
1:B:84:ASP:HB3	1:B:307:ARG:NH2	1.68	1.07
1:C:227:TYR:CD2	1:C:260:MET:HE1	1.88	1.07
1:C:76:LYS:C	1:C:77:GLU:HG2	1.76	1.06
1:A:227:TYR:CD2	1:A:260:MET:CE	2.37	1.06
1:C:28:ALA:HB2	1:C:35:ARG:HG2	1.31	1.06
1:D:284:GLY:O	1:D:285:GLU:HB3	1.56	1.06
1:D:186:ARG:NE	1:D:264:THR:O	1.89	1.05
1:D:186:ARG:HD2	1:D:263:LYS:C	1.82	1.04
1:C:186:ARG:NH1	1:C:190:MET:SD	2.30	1.04
1:A:121:VAL:HG13	1:A:209:LEU:CD2	1.89	1.01
1:B:53:ILE:HD12	1:B:53:ILE:O	1.60	1.01
1:A:124:LEU:C	1:A:124:LEU:CD2	2.30	1.01
1:D:33:ILE:HG21	1:D:38:ILE:HD11	1.32	1.01
1:B:54:ALA:O	1:C:51:VAL:HG22	1.61	1.00
1:D:269:MET:HE2	1:D:269:MET:HA	1.42	1.00
1:C:28:ALA:CB	1:C:35:ARG:CG	2.41	0.99
1:B:55:ILE:HA	1:C:51:VAL:HG22	1.42	0.97
1:C:25:ALA:HA	1:C:35:ARG:CD	1.95	0.96
1:C:186:ARG:CG	1:C:186:ARG:HH11	1.79	0.95
1:B:53:ILE:CG2	1:C:53:ILE:HB	1.97	0.94
1:D:33:ILE:HG21	1:D:38:ILE:HD13	1.49	0.93
1:A:283:MET:HE3	1:A:306:ASN:ND2	1.83	0.92
1:C:186:ARG:HH11	1:C:186:ARG:HG2	1.34	0.92
1:A:227:TYR:CE2	1:A:260:MET:HE1	2.03	0.92
1:B:269:MET:HE3	1:B:299:TYR:CD2	2.05	0.92
1:C:22:MET:HG2	1:C:26:GLN:HB3	1.52	0.91
1:B:238:ARG:O	1:B:239:HIS:HB2	1.71	0.90
1:D:182:ASN:OD1	1:D:184:LEU:N	2.03	0.90
1:A:186:ARG:HD2	1:A:262:GLU:O	1.69	0.90
1:D:23:THR:O	1:D:27:ILE:HG13	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ASN:OD1	1:D:183:PRO:N	2.05	0.90
1:D:215:PRO:HG3	1:D:223:TRP:CZ3	2.07	0.89
1:B:84:ASP:HB3	1:B:307:ARG:HH22	1.28	0.89
1:B:55:ILE:HA	1:C:51:VAL:HG23	0.88	0.88
1:D:23:THR:HG22	1:D:25:ALA:H	1.38	0.88
1:B:4:SER:CB	1:B:5:ASP:CA	2.36	0.88
1:A:306:ASN:OD1	1:A:309:THR:HG23	1.74	0.88
1:C:28:ALA:HB3	1:C:35:ARG:HG2	1.56	0.87
1:C:288:TYR:CE1	1:C:313:LEU:HD23	2.10	0.87
1:C:186:ARG:HD2	1:C:263:LYS:HA	1.54	0.87
1:B:285:GLU:HG2	1:B:312:LEU:CD2	2.05	0.86
1:A:186:ARG:HH11	1:A:187:ASN:ND2	1.73	0.86
1:C:285:GLU:HG3	1:C:286:GLU:OE2	1.76	0.86
1:C:155:HIS:HD2	1:C:157:ASN:H	1.20	0.85
1:D:118:GLY:HA3	2:D:1316:GOL:H31	1.57	0.85
1:A:146:PRO:HA	3:A:1317:MPD:HM1	1.58	0.85
1:A:284:GLY:N	1:A:309:THR:HG21	1.91	0.84
1:B:186:ARG:NH1	1:B:190:MET:SD	2.50	0.84
1:D:33:ILE:CG2	1:D:38:ILE:CD1	2.36	0.84
1:A:155:HIS:HD2	1:A:157:ASN:H	1.24	0.84
1:A:186:ARG:HH11	1:A:187:ASN:HD21	1.24	0.84
1:D:33:ILE:HG22	1:D:38:ILE:HD11	1.56	0.83
1:A:23:THR:CG2	1:A:26:GLN:HG3	2.09	0.83
1:B:85:GLY:C	1:B:86:LEU:HD12	2.03	0.83
1:C:25:ALA:HA	1:C:35:ARG:HD3	1.58	0.83
1:A:235:LEU:O	1:A:240:VAL:HG23	1.79	0.83
1:D:35:ARG:HA	1:D:38:ILE:HG12	0.88	0.82
1:C:186:ARG:CD	1:C:262:GLU:O	2.28	0.82
1:C:306:ASN:OD1	1:C:309:THR:HG23	1.78	0.82
1:A:30:GLU:HB3	1:A:31:LEU:HD12	1.62	0.82
1:C:47:GLU:CB	1:C:48:GLN:OE1	2.23	0.82
1:B:285:GLU:HG2	1:B:312:LEU:HD21	1.61	0.81
1:C:180:LEU:HD13	1:C:186:ARG:HB2	1.61	0.81
1:A:121:VAL:HG13	1:A:209:LEU:HD23	1.60	0.81
1:A:27:ILE:O	1:A:31:LEU:HD13	1.81	0.80
1:D:217:ILE:HG23	1:D:219:ASP:H	1.46	0.80
1:D:284:GLY:O	1:D:285:GLU:CB	2.30	0.80
1:C:51:VAL:CG1	1:C:51:VAL:O	2.30	0.80
1:C:284:GLY:N	1:C:309:THR:HG21	1.93	0.79
1:B:53:ILE:O	1:B:53:ILE:CD1	2.30	0.79
1:C:53:ILE:O	1:C:53:ILE:CD1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:HIS:CD2	1:C:157:ASN:H	2.01	0.79
1:D:11:VAL:HG12	1:D:12:LYS:N	1.96	0.79
1:D:34:TYR:O	1:D:35:ARG:HB3	1.83	0.79
1:D:23:THR:HB	1:D:26:GLN:HG3	1.65	0.78
1:A:284:GLY:H	1:A:309:THR:CG2	1.94	0.78
1:C:25:ALA:HA	1:C:35:ARG:HD2	1.64	0.78
1:C:284:GLY:H	1:C:309:THR:CG2	1.94	0.78
1:A:216:ALA:HB3	1:A:286:GLU:O	1.84	0.78
1:C:307:ARG:HG3	1:C:307:ARG:HH11	1.48	0.78
1:D:135:ARG:O	1:D:136:GLN:HB2	1.83	0.78
1:B:76:LYS:C	1:B:77:GLU:HG2	2.06	0.78
1:D:33:ILE:HG22	1:D:35:ARG:N	1.99	0.77
1:D:186:ARG:HE	1:D:264:THR:C	1.91	0.76
1:D:5:ASP:C	1:D:7:ILE:H	1.92	0.76
1:C:10:ILE:HA	1:C:13:ILE:HG22	1.67	0.76
1:C:235:LEU:O	1:C:240:VAL:HG23	1.84	0.76
1:B:4:SER:HB3	1:B:5:ASP:HA	0.78	0.76
1:A:155:HIS:CD2	1:A:157:ASN:H	2.03	0.76
1:C:10:ILE:HG12	1:C:41:LEU:HB3	1.67	0.76
1:B:53:ILE:HG22	1:C:53:ILE:HG21	1.68	0.76
1:A:259:ASN:OD1	1:A:259:ASN:C	2.30	0.75
