



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:58 PM UTC

PDB ID : 7ZHT / pdb_00007zht
Title : Leishmania donovani Glucose 6-Phosphate Dehydrogenase apo form
Authors : Fritz-Wolf, K.; Berneburg, I.
Deposited on : 2022-04-07
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

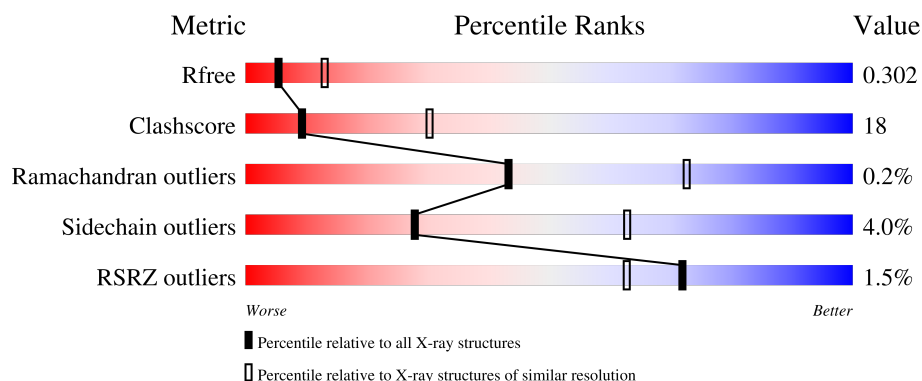
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	562	
1	B	562	
1	C	562	
1	D	562	

2 Entry composition [i](#)

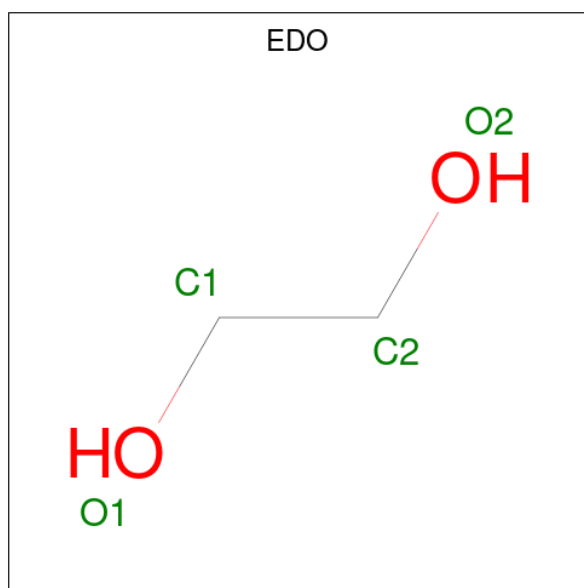
There are 4 unique types of molecules in this entry. The entry contains 16104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4208	2676	724	792	16			
1	B	525	Total	C	N	O	S	0	0	0
			4158	2647	713	782	16			
1	C	483	Total	C	N	O	S	0	0	0
			3823	2432	656	718	17			
1	D	485	Total	C	N	O	S	0	0	0
			3838	2442	658	721	17			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



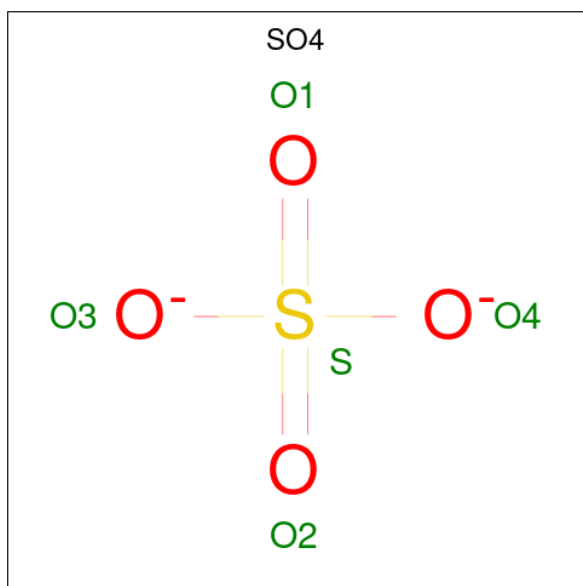
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

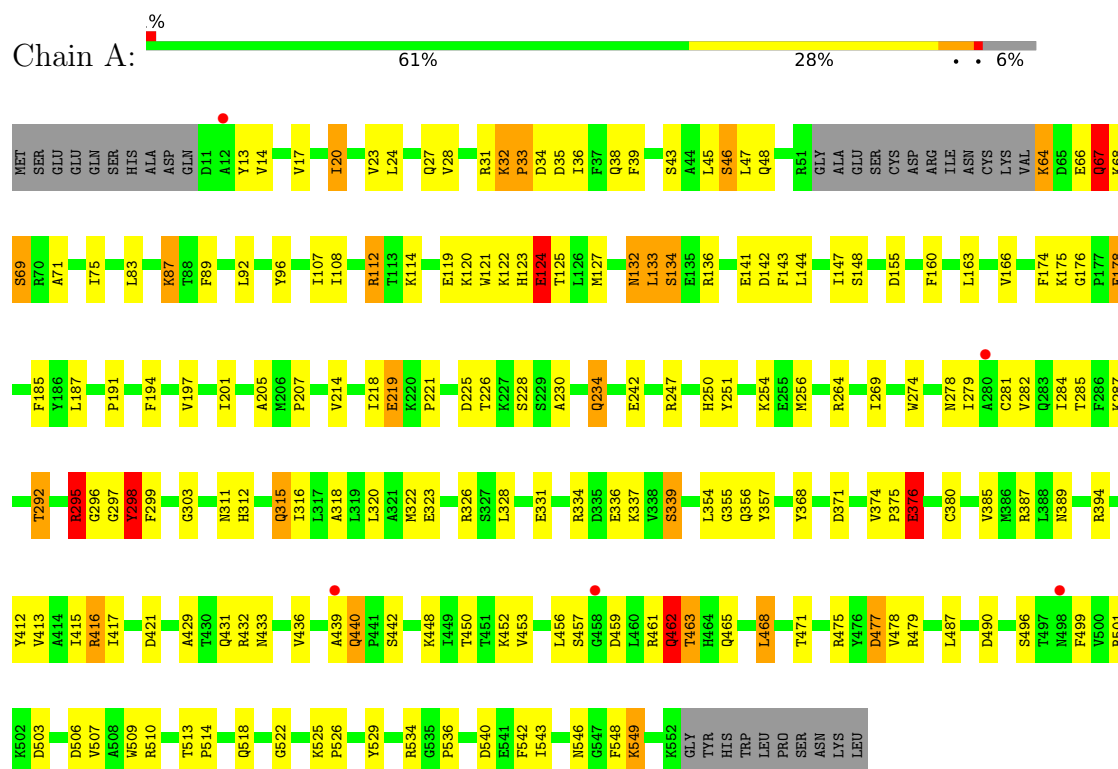
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	B	14	Total 14	O 14	0	0
4	C	4	Total 4	O 4	0	0
4	D	5	Total 5	O 5	0	0