1:D:6:ASP:OD1	1:D:6:ASP:C	2.30	0.75
1:D:185:ILE:HD13	1:D:185:ILE:N	2.01	0.75
1:A:269:MET:O	1:A:273:ARG:HG3	1.85	0.75
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.50	0.75
1:D:23:THR:HG22	1:D:25:ALA:N	2.01	0.75
1:A:27:ILE:HG22	1:A:38:ILE:HD12	1.69	0.74
1:D:182:ASN:OD1	1:D:182:ASN:C	2.29	0.74
1:C:56:ASN:OD1	1:C:56:ASN:C	2.30	0.74
1:D:186:ARG:HD3	1:D:262:GLU:O	1.87	0.74
1:B:23:THR:H	1:B:26:GLN:HE21	1.33	0.74
1:C:51:VAL:O	1:C:51:VAL:HG12	1.87	0.73
1:D:16:LEU:HD12	1:D:27:ILE:HG23	1.68	0.73
1:A:19:GLU:C	1:A:20:GLN:OE1	2.31	0.73
1:C:104:ASP:OD2	1:C:129:PRO:HG2	1.89	0.73
1:C:224:HIS:CE1	1:C:229:SER:HB3	2.24	0.73
1:A:175:ASP:H	1:A:194:HIS:HE1	1.36	0.73
1:C:5:ASP:O	1:C:8:ARG:HG3	1.89	0.73
1:A:243:ASP:OD1	1:A:243:ASP:C	2.29	0.72
1:A:121:VAL:HG13	1:A:209:LEU:HD21	1.72	0.72
1:A:104:ASP:OD2	1:A:129:PRO:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:MET:HA	1:C:269:MET:HE2	1.72	0.71
1:B:227:TYR:CG	1:B:260:MET:HE1	2.24	0.71
1:B:103:VAL:HG21	1:B:124:LEU:HD21	1.72	0.71
1:A:292:LEU:HD22	1:A:296:HIS:CE1	2.26	0.71
1:C:90:GLU:OE2	1:C:90:GLU:HA	1.91	0.71
1:B:51:VAL:CG2	1:B:51:VAL:O	2.39	0.70
1:B:55:ILE:HG12	1:C:51:VAL:HG21	1.73	0.70
1:C:234:ASP:O	1:C:238:ARG:HG2	1.91	0.70
1:C:292:LEU:HD22	1:C:296:HIS:CE1	2.25	0.70
1:A:224:HIS:CE1	1:A:229:SER:HB3	2.26	0.70
1:A:121:VAL:CG1	1:A:209:LEU:CD2	2.67	0.69
1:C:285:GLU:CG	1:C:286:GLU:OE2	2.39	0.69
1:D:103:VAL:HG21	1:D:124:LEU:HD21	1.74	0.69
1:A:117:TRP:NE1	3:A:1317:MPD:H12	2.07	0.69
1:D:186:ARG:HD2	1:D:263:LYS:O	1.90	0.69
1:B:182:ASN:OD1	1:B:182:ASN:C	2.35	0.69
1:B:224:HIS:O	1:B:228:GLY:HA2	1.92	0.69
1:C:240:VAL:HG11	1:C:248:PHE:HB3	1.75	0.69
1:A:23:THR:HG22	1:A:26:GLN:OE1	1.93	0.69
1:A:29:ARG:O	1:A:30:GLU:C	2.36	0.69
1:C:91:GLN:HE21	1:C:306:ASN:HD22	1.40	0.69
1:A:234:ASP:O	1:A:238:ARG:HG2	1.92	0.68
1:B:36:THR:HG22	1:B:37:THR:N	2.08	0.68
1:B:238:ARG:O	1:B:239:HIS:CB	2.36	0.68
1:A:258:THR:O	1:A:259:ASN:CB	2.30	0.68
1:D:180:LEU:HD11	1:D:265:LEU:CD1	2.22	0.68
1:A:23:THR:HG23	1:A:26:GLN:HG3	1.75	0.68
1:D:5:ASP:O	1:D:7:ILE:N	2.26	0.68
1:D:220:GLY:O	1:D:222:ASN:N	2.24	0.68
1:D:180:LEU:HD11	1:D:265:LEU:HD11	1.75	0.67
1:B:54:ALA:C	1:C:51:VAL:HG22	2.20	0.66
1:C:55:ILE:HG23	1:C:55:ILE:O	1.95	0.66
1:A:186:ARG:CD	1:A:262:GLU:O	2.42	0.66
1:C:28:ALA:HB3	1:C:35:ARG:CG	2.19	0.66
1:D:186:ARG:CD	1:D:263:LYS:C	2.66	0.66
1:B:80:VAL:HA	1:B:305:THR:O	1.95	0.66
1:D:35:ARG:O	1:D:38:ILE:N	2.29	0.66
1:C:175:ASP:H	1:C:194:HIS:HE1	1.44	0.66
1:A:6:ASP:O	1:A:10:ILE:HG13	1.96	0.66
1:A:60:ASN:HB3	1:A:63:LEU:HB3	1.78	0.66
1:A:20:GLN:OE1	1:A:20:GLN:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:CG1	1:C:51:VAL:HG21	2.26	0.65
1:B:234:ASP:O	1:B:238:ARG:HD2	1.96	0.65
1:B:274:GLN:O	5:B:1316:MRD:H1C1	1.96	0.65
1:A:240:VAL:HG11	1:A:248:PHE:HB3	1.78	0.65
1:D:186:ARG:HD2	1:D:263:LYS:CA	2.26	0.65
1:A:155:HIS:HD2	1:A:157:ASN:N	1.95	0.64
1:B:301:ASN:N	1:B:301:ASN:HD22	1.94	0.64
1:B:23:THR:H	1:B:26:GLN:NE2	1.96	0.64
1:C:48:GLN:OE1	1:C:48:GLN:N	2.30	0.64
1:C:76:LYS:C	1:C:77:GLU:CG	2.61	0.64
1:B:180:LEU:HD11	1:B:265:LEU:HD22	1.78	0.64
1:B:276:ARG:N	5:B:1316:MRD:H1C3	2.13	0.64
1:C:131:ARG:O	1:C:168:LYS:HD2	1.97	0.64
1:D:80:VAL:HA	1:D:305:THR:O	1.98	0.64
1:B:24:GLN:HA	1:B:27:ILE:HG22	1.80	0.64
1:B:141:PRO:HD3	1:B:172:HIS:O	1.97	0.64
1:C:180:LEU:HD21	1:C:189:ILE:HD12	1.80	0.64
1:D:35:ARG:CG	1:D:36:THR:N	2.52	0.64
1:A:269:MET:O	1:A:270:ALA:C	2.38	0.64
1:C:307:ARG:HG3	1:C:307:ARG:NH1	2.13	0.64
1:A:20:GLN:O	1:A:21:ASP:C	2.40	0.63
1:D:301:ASN:HD22	1:D:301:ASN:N	1.95	0.63
1:B:7:ILE:C	1:B:7:ILE:HD12	2.22	0.63
1:C:47:GLU:C	1:C:48:GLN:OE1	2.42	0.63
1:A:117:TRP:CE2	3:A:1317:MPD:H12	2.33	0.63
1:C:131:ARG:HG3	1:C:135:ARG:HD3	1.79	0.63
1:A:143:ILE:HD12	1:A:266:SER:HB3	1.80	0.63
1:C:155:HIS:HD2	1:C:157:ASN:N	1.96	0.63
1:D:81:ALA:O	1:D:306:ASN:HA	1.99	0.63
1:B:11:VAL:O	1:B:15:GLN:HG2	1.98	0.63
1:D:215:PRO:HG3	1:D:223:TRP:HZ3	1.61	0.63
1:D:35:ARG:C	1:D:38:ILE:HG12	2.23	0.63