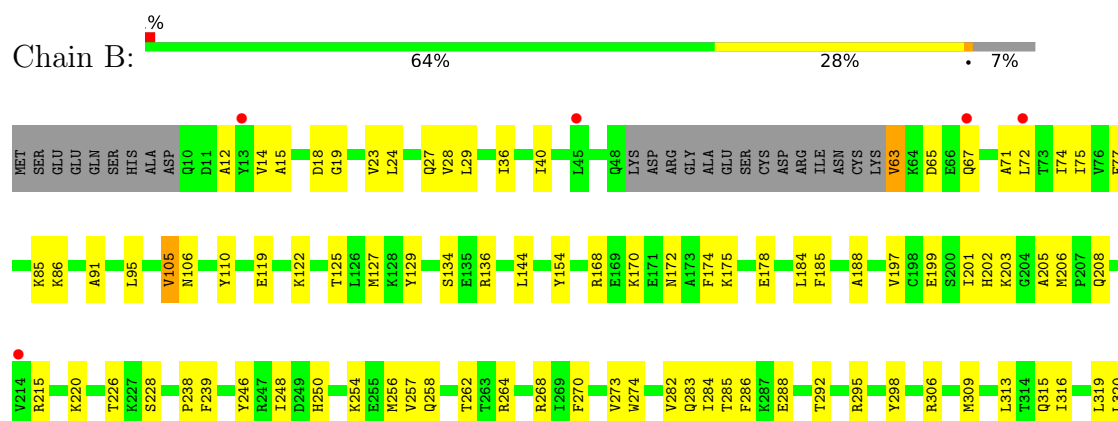
3 Residue-property plots

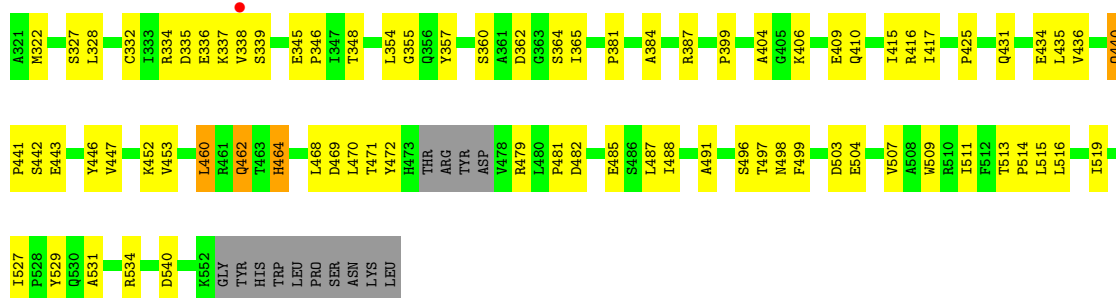
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucose-6-phosphate 1-dehydrogenase

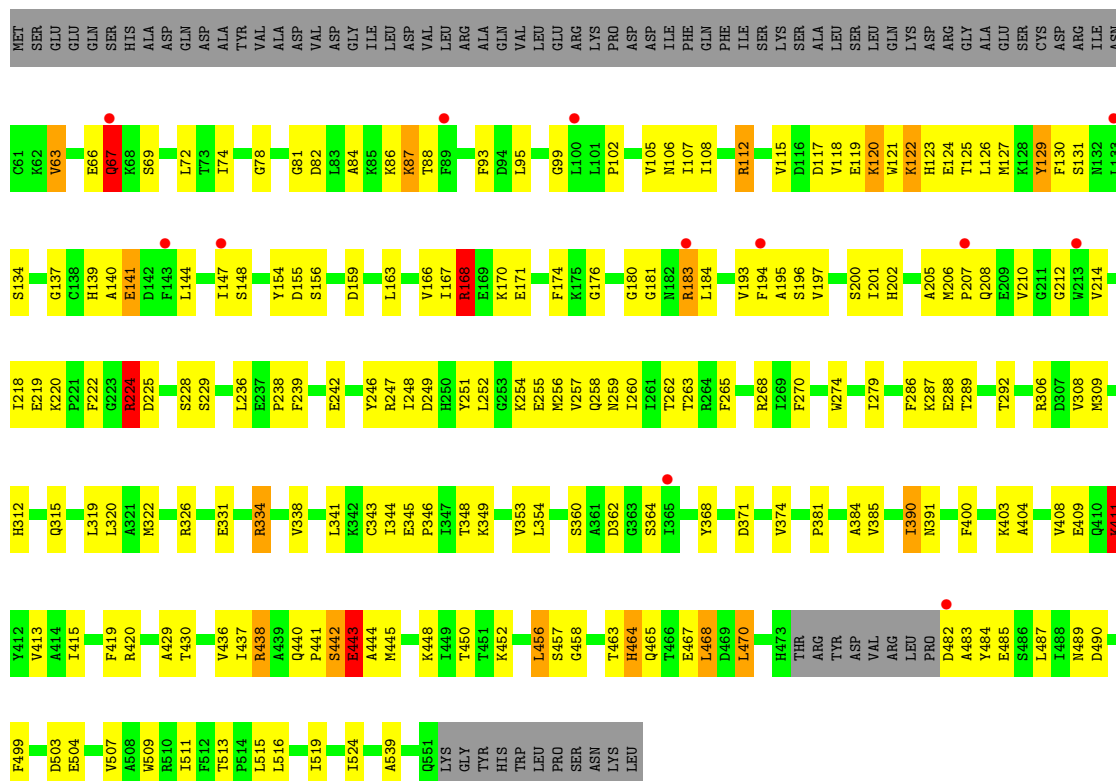


• Molecule 1: Glucose-6-phosphate 1-dehydrogenase

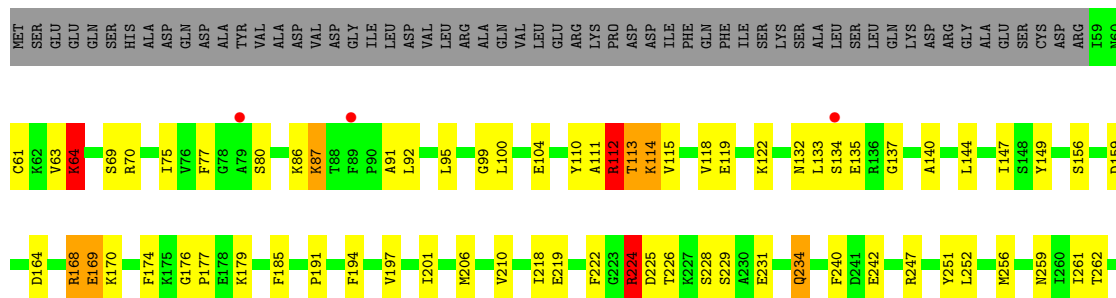


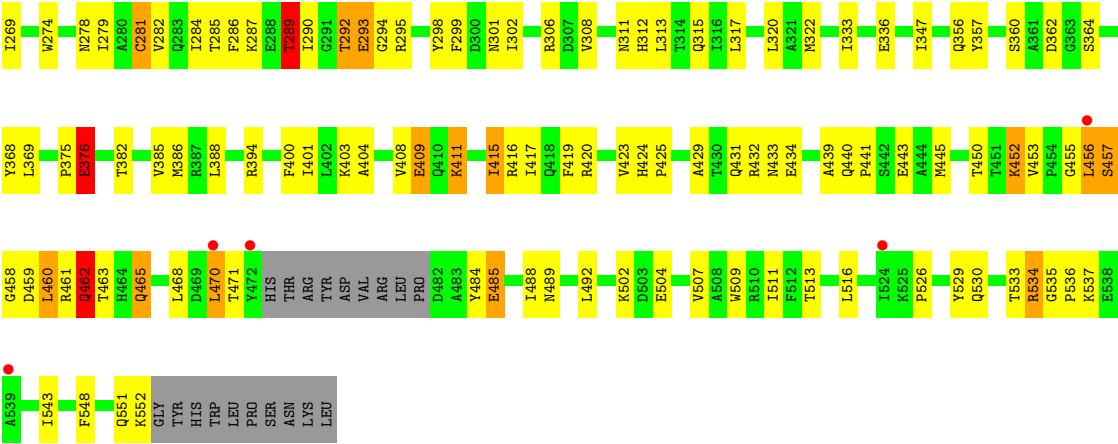


• Molecule 1: Glucose-6-phosphate 1-dehydrogenase



• Molecule 1: Glucose-6-phosphate 1-dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.69Å 65.82Å 189.22Å 90.00° 92.35° 90.00°	Depositor
Resolution (Å)	39.20 – 2.80 39.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.20-2.80) 98.4 (39.20-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.244 , 0.304 0.244 , 0.302	Depositor DCC
R_{free} test set	7073 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16104	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4996e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	3/4296 (0.1%)	0.89	25/5810 (0.4%)
1	B	0.28	0/4244	0.66	9/5740 (0.2%)
1	C	0.48	5/3905 (0.1%)	1.08	42/5281 (0.8%)
1	D	0.44	3/3919 (0.1%)	1.04	42/5299 (0.8%)
All	All	0.40	11/16364 (0.1%)	0.93	118/22130 (0.5%)

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	17
1	C	0	6
1	D	1	7
All	All	1	30