1:A:17:TYR:O	1:A:21:ASP:HA	1.98	0.63
1:C:76:LYS:O	1:C:77:GLU:CG	2.36	0.62
1:A:186:ARG:NH1	1:A:187:ASN:ND2	2.47	0.62
1:A:178:ALA:HB3	3:A:1317:MPD:H32	1.81	0.62
1:B:217:ILE:C	1:B:218:ARG:HG2	2.24	0.62
1:C:216:ALA:HB3	1:C:286:GLU:O	1.99	0.62
1:D:269:MET:HA	1:D:269:MET:CE	2.26	0.62
1:B:3:ASN:C	1:B:3:ASN:OD1	2.43	0.62
1:C:143:ILE:HD12	1:C:266:SER:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:HE2	1:C:15:GLN:HE21	1.47	0.62
1:A:29:ARG:HG2	1:A:30:GLU:N	2.12	0.62
1:C:155:HIS:HE1	1:D:175:ASP:OD1	1.83	0.62
1:A:180:LEU:HD21	1:A:189:ILE:HD12	1.80	0.61
1:C:16:LEU:HA	1:C:20:GLN:HG2	1.82	0.61
1:D:34:TYR:O	1:D:35:ARG:CB	2.40	0.61
1:A:30:GLU:HB3	1:A:31:LEU:CD1	2.29	0.61
1:B:107:LEU:HD23	1:B:137:VAL:HG11	1.83	0.61
1:A:62:ASN:O	1:A:63:LEU:C	2.43	0.61
1:B:4:SER:HB2	1:B:5:ASP:HA	1.72	0.61
1:C:227:TYR:HD2	1:C:260:MET:HE1	1.56	0.61
1:D:186:ARG:CZ	1:D:264:THR:O	2.48	0.61
1:C:50:ILE:O	1:C:50:ILE:HG22	2.00	0.61
1:A:55:ILE:HD13	1:A:57:TYR:CZ	2.36	0.61
1:A:15:GLN:O	1:A:19:GLU:HB2	2.00	0.60
1:B:183:PRO:O	1:B:187:ASN:OD1	2.19	0.60
1:B:276:ARG:H	5:B:1316:MRD:H1C3	1.66	0.60
1:D:107:LEU:HD23	1:D:137:VAL:HG11	1.81	0.60
1:C:124:LEU:HD22	1:C:209:LEU:HD21	1.81	0.60
1:D:141:PRO:HD3	1:D:172:HIS:O	2.01	0.60
1:A:307:ARG:HG3	1:A:307:ARG:NH1	2.16	0.60
1:D:23:THR:HG22	1:D:24:GLN:N	2.15	0.60
1:B:86:LEU:HB2	1:B:91:GLN:NE2	2.17	0.60
1:D:111:ASP:OD2	1:D:276:ARG:NH2	2.35	0.60
1:D:35:ARG:O	1:D:38:ILE:HB	2.03	0.59
1:C:227:TYR:CD2	1:C:260:MET:CE	2.76	0.59
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.67	0.59
1:B:285:GLU:HG3	1:B:308:GLU:OE2	2.02	0.59
1:D:135:ARG:O	1:D:136:GLN:CB	2.49	0.59
1:B:44:ARG:HH11	1:B:48:GLN:CD	2.09	0.59
1:C:60:ASN:CG	1:C:63:LEU:HB2	2.28	0.59
1:C:5:ASP:C	1:C:7:ILE:H	2.11	0.58
1:D:175:ASP:H	1:D:194:HIS:HE1	1.51	0.58
1:B:180:LEU:HD22	1:B:185:ILE:HG22	1.85	0.58
1:B:215:PRO:C	1:B:217:ILE:H	2.11	0.58
1:C:15:GLN:HG2	1:C:16:LEU:HD12	1.86	0.58
1:C:240:VAL:CG1	1:C:248:PHE:HB3	2.33	0.58
1:A:186:ARG:O	1:A:186:ARG:HG2	1.99	0.58
1:B:23:THR:O	1:B:27:ILE:HB	2.04	0.58
1:D:23:THR:CG2	1:D:24:GLN:N	2.67	0.58
1:D:269:MET:O	1:D:270:ALA:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HG12	1:A:268:GLU:O	2.04	0.57
1:B:76:LYS:O	1:B:77:GLU:HG2	2.03	0.57
1:D:9:LEU:O	1:D:13:ILE:HG23	2.03	0.57
1:A:227:TYR:CD2	1:A:260:MET:HE3	2.36	0.57
1:A:79:VAL:CG1	1:A:102:LEU:HD22	2.34	0.57
1:C:106:LEU:HG	1:C:277:TYR:CE2	2.40	0.57
1:B:240:VAL:O	1:B:240:VAL:HG23	2.04	0.57
1:A:106:LEU:HG	1:A:277:TYR:CE2	2.40	0.57
1:C:10:ILE:HA	1:C:13:ILE:CG2	2.33	0.57
1:D:38:ILE:HD13	1:D:38:ILE:N	2.20	0.57
1:C:5:ASP:O	1:C:8:ARG:CG	2.53	0.57
1:C:186:ARG:HD2	1:C:262:GLU:O	2.04	0.57
1:B:197:THR:O	1:B:200:SER:HB3	2.05	0.56
1:C:269:MET:O	1:C:270:ALA:C	2.48	0.56
1:D:220:GLY:C	1:D:222:ASN:H	2.11	0.56
1:A:258:THR:O	1:A:258:THR:HG23	1.98	0.56
1:C:79:VAL:CG1	1:C:102:LEU:HD22	2.35	0.56
1:D:122:ARG:HA	1:D:159:LEU:HD22	1.86	0.56
1:D:283:MET:HE3	1:D:306:ASN:ND2	2.21	0.56
1:A:122:ARG:HB2	1:A:159:LEU:HD21	1.86	0.56
1:C:45:GLY:HA2	1:C:50:ILE:HD12	1.88	0.56
1:C:186:ARG:NH1	1:C:186:ARG:HG2	2.13	0.56
1:D:283:MET:HE3	1:D:306:ASN:HD21	1.70	0.56
1:D:35:ARG:C	1:D:38:ILE:H	2.14	0.56
1:B:15:GLN:O	1:B:19:GLU:HB2	2.07	0.55
1:C:124:LEU:HD13	1:C:209:LEU:HD11	1.87	0.55
1:C:288:TYR:HE1	1:C:313:LEU:HD23	1.66	0.55
1:B:16:LEU:HD23	1:B:16:LEU:N	2.20	0.55
1:C:13:ILE:HD11	1:C:38:ILE:HG23	1.89	0.55
1:D:35:ARG:O	1:D:38:ILE:CB	2.55	0.55
1:D:104:ASP:O	1:D:135:ARG:NH2	2.40	0.55
1:A:240:VAL:CG1	1:A:248:PHE:HB3	2.36	0.55
1:A:273:ARG:C	1:A:275:ALA:H	2.14	0.55
1:B:287:LYS:O	1:B:291:ILE:HG13	2.07	0.55
1:C:13:ILE:HG23	1:C:14:ALA:N	2.21	0.54
1:D:11:VAL:O	1:D:14:ALA:HB3	2.06	0.54
1:A:122:ARG:HA	1:A:159:LEU:HD22	1.89	0.54
1:A:131:ARG:O	1:A:168:LYS:HD2	2.07	0.54
1:A:4:SER:OG	1:A:5:ASP:N	2.38	0.54
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.23	0.54
1:A:143:ILE:HG13	1:A:144:GLY:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HB	1:A:269:MET:HE1	1.90	0.54
1:C:33:ILE:HG22	1:C:37:THR:OG1	2.08	0.54
1:B:51:VAL:O	1:B:51:VAL:HG23	2.03	0.54
1:B:175:ASP:H	1:B:194:HIS:HE1	1.56	0.54
1:C:287:LYS:O	1:C:291:ILE:HG13	2.06	0.54
1:B:301:ASN:N	1:B:301:ASN:ND2	2.55	0.54
1:C:10:ILE:CA	1:C:13:ILE:HG22	2.36	0.54
1:C:10:ILE:CG1	1:C:41:LEU:HD22	2.38	0.54
1:C:273:ARG:C	1:C:275:ALA:H	2.13	0.54
1:A:31:LEU:N	1:A:31:LEU:CD1	2.30	0.54
1:A:191:GLN:O	1:A:196:LYS:HE2	2.07	0.54
1:B:53:ILE:HA	1:C:53:ILE:HB	1.88	0.54
1:B:238:ARG:NH1	1:B:257:ASP:O	2.40	0.54
1:A:227:TYR:CG	1:A:260:MET:HE1	2.36	0.54
1:C:186:ARG:HD3	1:C:262:GLU:O	2.08	0.54
1:C:28:ALA:CB	1:C:35:ARG:HG3	2.36	0.53
1:D:15:GLN:O	1:D:19:GLU:HB2	2.07	0.53
1:D:193:GLN:HA	1:D:193:GLN:NE2	2.24	0.53
1:A:186:ARG:NH1	1:A:187:ASN:HD21	1.99	0.53
1:B:10:ILE:HD13	1:B:44:ARG:HD2	1.90	0.53
1:A:227:TYR:CE2	1:A:260:MET:CE	2.79	0.53
1:B:34:TYR:HB2	1:B:37:THR:HB	1.89	0.53
1:B:15:GLN:O	1:B:16:LEU:C	2.43	0.53
1:B:83:SER:HA	1:B:86:LEU:HD13	1.90	0.53
1:D:301:ASN:N	1:D:301:ASN:ND2	2.56	0.53
1:A:115:PHE:O	1:A:142:ILE:HG12	2.08	0.53
1:D:219:ASP:O	1:D:220:GLY:C	2.49	0.53
1:D:31:LEU:C	1:D:33:ILE:H	2.16	0.53
1:A:13:ILE:HG22	1:A:42:LEU:HD21	1.90	0.53
1:B:53:ILE:HA	1:C:53:ILE:HA	1.91	0.53
1:B:107:LEU:HD21	1:B:113:ILE:HD11	1.90	0.53
1:D:122:ARG:HB2	1:D:159:LEU:HD21	1.91	0.52
1:A:23:THR:HG22	1:A:26:GLN:HG3	1.87	0.52
1:C:124:LEU:CD2	1:C:209:LEU:HD21	2.40	0.52
1:D:35:ARG:HG2	1:D:36:THR:N	2.23	0.52
1:C:5:ASP:C	1:C:7:ILE:N	2.66	0.52
1:C:143:ILE:HG13	1:C:144:GLY:N	2.24	0.52
1:A:269:MET:C	1:A:271:LYS:N	2.58	0.52
1:C:28:ALA:HB2	1:C:35:ARG:CG	2.19	0.52
1:C:34:TYR:HB3	1:C:36:THR:HG22	1.91	0.52
1:D:43:LYS:O	1:D:47:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:SD	1:A:283:MET:SD	3.08	0.52
1:D:287:LYS:O	1:D:291:ILE:HG13	2.09	0.52
1:B:7:ILE:HA	1:B:10:ILE:HD12	1.92	0.51
1:C:183:PRO:HD3	1:C:263:LYS:HD3	1.91	0.51
1:C:219:ASP:OD1	1:C:220:GLY:N	2.43	0.51
1:D:137:VAL:HG22	1:D:169:ALA:HB2	1.92	0.51
1:B:276:ARG:HG2	1:B:277:TYR:CD2	2.45	0.51
1:D:186:ARG:NH2	1:D:264:THR:O	2.43	0.51
1:A:232:SER:HA	1:A:235:LEU:HG	1.92	0.51
1:B:137:VAL:CG2	1:B:169:ALA:HB2	2.41	0.51
1:C:186:ARG:NE	1:C:262:GLU:O	2.43	0.51
1:B:6:ASP:O	1:B:9:LEU:N	2.38	0.51
1:B:24:GLN:O	1:B:27:ILE:HG22	2.10	0.51
1:A:155:HIS:CD2	1:A:156:VAL:N	2.79	0.51
1:C:22:MET:HG2	1:C:26:GLN:CB	2.33	0.51
1:A:243:ASP:OD1	1:A:243:ASP:O	2.29	0.51
1:C:124:LEU:HD23	1:C:124:LEU:C	2.36	0.51
1:D:130:GLN:C	1:D:130:GLN:HE21	2.19	0.51
1:C:10:ILE:HG12	1:C:41:LEU:HD22	1.93	0.50
1:B:137:VAL:HG22	1:B:169:ALA:HB2	1.92	0.50
1:C:16:LEU:HA	1:C:20:GLN:CG	2.41	0.50
1:D:125:VAL:HA	1:D:128:LEU:HG	1.93	0.50
1:A:42:LEU:O	1:A:43:LYS:C	2.53	0.50
1:A:259:ASN:OD1	1:A:259:ASN:O	2.29	0.50
1:B:3:ASN:OD1	1:B:3:ASN:O	2.30	0.50
1:B:185:ILE:O	1:B:189:ILE:HG13	2.11	0.50
1:A:92:LEU:CD2	1:A:119:ARG:HG2	2.41	0.50
1:C:143:ILE:HD12	1:C:266:SER:CB	2.42	0.50
1:C:186:ARG:HD2	1:C:263:LYS:CA	2.35	0.50
1:A:16:LEU:HD23	1:A:22:MET:SD	2.52	0.50
1:A:18:TYR:CD1	1:D:53:ILE:HD13	2.47	0.50
1:A:43:LYS:O	1:A:47:GLU:HG3	2.11	0.50
1:A:9:LEU:HD12	1:A:13:ILE:HG13	1.94	0.50
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.77	0.50
1:B:3:ASN:O	1:B:4:SER:O	2.29	0.49
1:A:218:ARG:O	1:A:218:ARG:HG2	2.12	0.49
1:B:44:ARG:NH1	1:B:48:GLN:CD	2.60	0.49
1:C:48:GLN:O	1:C:48:GLN:HG2	2.12	0.49
1:A:180:LEU:HD22	1:A:185:ILE:HG22	1.94	0.49
1:A:217:ILE:HD11	1:A:287:LYS:NZ	2.27	0.49
1:A:283:MET:HE3	1:A:306:ASN:HD22	1.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLU:HG3	1:B:89:GLU:N	2.28	0.49
1:C:58:ASP:O	1:C:58:ASP:OD2	2.30	0.49
1:C:273:ARG:C	1:C:275:ALA:N	2.70	0.49
1:A:244:ILE:O	1:A:245:CYS:C	2.50	0.49
1:B:46:ARG:HG2	1:B:46:ARG:NH1	2.27	0.49
1:B:139:CYS:HB3	1:B:160:THR:HG23	1.94	0.49
1:C:16:LEU:HG	1:C:20:GLN:HG3	1.95	0.49
1:D:33:ILE:CG2	1:D:38:ILE:HD13	2.27	0.49
1:D:120:ALA:HB3	2:D:1316:GOL:O3	2.12	0.49
1:B:23:THR:OG1	1:B:26:GLN:HG2	2.11	0.49
1:B:63:LEU:O	1:B:63:LEU:HD12	2.13	0.49