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	326	ARG	CD-NE	-7.01	1.36	1.46
1	D	462	GLN	CB-CG	-6.71	1.32	1.52
1	C	326	ARG	CZ-NH2	6.58	1.42	1.33
1	A	326	ARG	CZ-NH2	6.23	1.41	1.33
1	A	112	ARG	CG-CD	-5.94	1.34	1.52
1	D	534	ARG	CG-CD	-5.75	1.35	1.52
1	C	140	ALA	C-N	5.58	1.41	1.33
1	A	124	GLU	CG-CD	5.43	1.65	1.52
1	C	120	LYS	CD-CE	5.32	1.68	1.52
1	C	141	GLU	CA-C	-5.32	1.44	1.52
1	D	111	ALA	C-N	5.05	1.40	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	534	ARG	CB-CG-CD	-18.64	68.43	111.30
1	C	140	ALA	CA-C-N	-16.20	95.75	122.65
1	C	140	ALA	C-N-CA	-16.20	95.75	122.65
1	A	376	GLU	CG-CD-OE1	15.10	153.12	118.40
1	A	376	GLU	CG-CD-OE2	-14.37	85.36	118.40
1	D	112	ARG	CB-CA-C	-14.19	88.49	110.90
1	A	295	ARG	CB-CG-CD	-13.72	79.73	111.30
1	D	112	ARG	CB-CG-CD	13.49	142.33	111.30
1	C	112	ARG	CB-CG-CD	-13.11	81.15	111.30
1	D	462	GLN	CB-CG-CD	-13.00	90.50	112.60
1	C	67	GLN	CB-CA-C	-12.15	90.61	110.79
1	C	67	GLN	CA-CB-CG	12.01	138.12	114.10
1	A	295	ARG	CG-CD-NE	11.51	137.31	112.00
1	D	462	GLN	CA-C-N	11.29	141.77	122.81
1	D	462	GLN	C-N-CA	11.29	141.77	122.81
1	D	112	ARG	N-CA-CB	10.46	125.24	110.07
1	C	112	ARG	CG-CD-NE	10.36	134.78	112.00
1	C	112	ARG	CA-CB-CG	10.25	134.60	114.10
1	C	168	ARG	CG-CD-NE	10.18	134.39	112.00
1	A	124	GLU	CA-CB-CG	10.13	134.37	114.10
1	A	462	GLN	N-CA-CB	-10.05	98.27	110.53
1	B	175	LYS	CG-CD-CE	9.87	134.00	111.30
1	C	411	LYS	CD-CE-NZ	9.40	141.98	111.90
1	C	67	GLN	N-CA-CB	9.25	123.72	110.12
1	D	411	LYS	CA-CB-CG	9.25	132.59	114.10
1	B	175	LYS	CD-CE-NZ	-9.23	82.36	111.90
1	D	375	PRO	CA-C-N	-9.00	103.75	122.82
1	D	375	PRO	C-N-CA	-9.00	103.75	122.82
1	D	411	LYS	CB-CG-CD	-8.70	91.29	111.30
1	D	293	GLU	CB-CG-CD	-8.59	97.99	112.60
1	A	298	TYR	N-CA-C	-8.49	102.73	113.43
1	C	438	ARG	CA-CB-CG	8.44	130.98	114.10
1	A	295	ARG	CB-CA-C	-8.28	98.23	111.06
1	C	120	LYS	CA-CB-CG	8.10	130.31	114.10
1	C	141	GLU	CG-CD-OE2	-7.99	100.03	118.40
1	A	461	ARG	CA-C-N	7.95	133.81	122.05
1	A	461	ARG	C-N-CA	7.95	133.81	122.05
1	C	456	LEU	CA-CB-CG	7.92	144.01	116.30
1	C	411	LYS	CB-CG-CD	-7.88	93.17	111.30
1	B	440	GLN	CA-CB-CG	7.75	129.61	114.10
1	C	456	LEU	CB-CA-C	-7.73	95.04	110.42
1	C	168	ARG	CA-CB-CG	7.59	129.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	LYS	CB-CG-CD	7.57	128.71	111.30
1	D	376	GLU	CG-CD-OE2	-7.45	101.26	118.40
1	A	112	ARG	CG-CD-NE	-7.43	95.66	112.00
1	D	534	ARG	N-CA-CB	-7.38	98.14	110.39
1	C	120	LYS	CB-CG-CD	7.20	127.87	111.30
1	D	87	LYS	CA-CB-CG	-7.16	99.78	114.10
1	D	465	GLN	CA-CB-CG	-7.12	99.87	114.10
1	D	234	GLN	CA-CB-CG	7.11	128.32	114.10
1	D	224	ARG	CB-CG-CD	-7.00	95.21	111.30
1	D	112	ARG	CA-CB-CG	6.94	127.99	114.10
1	D	86	LYS	CG-CD-CE	-6.83	95.60	111.30
1	D	64	LYS	CA-CB-CG	6.78	127.66	114.10