1:D:33:ILE:C	1:D:35:ARG:N	2.70	0.49
1:D:120:ALA:HB1	1:D:281:ILE:HG12	1.95	0.49
1:B:10:ILE:HD13	1:B:44:ARG:CD	2.42	0.49
1:D:103:VAL:CG2	1:D:124:LEU:HD21	2.43	0.49
1:B:12:LYS:O	1:B:15:GLN:HG3	2.13	0.48
1:C:232:SER:HA	1:C:235:LEU:HG	1.95	0.48
1:D:103:VAL:O	1:D:107:LEU:HD12	2.12	0.48
1:D:33:ILE:C	1:D:35:ARG:H	2.19	0.48
1:D:35:ARG:C	1:D:37:THR:N	2.65	0.48
1:D:130:GLN:C	1:D:130:GLN:NE2	2.71	0.48
1:D:210:VAL:O	1:D:280:GLY:HA2	2.12	0.48
1:B:24:GLN:HA	1:B:27:ILE:CG2	2.42	0.48
1:A:29:ARG:O	1:A:30:GLU:O	2.30	0.48
1:A:258:THR:HG23	1:A:260:MET:H	1.79	0.48
1:A:279:ILE:HA	1:A:302:CYS:HB2	1.95	0.48
1:D:220:GLY:C	1:D:222:ASN:N	2.70	0.48
1:A:133:GLN:OE1	1:C:105:ARG:HD2	2.14	0.48
1:D:23:THR:O	1:D:27:ILE:CG1	2.56	0.48
1:D:217:ILE:HG21	1:D:221:ALA:O	2.14	0.48
1:D:224:HIS:O	1:D:228:GLY:HA2	2.14	0.48
1:A:283:MET:CE	1:A:306:ASN:ND2	2.69	0.48
1:A:146:PRO:CA	3:A:1317:MPD:HM1	2.39	0.47
1:A:273:ARG:C	1:A:275:ALA:N	2.72	0.47
1:B:53:ILE:CD1	1:B:53:ILE:C	2.85	0.47
1:D:63:LEU:O	1:D:63:LEU:HD12	2.14	0.47
1:B:3:ASN:C	1:B:4:SER:O	2.56	0.47
1:B:55:ILE:O	1:B:55:ILE:HG22	2.08	0.47
1:B:103:VAL:O	1:B:107:LEU:HD12	2.14	0.47
1:D:279:ILE:HG12	1:D:302:CYS:HB2	1.97	0.47
1:A:297:GLY:O	1:A:298:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG21	1:B:209:LEU:HD11	1.96	0.47
1:B:103:VAL:CG2	1:B:124:LEU:HD21	2.43	0.47
1:C:25:ALA:CA	1:C:35:ARG:HD2	2.41	0.47
1:C:51:VAL:O	1:C:51:VAL:HG13	2.11	0.47
1:B:269:MET:HE3	1:B:299:TYR:CG	2.48	0.47
1:B:288:TYR:CE1	1:B:313:LEU:HD23	2.49	0.47
1:A:217:ILE:HD11	1:A:287:LYS:HZ2	1.80	0.47
1:B:210:VAL:O	1:B:280:GLY:HA2	2.13	0.47
1:D:91:GLN:O	1:D:95:MET:HG3	2.14	0.47
1:A:75:LEU:HD21	1:A:295:LEU:CD2	2.45	0.47
1:B:227:TYR:CD2	1:B:260:MET:HE1	2.49	0.47
1:D:185:ILE:O	1:D:189:ILE:HG13	2.14	0.47
1:B:117:TRP:CE3	1:B:150:LEU:HD11	2.49	0.47
1:C:199:SER:O	1:C:202:TRP:HB2	2.15	0.47
1:A:219:ASP:OD1	1:A:220:GLY:N	2.43	0.47
1:D:186:ARG:O	1:D:190:MET:HG3	2.15	0.47
1:B:20:GLN:O	1:B:21:ASP:HB2	2.15	0.46
1:A:180:LEU:HD11	1:A:265:LEU:HD12	1.96	0.46
1:A:229:SER:O	1:A:230:GLU:C	2.57	0.46
1:B:57:TYR:CE2	1:C:15:GLN:NE2	2.83	0.46
1:A:59:TYR:CE1	1:D:7:ILE:CD1	2.98	0.46
1:B:51:VAL:O	1:B:51:VAL:HG22	2.14	0.46
1:C:244:ILE:O	1:C:245:CYS:C	2.56	0.46
1:D:10:ILE:O	1:D:10:ILE:HG22	2.09	0.46
1:D:288:TYR:O	1:D:289:SER:C	2.59	0.46
1:B:55:ILE:CA	1:C:51:VAL:HG22	2.21	0.46
1:D:117:TRP:CE3	1:D:150:LEU:HD11	2.51	0.46
1:D:137:VAL:CG2	1:D:169:ALA:HB2	2.45	0.46
1:A:117:TRP:NE1	3:A:1317:MPD:C1	2.78	0.46
1:B:273:ARG:HD2	1:B:298:ARG:O	2.15	0.46
1:C:279:ILE:HA	1:C:302:CYS:HB2	1.97	0.46
1:D:10:ILE:HG12	1:D:41:LEU:HD22	1.98	0.46
1:D:205:LEU:HD21	1:D:208:ALA:HB2	1.97	0.46
1:A:149:LYS:HB3	1:A:226:PHE:CE2	2.51	0.46
1:C:22:MET:O	1:C:27:ILE:HG13	2.16	0.46
1:C:288:TYR:CD1	1:C:313:LEU:HD23	2.51	0.46
1:B:6:ASP:OD1	1:B:6:ASP:N	2.48	0.46
1:A:113:ILE:HA	1:A:207:VAL:O	2.16	0.46
1:A:227:TYR:HD2	1:A:260:MET:CE	2.16	0.46
1:C:269:MET:O	1:C:272:LEU:N	2.50	0.45
1:A:63:LEU:HA	1:A:63:LEU:HD12	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:CD	1:B:262:GLU:O	2.64	0.45
1:D:88:GLU:O	1:D:88:GLU:HG3	2.16	0.45
1:D:217:ILE:HG23	1:D:219:ASP:HB2	1.99	0.45
1:A:186:ARG:HD2	1:A:263:LYS:HA	1.98	0.45
1:B:182:ASN:OD1	1:B:184:LEU:N	2.49	0.45
1:D:87:LEU:HD12	1:D:87:LEU:HA	1.68	0.45
1:A:28:ALA:HB2	1:A:35:ARG:HA	1.99	0.45
1:A:180:LEU:HD11	1:A:265:LEU:CD1	2.47	0.45
1:B:111:ASP:OD1	1:B:276:ARG:NH2	2.49	0.45
1:B:228:GLY:O	1:B:229:SER:C	2.59	0.45
1:B:240:VAL:O	1:B:240:VAL:CG2	2.62	0.45
1:D:107:LEU:HD21	1:D:113:ILE:HD11	1.99	0.45
1:A:190:MET:HE2	1:A:190:MET:HB3	1.69	0.45
1:B:53:ILE:HG22	1:C:53:ILE:HG22	1.87	0.45
1:B:288:TYR:CZ	1:B:292:LEU:HD13	2.52	0.45
1:C:297:GLY:O	1:C:298:ARG:HB2	2.16	0.45
1:D:308:GLU:HG2	1:D:309:THR:N	2.27	0.45
1:C:56:ASN:OD1	1:C:58:ASP:N	2.50	0.45
1:C:186:ARG:NH1	1:C:186:ARG:CG	2.50	0.45
1:A:80:VAL:HA	1:A:305:THR:O	2.16	0.45
1:C:243:ASP:HB2	1:C:248:PHE:CD1	2.52	0.45
1:D:92:LEU:HD12	1:D:283:MET:SD	2.57	0.45