1	D	168	ARG	CA-C-N	6.68	129.23	120.28
1	D	168	ARG	C-N-CA	6.68	129.23	120.28
1	A	298	TYR	CA-C-N	6.65	130.42	120.31
1	A	298	TYR	C-N-CA	6.65	130.42	120.31
1	C	141	GLU	CA-CB-CG	-6.51	101.08	114.10
1	C	411	LYS	CA-CB-CG	6.51	127.12	114.10
1	C	120	LYS	CD-CE-NZ	6.44	132.51	111.90
1	D	376	GLU	CB-CG-CD	-6.43	101.67	112.60
1	D	289	THR	OG1-CB-CG2	6.40	122.09	109.30
1	A	549	LYS	CA-CB-CG	6.38	126.86	114.10
1	A	376	GLU	OE1-CD-OE2	-6.37	107.61	122.90
1	D	112	ARG	N-CA-C	-6.34	104.29	111.14
1	C	390	ILE	CA-C-N	-6.33	112.99	123.37
1	C	390	ILE	C-N-CA	-6.33	112.99	123.37
1	D	234	GLN	CB-CA-C	-6.31	98.56	110.67
1	C	129	TYR	CA-CB-CG	-6.19	102.75	113.90
1	B	178	GLU	CA-CB-CG	6.11	126.33	114.10
1	C	141	GLU	N-CA-CB	5.94	118.76	110.56
1	D	111	ALA	CA-C-N	-5.90	112.41	120.44
1	D	111	ALA	C-N-CA	-5.90	112.41	120.44
1	D	534	ARG	CG-CD-NE	5.90	124.98	112.00
1	D	289	THR	CA-CB-OG1	5.89	118.44	109.60
1	B	462	GLN	CA-CB-CG	-5.88	102.34	114.10
1	C	141	GLU	CB-CG-CD	5.87	122.57	112.60
1	C	224	ARG	CA-CB-CG	5.84	125.77	114.10
1	C	141	GLU	CG-CD-OE1	5.83	131.81	118.40
1	A	178	GLU	CA-CB-CG	5.81	125.72	114.10
1	C	168	ARG	N-CA-CB	5.78	120.26	110.49
1	A	87	LYS	CA-CB-CG	5.78	125.66	114.10
1	D	169	GLU	CA-CB-CG	5.74	125.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	LYS	CB-CG-CD	-5.72	98.15	111.30
1	C	87	LYS	CB-CG-CD	-5.68	98.23	111.30
1	D	114	LYS	CB-CG-CD	5.67	124.35	111.30
1	C	438	ARG	N-CA-CB	5.62	119.51	110.85
1	A	67	GLN	CA-CB-CG	-5.55	102.99	114.10
1	A	376	GLU	CB-CG-CD	-5.55	103.16	112.60
1	B	105	VAL	CA-C-N	-5.55	114.62	122.94
1	B	105	VAL	C-N-CA	-5.55	114.62	122.94
1	C	224	ARG	CB-CG-CD	-5.54	98.55	111.30
1	B	440	GLN	CB-CA-C	5.54	117.77	109.63
1	A	326	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	D	462	GLN	N-CA-C	5.51	117.44	108.63
1	C	183	ARG	CD-NE-CZ	-5.48	116.72	124.40
1	C	112	ARG	CD-NE-CZ	5.36	131.90	124.40
1	D	104	GLU	CA-CB-CG	5.35	124.80	114.10
1	C	87	LYS	CA-CB-CG	5.30	124.71	114.10
1	B	460	LEU	N-CA-CB	-5.29	102.15	110.30
1	A	295	ARG	CA-CB-CG	5.28	124.66	114.10
1	D	224	ARG	CA-CB-CG	5.25	124.60	114.10
1	D	375	PRO	CA-C-O	-5.25	115.05	121.03
1	C	443	GLU	CA-CB-CG	5.20	124.50	114.10
1	D	289	THR	CA-CB-CG2	5.20	119.33	110.50
1	C	443	GLU	CB-CA-C	-5.18	100.12	110.42
1	D	462	GLN	CA-CB-CG	-5.16	103.78	114.10
1	D	462	GLN	CB-CA-C	5.15	119.12	110.88
1	A	326	ARG	CB-CA-C	5.14	119.53	110.37
1	C	238	PRO	CA-C-N	-5.13	113.70	122.11
1	C	238	PRO	C-N-CA	-5.13	113.70	122.11
1	D	224	ARG	CG-CD-NE	5.09	123.20	112.00
1	C	438	ARG	CA-C-N	5.08	131.84	122.79
1	C	438	ARG	C-N-CA	5.08	131.84	122.79
1	A	132	ASN	CA-C-N	5.07	131.21	121.54
1	A	132	ASN	C-N-CA	5.07	131.21	121.54
1	A	295	ARG	N-CA-C	-5.04	106.88	112.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	289	THR	CB

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	A	134	SER	Peptide
1	A	20	ILE	Peptide
1	A	219	GLU	Peptide
1	A	295	ARG	Sidechain
1	A	297	GLY	Peptide
1	A	298	TYR	Sidechain
1	A	375	PRO	Peptide
1	A	376	GLU	Sidechain
1	A	416	ARG	Sidechain
1	A	440	GLN	Peptide
1	A	456	LEU	Peptide
1	A	477	ASP	Peptide
1	A	478	VAL	Peptide
1	A	67	GLN	Sidechain,Peptide
1	A	69	SER	Mainchain
1	C	112	ARG	Sidechain
1	C	168	ARG	Sidechain
1	C	224	ARG	Sidechain
1	C	442	SER	Peptide
1	C	443	GLU	Peptide
1	C	63	VAL	Peptide
1	D	112	ARG	Sidechain
1	D	224	ARG	Sidechain
1	D	292	THR	Peptide
1	D	376	GLU	Peptide
1	D	456	LEU	Peptide
1	D	457	SER	Peptide
1	D	64	LYS	Peptide

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	4208	0	4181	149	2
1	B	4158	0	4135	125	0
1	C	3823	0	3791	176	1
1	D	3838	0	3814	158	0
2	A	8	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	18	0	0
2	C	12	0	18	0	0
2	D	4	0	6	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	3	0	0	3	0
4	B	14	0	0	2	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
All	All	16104	0	15974	579	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (579) 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:C:120:LYS:HD3	1:C:124:GLU:OE1	1.32	1.23
1:D:112:ARG:NH1	1:D:113:THR:HG23	1.57	1.18
1:D:112:ARG:HH12	1:D:113:THR:CG2	1.57	1.17
1:D:112:ARG:NH1	1:D:113:THR:CG2	2.09	1.14
1:D:112:ARG:HH12	1:D:113:THR:HG22	1.13	1.04
1:C:63:VAL:HG13	1:C:67:GLN:NE2	1.73	1.02
1:A:440:GLN:HB2	1:A:442:SER:H	1.22	1.00
1:C:63:VAL:HG13	1:C:67:GLN:HE22	1.22	0.98
1:A:413:VAL:H	1:A:440:GLN:NE2	1.63	0.97
1:A:413:VAL:H	1:A:440:GLN:HE22	1.04	0.94
1:B:106:ASN:HD22	1:B:170:LYS:HD2	1.35	0.89
1:C:120:LYS:HD3	1:C:124:GLU:CD	1.99	0.88
1:C:255:GLU:O	1:D:452:LYS:NZ	2.07	0.88
1:B:168:ARG:O	1:B:172:ASN:ND2	2.09	0.85
1:B:106:ASN:ND2	1:B:170:LYS:HD2	1.92	0.83
1:A:450:THR:HG22	1:A:465:GLN:HG3	1.61	0.83
1:C:121:TRP:O	1:C:125:THR:OG1	1.96	0.83
1:A:413:VAL:N	1:A:440:GLN:HE22	1.76	0.82
1:A:440:GLN:HB2	1:A:442:SER:N	1.94	0.82
1:C:338:VAL:HG22	1:C:504:GLU:HB3	1.61	0.82
1:A:356:GLN:OE1	4:A:701:HOH:O	1.96	0.82
1:C:122:LYS:NZ	1:C:144:LEU:O	2.13	0.82
1:A:540:ASP:HA	1:A:543:ILE:HD12	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:LEU:HD22	1:D:376:GLU:OE2	1.81	0.81
1:B:309:MET:HE2	1:B:404:ALA:HB3	1.62	0.81
1:C:456:LEU:HD21	1:D:100:LEU:HD13	1.62	0.81
1:A:31:ARG:NH1	1:A:32:LYS:O	2.14	0.80
1:D:369:LEU:HD13	1:D:376:GLU:OE1	1.82	0.80
1:B:534:ARG:NH2	1:B:540:ASP:OD1	2.16	0.79
1:C:319:LEU:HA	1:C:322:MET:HE3	1.63	0.79
1:C:183:ARG:NH1	1:C:205:ALA:O	2.15	0.79
1:A:27:GLN:OE1	1:A:43:SER:OG	2.01	0.79
1:B:354:LEU:HD21	1:B:519:ILE:HD13	1.65	0.79
1:B:534:ARG:HH21	1:B:540:ASP:CG	1.90	0.79
1:C:120:LYS:CD	1:C:124:GLU:OE1	2.25	0.78
1:C:206:MET:HA	1:C:206:MET:HE2	1.67	0.77
1:D:533:THR:HG23	1:D:535:GLY:H	1.49	0.76
1:D:226:THR:H	1:D:513:THR:HG21	1.50	0.76
1:C:288:GLU:HA	1:C:411:LYS:HB2	1.66	0.76
1:A:119:GLU:HA	1:A:122:LYS:HD3	1.68	0.75
1:C:141:GLU:OE2	1:C:144:LEU:HD22	1.84	0.75
1:D:133:LEU:O	1:D:137:GLY:N	2.18	0.75
1:C:262:THR:HG21	1:D:452:LYS:H	1.52	0.74
1:D:450:THR:HG22	1:D:465:GLN:HG2	1.70	0.74
1:C:485:GLU:CD	1:C:485:GLU:H	1.95	0.74
1:B:320:LEU:HD11	1:B:415:ILE:HD13	1.69	0.73
1:D:347:ILE:HD13	1:D:386:MET:HE2	1.69	0.73
1:A:69:SER:C	1:A:178:GLU:HG3	2.14	0.73
1:B:36:ILE:O	1:B:40:ILE:HG13	1.89	0.73
1:A:68:LYS:O	1:A:68:LYS:HG2	1.88	0.73
1:A:412:TYR:HA	1:A:440:GLN:HE22	1.52	0.73
1:B:322:MET:HE3	1:B:336:GLU:HB2	1.71	0.73
1:C:122:LYS:NZ	1:C:147:ILE:O	2.21	0.72