1:D:156:VAL:HG13	1:D:157:ASN:N	2.31	0.45
1:A:31:LEU:H	1:A:31:LEU:HD13	1.68	0.45
1:B:130:GLN:HE21	1:B:130:GLN:C	2.25	0.45
1:D:121:VAL:H	2:D:1316:GOL:HO3	1.63	0.45
1:D:156:VAL:CG1	1:D:157:ASN:N	2.79	0.45
1:C:25:ALA:CA	1:C:35:ARG:HD3	2.38	0.45
1:C:93:SER:O	1:C:97:GLN:HG3	2.17	0.45
1:D:69:LEU:HD23	1:D:314:LEU:HD21	1.99	0.45
1:B:28:ALA:HB2	1:B:38:ILE:HG13	1.98	0.45
1:B:137:VAL:O	1:B:169:ALA:HB1	2.17	0.45
1:D:186:ARG:HD2	1:D:263:LYS:HA	1.98	0.45
1:D:34:TYR:O	1:D:36:THR:N	2.50	0.44
1:A:7:ILE:HD13	1:D:59:TYR:HD2	1.82	0.44
1:B:102:LEU:O	1:B:106:LEU:HD13	2.17	0.44
1:B:130:GLN:NE2	1:B:131:ARG:O	2.50	0.44
1:B:163:ALA:O	1:B:164:ALA:C	2.60	0.44
1:D:182:ASN:OD1	1:D:183:PRO:CD	2.64	0.44
1:A:199:SER:O	1:A:202:TRP:HB2	2.17	0.44
1:C:268:GLU:O	1:C:269:MET:C	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:GLU:O	1:D:235:LEU:HG	2.17	0.44
1:A:133:GLN:OE1	1:C:105:ARG:CD	2.66	0.44
1:A:155:HIS:HD2	1:A:156:VAL:N	2.14	0.44
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.69	0.44
1:B:107:LEU:CD2	1:B:113:ILE:HD11	2.47	0.44
1:C:244:ILE:HG13	1:C:249:TYR:HE1	1.82	0.44
1:D:33:ILE:O	1:D:35:ARG:N	2.50	0.44
1:A:256:VAL:O	1:A:256:VAL:HG12	2.16	0.44
1:B:34:TYR:O	1:B:38:ILE:HG12	2.17	0.44
1:C:10:ILE:HG12	1:C:41:LEU:CB	2.42	0.44
1:C:229:SER:O	1:C:230:GLU:C	2.61	0.44
1:D:216:ALA:O	1:D:217:ILE:C	2.60	0.44
1:D:283:MET:HE3	1:D:283:MET:HB2	1.59	0.44
1:A:60:ASN:CG	1:A:63:LEU:CB	2.91	0.44
1:A:64:TRP:CZ2	1:D:48:GLN:HA	2.53	0.44
1:B:55:ILE:CG1	1:C:51:VAL:CG2	2.95	0.44
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.80	0.44
1:A:197:THR:O	1:A:200:SER:HB3	2.18	0.44
1:A:224:HIS:O	1:A:228:GLY:HA2	2.18	0.44
1:C:113:ILE:HA	1:C:207:VAL:O	2.18	0.44
1:C:186:ARG:HH11	1:C:186:ARG:HG3	1.70	0.44
1:D:197:THR:O	1:D:200:SER:HB3	2.17	0.44
1:A:23:THR:HG22	1:A:26:GLN:CG	2.48	0.44
1:A:59:TYR:HE1	1:D:7:ILE:HD11	1.82	0.44
1:A:188:GLY:HA3	1:B:185:ILE:HD11	2.00	0.44
1:A:156:VAL:HG13	1:A:157:ASN:N	2.32	0.43
1:B:156:VAL:HG13	1:B:157:ASN:N	2.32	0.43
1:C:243:ASP:CB	1:C:248:PHE:CD1	3.01	0.43
1:C:13:ILE:CG2	1:C:14:ALA:N	2.80	0.43
1:C:80:VAL:HA	1:C:305:THR:O	2.18	0.43
1:D:130:GLN:NE2	1:D:131:ARG:O	2.51	0.43
1:A:227:TYR:HD2	1:A:260:MET:HE3	1.80	0.43
1:D:35:ARG:O	1:D:36:THR:C	2.60	0.43
1:D:35:ARG:O	1:D:38:ILE:HG12	2.18	0.43
1:B:131:ARG:HG3	1:B:135:ARG:HH21	1.82	0.43
1:C:75:LEU:HD21	1:C:295:LEU:CD2	2.48	0.43
1:C:213:GLY:HA3	1:C:243:ASP:OD1	2.19	0.43
1:B:156:VAL:CG1	1:B:157:ASN:N	2.81	0.43
1:D:186:ARG:HD3	1:D:262:GLU:C	2.43	0.43
1:A:143:ILE:HD12	1:A:266:SER:CB	2.46	0.43
1:B:15:GLN:HB2	1:B:19:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLN:C	1:B:130:GLN:NE2	2.76	0.43
1:C:23:THR:HG22	1:C:26:GLN:OE1	2.18	0.43
1:C:48:GLN:O	1:C:50:ILE:HG13	2.18	0.43
1:C:228:GLY:O	1:C:230:GLU:N	2.51	0.43
1:A:149:LYS:O	1:A:150:LEU:HD23	2.18	0.43
1:B:215:PRO:C	1:B:217:ILE:N	2.73	0.43
1:C:92:LEU:CD2	1:C:119:ARG:HG2	2.49	0.43
1:D:86:LEU:HD23	1:D:86:LEU:O	2.19	0.43
1:A:250:ASP:OD1	1:A:250:ASP:C	2.62	0.43
1:B:81:ALA:O	1:B:306:ASN:HA	2.18	0.43
5:B:1316:MRD:H1C2	5:B:1316:MRD:H4	1.70	0.43
1:C:314:LEU:O	1:C:315:LYS:C	2.60	0.43
1:D:101:LEU:HD23	1:D:101:LEU:HA	1.85	0.43
1:D:142:ILE:HD11	1:D:210:VAL:HG23	2.00	0.43
1:D:75:LEU:HD21	1:D:295:LEU:HD22	2.01	0.43
1:D:269:MET:HE2	1:D:269:MET:CA	2.31	0.43
1:C:155:HIS:CD2	1:C:156:VAL:N	2.87	0.43
1:D:28:ALA:CB	1:D:35:ARG:HB2	2.49	0.43
1:C:250:ASP:OD1	1:C:250:ASP:C	2.61	0.42
1:A:92:LEU:HD23	1:A:119:ARG:HG2	2.01	0.42
1:A:283:MET:CE	1:A:306:ASN:HD22	2.31	0.42
1:B:8:ARG:HD2	1:B:8:ARG:HA	1.85	0.42
1:B:142:ILE:HD11	1:B:210:VAL:HG23	2.01	0.42
1:B:312:LEU:HD12	1:B:312:LEU:HA	1.58	0.42
1:C:6:ASP:O	1:C:9:LEU:HB2	2.20	0.42
1:C:128:LEU:HA	1:C:129:PRO:HD3	1.81	0.42
1:C:166:ARG:HH11	1:C:166:ARG:HG3	1.85	0.42
1:A:287:LYS:O	1:A:291:ILE:HG13	2.20	0.42
1:B:181:ASP:OD2	1:B:181:ASP:N	2.52	0.42
1:B:205:LEU:HD21	1:B:208:ALA:HB2	2.00	0.42
1:C:33:ILE:CG2	1:C:37:THR:OG1	2.68	0.42
1:D:62:ASN:O	1:D:66:GLU:HG3	2.20	0.42