1:D:408:VAL:HG12	1:D:409:GLU:H	1.54	0.71
1:A:452:LYS:NZ	1:B:443:GLU:OE2	2.19	0.71
1:A:295:ARG:O	1:A:298:TYR:HB2	1.89	0.71
1:A:412:TYR:HA	1:A:440:GLN:NE2	2.06	0.71
1:A:315:GLN:NE2	4:A:702:HOH:O	2.21	0.71
1:C:456:LEU:CD2	1:D:100:LEU:HD13	2.21	0.70
1:C:193:VAL:HG12	1:C:197:VAL:HG23	1.72	0.70
1:A:468:LEU:HB3	1:B:468:LEU:HD11	1.74	0.70
1:D:439:ALA:O	1:D:440:GLN:NE2	2.25	0.69
1:A:132:ASN:HB3	1:A:136:ARG:HD3	1.75	0.69
1:A:320:LEU:HD11	1:A:415:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLY:O	1:A:525:LYS:NZ	2.26	0.69
1:A:354:LEU:HB2	1:A:526:PRO:HA	1.75	0.69
1:A:69:SER:O	1:A:178:GLU:HG3	1.92	0.68
1:D:295:ARG:NE	1:D:298:TYR:HB2	2.07	0.68
1:D:534:ARG:HH22	1:D:537:LYS:HG2	1.58	0.68
1:C:452:LYS:HZ3	1:D:259:ASN:HD22	1.42	0.68
1:C:86:LYS:HD3	1:C:129:TYR:HE1	1.60	0.67
1:A:318:ALA:HB1	1:A:337:LYS:HG2	1.76	0.67
1:A:274:TRP:O	1:A:394:ARG:NH1	2.27	0.67
1:C:438:ARG:NH2	1:C:442:SER:HB2	2.09	0.67
1:C:468:LEU:HD12	1:D:468:LEU:HB2	1.76	0.67
1:B:365:ILE:HD12	1:B:365:ILE:O	1.95	0.66
1:D:295:ARG:HD3	1:D:295:ARG:O	1.96	0.66
1:A:336:GLU:HA	1:A:339:SER:HB3	1.77	0.66
1:C:490:ASP:OD1	1:D:457:SER:HB2	1.95	0.66
1:D:289:THR:HB	1:D:411:LYS:HD3	1.76	0.66
1:A:416:ARG:NH2	1:A:548:PHE:CE2	2.64	0.66
1:A:66:GLU:O	1:A:69:SER:HB3	1.95	0.66
1:C:115:VAL:HG13	1:C:117:ASP:O	1.96	0.66
1:C:95:LEU:HD21	1:C:489:ASN:HB2	1.78	0.66
1:C:168:ARG:HA	1:C:171:GLU:CG	2.25	0.66
1:A:108:ILE:HD11	1:A:163:LEU:HD11	1.78	0.65
1:A:20:ILE:HA	1:A:23:VAL:HG13	1.77	0.65
1:D:112:ARG:NH1	1:D:113:THR:HG22	1.88	0.65
1:D:362:ASP:HB3	1:D:364:SER:HB2	1.78	0.65
1:B:447:VAL:HG23	1:B:470:LEU:HD11	1.78	0.65
1:C:206:MET:HE1	1:C:214:VAL:HG11	1.76	0.65
1:A:226:THR:H	1:A:513:THR:HG21	1.61	0.65
1:A:542:PHE:O	1:A:546:ASN:ND2	2.25	0.65
1:A:218:ILE:HD11	1:A:247:ARG:HG2	1.79	0.64
1:A:225:ASP:OD1	1:A:228:SER:OG	2.09	0.64
1:D:347:ILE:CD1	1:D:386:MET:HE2	2.26	0.64
1:C:108:ILE:HG22	1:C:148:SER:HB2	1.80	0.64
1:B:360:SER:HB3	1:B:365:ILE:HD11	1.79	0.64
1:C:343:CYS:O	1:C:391:ASN:HB2	1.97	0.64
1:A:230:ALA:O	1:A:234:GLN:HG2	1.97	0.64
1:A:432:ARG:HD2	1:A:549:LYS:HD2	1.80	0.64
1:D:362:ASP:CB	1:D:364:SER:HB2	2.27	0.63
1:A:413:VAL:N	1:A:440:GLN:NE2	2.38	0.63
1:B:435:LEU:HD13	1:B:447:VAL:HG22	1.79	0.63
1:D:287:LYS:NZ	1:D:409:GLU:OE1	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:O	1:A:69:SER:CB	2.46	0.62
1:A:278:ASN:HD21	2:A:602:EDO:H12	1.64	0.62
1:D:298:TYR:CE2	1:D:302:ILE:HD11	2.34	0.62
1:A:66:GLU:O	1:A:69:SER:N	2.27	0.62
1:D:357:TYR:CE1	1:D:368:TYR:HB2	2.34	0.62
1:A:83:LEU:O	1:A:87:LYS:HB2	2.00	0.62
1:A:33:PRO:C	1:A:35:ASP:H	2.08	0.61
1:D:92:LEU:HA	1:D:95:LEU:HD12	1.82	0.61
1:A:160:PHE:HE2	1:A:201:ILE:HG13	1.65	0.61
1:C:72:LEU:HD23	1:C:105:VAL:HG23	1.82	0.61
1:C:258:GLN:HB2	1:D:452:LYS:HE3	1.82	0.61
1:C:219:GLU:O	1:C:220:LYS:HG2	2.00	0.61
1:A:279:ILE:HG12	1:A:417:ILE:HD11	1.83	0.61
1:C:385:VAL:HG22	1:C:403:LYS:HG3	1.82	0.61
1:D:174:PHE:CE2	1:D:176:GLY:HA3	2.34	0.61
1:D:440:GLN:HG3	1:D:441:PRO:HA	1.82	0.61
1:C:445:MET:HB3	1:C:470:LEU:HD22	1.83	0.61
1:C:154:TYR:HB3	1:C:197:VAL:HG22	1.83	0.60
1:A:380:CYS:N	4:A:701:HOH:O	2.34	0.60
1:B:201:ILE:HA	1:B:205:ALA:HB3	1.83	0.60
1:D:122:LYS:NZ	1:D:144:LEU:O	2.34	0.60
1:D:530:GLN:O	1:D:533:THR:HG22	2.00	0.60
1:C:74:ILE:HD13	1:C:184:LEU:HB3	1.83	0.60
1:B:154:TYR:HB3	1:B:197:VAL:HG22	1.84	0.60
1:C:279:ILE:O	1:C:420:ARG:NH1	2.34	0.60
1:B:282:VAL:HG22	1:B:417:ILE:HG12	1.83	0.60
1:A:448:LYS:HE3	1:A:465:GLN:HB3	1.83	0.59
1:C:354:LEU:HD11	1:C:519:ILE:HD13	1.84	0.59