1:A:238:ARG:HG2	1:A:238:ARG:H	1.74	0.42
1:B:20:GLN:O	1:B:21:ASP:CB	2.65	0.42
1:B:53:ILE:CG2	1:C:53:ILE:HG21	2.45	0.42
1:B:215:PRO:O	1:B:217:ILE:N	2.53	0.42
1:C:16:LEU:HD23	1:C:22:MET:HE2	2.02	0.42
1:C:149:LYS:O	1:C:150:LEU:HD23	2.19	0.42
1:A:117:TRP:HE1	3:A:1317:MPD:C1	2.33	0.42
1:A:199:SER:HA	1:A:202:TRP:CD2	2.54	0.42
1:B:46:ARG:HH12	1:B:53:ILE:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG21	1:D:209:LEU:HD11	2.01	0.42
1:D:292:LEU:HD23	1:D:296:HIS:CE1	2.54	0.42
1:A:111:ASP:HB2	1:A:137:VAL:HG12	2.01	0.41
1:A:175:ASP:H	1:A:194:HIS:CE1	2.27	0.41
1:A:180:LEU:CD2	1:A:185:ILE:HG22	2.50	0.41
1:B:182:ASN:HA	1:B:183:PRO:HD3	1.70	0.41
1:C:260:MET:H	1:C:260:MET:HG2	1.28	0.41
1:D:31:LEU:C	1:D:33:ILE:N	2.77	0.41
1:A:34:TYR:O	1:A:35:ARG:C	2.63	0.41
1:A:41:LEU:HA	1:A:41:LEU:HD23	1.76	0.41
1:A:104:ASP:OD1	1:A:135:ARG:NH2	2.52	0.41
1:B:10:ILE:H	1:B:10:ILE:HG13	1.69	0.41
1:C:199:SER:HA	1:C:202:TRP:CD2	2.55	0.41
1:D:217:ILE:HG23	1:D:219:ASP:N	2.25	0.41
1:D:137:VAL:O	1:D:169:ALA:HB1	2.20	0.41
1:B:44:ARG:HH11	1:B:44:ARG:CG	2.34	0.41
1:D:16:LEU:N	1:D:16:LEU:HD23	2.36	0.41
1:D:108:GLU:CD	1:D:276:ARG:NH1	2.79	0.41
1:A:9:LEU:HA	1:A:12:LYS:HB3	2.01	0.41
1:A:255:LEU:HD12	1:A:299:TYR:OH	2.20	0.41
1:D:210:VAL:O	1:D:210:VAL:HG12	2.21	0.41
1:B:75:LEU:HD21	1:B:295:LEU:HD22	2.02	0.41
1:B:231:GLU:O	1:B:235:LEU:HG	2.20	0.41
1:D:13:ILE:HD13	1:D:13:ILE:HG21	1.76	0.41
1:D:76:LYS:C	1:D:77:GLU:HG2	2.45	0.41
1:C:191:GLN:O	1:C:196:LYS:HE2	2.20	0.41
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.82	0.41
1:B:125:VAL:HA	1:B:128:LEU:HD22	2.02	0.41
1:B:258:THR:O	1:B:259:ASN:C	2.62	0.41
1:B:258:THR:C	1:B:260:MET:N	2.75	0.41
1:C:53:ILE:O	1:C:53:ILE:CG1	2.61	0.41
1:C:13:ILE:HG23	1:C:42:LEU:CD2	2.51	0.41
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.88	0.41
1:D:180:LEU:HD13	1:D:186:ARG:HA	2.03	0.41
1:A:23:THR:HG22	1:A:26:GLN:CD	2.45	0.40
1:A:249:TYR:OH	1:A:294:ALA:HB2	2.20	0.40
1:A:44:ARG:O	1:A:45:GLY:C	2.65	0.40
1:A:198:ILE:HD13	1:A:198:ILE:HA	1.93	0.40
1:C:48:GLN:N	1:C:48:GLN:CD	2.80	0.40
1:D:228:GLY:O	1:D:229:SER:C	2.65	0.40
1:D:292:LEU:CD2	1:D:296:HIS:CE1	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:C	1:B:9:LEU:N	2.77	0.40
1:D:186:ARG:CD	1:D:263:LYS:CA	2.97	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:TYR:CG	1:D:311:GLU:OE1[1_655]	1.66	0.54
1:B:34:TYR:CB	1:D:311:GLU:OE1[1_655]	1.95	0.25
1:B:35:ARG:N	1:D:311:GLU:OE2[1_655]	2.00	0.20
1:B:34:TYR:CD1	1:D:311:GLU:OE1[1_655]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/315 (96%)	282 (93%)	19 (6%)	3 (1%)	12	45
1	B	311/315 (99%)	288 (93%)	18 (6%)	5 (2%)	7	36
1	C	291/315 (92%)	270 (93%)	17 (6%)	4 (1%)	9	39
1	D	304/315 (96%)	281 (92%)	17 (6%)	6 (2%)	6	31
All	All	1210/1260 (96%)	1121 (93%)	71 (6%)	18 (2%)	8	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	SER
1	B	4	SER
1	B	229	SER
1	C	229	SER
1	D	6	ASP

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Mol	Chain	Res	Type
1	D	229	SER
1	D	34	TYR
1	D	285	GLU
1	C	51	VAL
1	D	221	ALA
1	A	21	ASP
1	A	30	GLU
1	B	216	ALA
1	D	5	ASP
1	B	84	ASP
1	C	23	THR
1	B	215	PRO
1	C	253	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	253/262 (97%)	225 (89%)	28 (11%)	6	25
1	B	257/262 (98%)	221 (86%)	36 (14%)	3	17
1	C	245/262 (94%)	215 (88%)	30 (12%)	5	22
1	D	253/262 (97%)	222 (88%)	31 (12%)	4	22
All	All	1008/1048 (96%)	883 (88%)	125 (12%)	4	21

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	9	LEU
1	A	20	GLN
1	A	31	LEU
1	A	36	THR
1	A	51	VAL
1	A	55	ILE
1	A	77	GLU

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Mol	Chain	Res	Type
1	A	79	VAL
1	A	106	LEU
1	A	113	ILE
1	A	123	SER
1	A	124	LEU
1	A	135	ARG
1	A	140	VAL
1	A	143	ILE
1	A	210	VAL
1	A	226	PHE
1	A	230	GLU
1	A	240	VAL
1	A	243	ASP
1	A	251	ILE
1	A	255	LEU
1	A	258	THR
1	A	259	ASN
1	A	307	ARG
1	A	309	THR
1	A	311	GLU
1	B	7	ILE
1	B	9	LEU
1	B	21	ASP
1	B	33	ILE
1	B	36	THR
1	B	37	THR
1	B	39	SER
1	B	44	ARG
1	B	46	ARG
1	B	50	ILE
1	B	51	VAL
1	B	52	THR
1	B	53	ILE
1	B	63	LEU
1	B	68	GLN
1	B	77	GLU
1	B	79	VAL
1	B	82	SER
1	B	93	SER
1	B	113	ILE
1	B	128	LEU
1	B	137	VAL

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Mol	Chain	Res	Type
1	B	159	LEU
1	B	181	ASP
1	B	182	ASN
1	B	210	VAL
1	B	218	ARG
1	B	255	LEU
1	B	260	MET
1	B	265	LEU
1	B	281	ILE
1	B	286	GLU
1	B	287	LYS
1	B	292	LEU
1	B	301	ASN
1	B	312	LEU
1	C	6	ASP
1	C	8	ARG
1	C	11	VAL
1	C	20	GLN
1	C	22	MET
1	C	23	THR
1	C	30	GLU
1	C	51	VAL
1	C	53	ILE
1	C	55	ILE
1	C	63	LEU
1	C	77	GLU
1	C	79	VAL
1	C	106	LEU
1	C	140	VAL
1	C	159	LEU
1	C	186	ARG
1	C	200	SER
1	C	209	LEU
1	C	210	VAL
1	C	219	ASP
1	C	226	PHE
1	C	240	VAL
1	C	243	ASP
1	C	251	ILE
1	C	260	MET
1	C	262	GLU
1	C	307	ARG

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Mol	Chain	Res	Type
1	C	309	THR
1	C	311	GLU
1	D	7	ILE
1	D	10	ILE
1	D	11	VAL
1	D	13	ILE
1	D	16	LEU
1	D	27	ILE
1	D	33	ILE
1	D	35	ARG
1	D	39	SER
1	D	51	VAL
1	D	63	LEU
1	D	68	GLN
1	D	79	VAL
1	D	86	LEU
1	D	93	SER
1	D	113	ILE
1	D	124	LEU
1	D	135	ARG
1	D	137	VAL
1	D	185	ILE
1	D	200	SER
1	D	210	VAL
1	D	217	ILE
1	D	281	ILE
1	D	285	GLU
1	D	286	GLU
1	D	287	LYS
1	D	292	LEU
1	D	301	ASN
1	D	305	THR
1	D	309	THR

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	68	GLN
1	A	127	ASN
1	A	155	HIS
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	194	HIS
1	A	224	HIS
1	B	26	GLN
1	B	127	ASN
1	B	130	GLN
1	B	187	ASN
1	B	194	HIS
1	B	252	ASN
1	B	259	ASN
1	B	301	ASN
1	C	15	GLN
1	C	20	GLN
1	C	68	GLN
1	C	91	GLN
1	C	127	ASN
1	C	155	HIS
1	C	194	HIS
1	C	224	HIS
1	D	48	GLN
1	D	127	ASN
1	D	130	GLN
1	D	193	GLN
1	D	194	HIS
1	D	252	ASN
1	D	301	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	MRD	B	1316	-	7,7,7	0.33	0	9,10,10	0.35	0
3	MPD	A	1317	-	7,7,7	0.51	0	9,10,10	0.71	0
2	GOL	D	1316	-	5,5,5	0.33	0	5,5,5	0.33	0
2	GOL	A	1316	-	5,5,5	0.43	0	5,5,5	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MRD	B	1316	-	-	2/5/5/5	-
3	MPD	A	1317	-	-	5/5/5/5	-
2	GOL	D	1316	-	-	2/4/4/4	-
2	GOL	A	1316	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1316	GOL	O1-C1-C2-C3
3	A	1317	MPD	CM-C2-C3-C4
3	A	1317	MPD	C2-C3-C4-O4
3	A	1317	MPD	C2-C3-C4-C5
2	D	1316	GOL	O1-C1-C2-O2
3	A	1317	MPD	O2-C2-C3-C4
3	A	1317	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	B	1316	MRD	C2-C3-C4-C5
5	B	1316	MRD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1316	MRD	4	0
3	A	1317	MPD	7	0
2	D	1316	GOL	3	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	308/315 (97%)	-0.21	3 (0%) 79 63	22, 47, 91, 149	0
1	B	313/315 (99%)	-0.05	6 (1%) 66 46	17, 57, 116, 185	0
1	C	299/315 (94%)	0.54	22 (7%) 20 13	43, 89, 184, 238	0
1	D	308/315 (97%)	0.38	9 (2%) 53 35	47, 79, 139, 200	0
All	All	1228/1260 (97%)	0.16	40 (3%) 49 30	17, 70, 142, 238	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	50	ILE	4.9
1	C	11	VAL	4.5
1	C	9	LEU	4.4
1	D	221	ALA	4.3
1	C	37	THR	3.8
1	C	4	SER	3.7
1	C	7	ILE	3.4
1	B	35	ARG	3.4
1	C	42	LEU	3.4
1	C	216	ALA	3.3
1	C	27	ILE	3.2
1	C	41	LEU	3.0
1	D	21	ASP	2.8
1	C	16	LEU	2.8
1	C	233	ASP	2.7
1	D	86	LEU	2.7
1	C	222	ASN	2.6
1	C	31	LEU	2.6
1	C	54	ALA	2.6
1	B	181	ASP	2.5
1	A	286	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	308	GLU	2.5
1	D	5	ASP	2.5
1	A	219	ASP	2.4
1	C	40	ARG	2.4
1	D	307	ARG	2.4
1	D	219	ASP	2.4
1	C	258	THR	2.3
1	C	185	ILE	2.3
1	C	81	ALA	2.3
1	A	83	SER	2.3
1	B	59	TYR	2.3
1	D	230	GLU	2.2
1	C	46	ARG	2.2
1	B	36	THR	2.2
1	B	57	TYR	2.2
1	B	61	GLU	2.2
1	C	90	GLU	2.2
1	D	216	ALA	2.1
1	C	187	ASN	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 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(Å ²)	Q<0.9
2	GOL	D	1316	6/6	0.70	0.23	88,88,88,88	0
5	MRD	B	1316	8/8	0.80	0.21	90,90,90,90	0
4	CL	A	1318	1/1	0.90	0.11	69,69,69,69	0
3	MPD	A	1317	8/8	0.94	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	1316	6/6	0.95	0.09	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.