1:C:484:TYR:N	1:C:485:GLU:OE1	2.35	0.59
1:A:387:ARG:NH1	1:A:389:ASN:OD1	2.35	0.59
1:C:120:LYS:CD	1:C:124:GLU:CD	2.75	0.59
1:C:448:LYS:HG2	1:C:467:GLU:HG2	1.84	0.59
1:A:256:MET:HB2	1:A:439:ALA:CB	2.33	0.59
1:C:362:ASP:OD2	1:C:364:SER:OG	2.18	0.59
1:A:66:GLU:C	1:A:69:SER:H	2.10	0.59
1:B:215:ARG:HD3	1:B:246:TYR:CE1	2.38	0.59
1:B:286:PHE:O	1:B:404:ALA:HA	2.03	0.59
1:C:242:GLU:OE2	1:C:247:ARG:NH2	2.33	0.59
1:B:256:MET:HE3	1:B:415:ILE:HD11	1.85	0.58
1:D:224:ARG:HH22	1:D:301:ASN:ND2	2.01	0.58
1:D:231:GLU:HA	1:D:234:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ARG:HA	1:B:337:LYS:HE2	1.84	0.58
1:B:309:MET:HE1	1:B:384:ALA:HB3	1.85	0.58
1:C:288:GLU:HG2	1:C:411:LYS:HE2	1.84	0.58
1:B:23:VAL:O	1:B:27:GLN:HG3	2.02	0.58
1:D:292:THR:HG21	1:D:299:PHE:HD1	1.69	0.58
1:A:439:ALA:C	1:A:440:GLN:HG2	2.29	0.58
1:C:122:LYS:HB2	1:C:144:LEU:HD23	1.86	0.57
1:A:132:ASN:HB3	1:A:136:ARG:CD	2.33	0.57
1:A:43:SER:HA	1:A:46:SER:OG	2.04	0.57
1:C:67:GLN:HB3	1:C:102:PRO:HG3	1.87	0.57
1:D:315:GLN:NE2	1:D:504:GLU:OE2	2.33	0.57
1:B:248:ILE:HD12	1:B:499:PHE:HE2	1.70	0.57
1:C:287:LYS:NZ	1:C:409:GLU:OE2	2.36	0.57
1:C:219:GLU:HG3	1:C:484:TYR:HE1	1.70	0.57
1:B:504:GLU:HA	1:B:507:VAL:HG12	1.86	0.57
1:A:416:ARG:NH2	1:A:548:PHE:HE2	2.02	0.57
1:A:506:ASP:O	1:A:510:ARG:HG2	2.05	0.57
1:A:316:ILE:CG2	1:A:415:ILE:HD11	2.35	0.56
1:C:168:ARG:HA	1:C:171:GLU:HG2	1.87	0.56
1:D:456:LEU:HD12	1:D:456:LEU:H	1.70	0.56
1:A:226:THR:N	1:A:513:THR:HG21	2.20	0.56
1:A:285:THR:HG21	1:A:287:LYS:HE3	1.87	0.56
1:B:27:GLN:OE1	1:B:134:SER:HA	2.05	0.56
1:C:127:MET:HA	1:C:130:PHE:CD1	2.41	0.56
1:C:452:LYS:HZ2	1:D:259:ASN:HB2	1.70	0.56
1:D:453:VAL:C	1:D:455:GLY:H	2.13	0.56
1:B:286:PHE:HB2	1:B:313:LEU:HD21	1.88	0.56
1:C:123:HIS:ND1	1:C:141:GLU:OE1	2.39	0.56
1:D:252:LEU:HD21	1:D:315:GLN:HB3	1.86	0.56
1:B:515:LEU:O	1:B:519:ILE:HG13	2.06	0.56
1:C:353:VAL:HG21	1:C:539:ALA:HA	1.88	0.56
1:B:257:VAL:HG21	1:B:498:ASN:ND2	2.20	0.56
1:B:284:ILE:HD13	1:B:316:ILE:HG22	1.88	0.56
1:C:344:ILE:HG12	1:C:390:ILE:HG12	1.88	0.56
1:A:121:TRP:O	1:A:125:THR:OG1	2.22	0.55
1:C:63:VAL:O	1:C:67:GLN:NE2	2.40	0.55
1:C:202:HIS:CB	1:C:239:PHE:HD1	2.20	0.55
1:C:252:LEU:HD21	1:C:315:GLN:HB3	1.86	0.55
1:C:222:PHE:CE2	1:C:247:ARG:HB3	2.41	0.55
1:B:257:VAL:HG13	1:B:319:LEU:HD13	1.88	0.55
1:B:63:VAL:HB	1:B:65:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:NH2	1:D:301:ASN:ND2	2.55	0.55
1:C:259:ASN:N	1:D:452:LYS:HZ2	2.04	0.55
1:D:122:LYS:HB3	1:D:144:LEU:HD22	1.89	0.55
1:B:295:ARG:HB3	1:B:298:TYR:HD2	1.70	0.55
1:C:248:ILE:HG12	1:C:499:PHE:CE1	2.42	0.55
1:C:183:ARG:HH12	1:C:205:ALA:C	2.13	0.55
1:C:84:ALA:HA	1:C:88:THR:HG22	1.89	0.54
1:C:483:ALA:N	1:C:485:GLU:OE1	2.40	0.54
1:B:226:THR:H	1:B:513:THR:HG21	1.71	0.54
1:B:482:ASP:N	1:B:485:GLU:OE2	2.35	0.54
1:C:66:GLU:HG3	1:C:66:GLU:O	2.07	0.54
1:A:64:LYS:HB3	1:A:67:GLN:NE2	2.21	0.54
1:B:19:GLY:O	1:B:23:VAL:HG13	2.07	0.54
1:C:251:TYR:O	1:C:257:VAL:HG21	2.08	0.54
1:C:485:GLU:OE1	1:C:485:GLU:N	2.26	0.54
1:A:201:ILE:HA	1:A:205:ALA:HB3	1.90	0.54
1:A:66:GLU:O	1:A:66:GLU:HG2	2.06	0.54
1:D:226:THR:N	1:D:513:THR:HG21	2.21	0.54
1:C:120:LYS:O	1:C:124:GLU:HG2	2.08	0.54
1:C:168:ARG:HA	1:C:171:GLU:HG3	1.90	0.54
1:D:256:MET:HG3	1:D:443:GLU:CG	2.37	0.54
1:A:281:CYS:SG	1:A:548:PHE:HD1	2.31	0.53
1:B:254:LYS:O	1:B:258:GLN:HG2	2.09	0.53
1:D:169:GLU:HB3	1:D:170:LYS:HG3	1.90	0.53
1:C:222:PHE:HE2	1:C:247:ARG:HB3	1.74	0.53
1:C:274:TRP:HA	1:C:279:ILE:HD11	1.89	0.53
1:C:430:THR:HA	1:C:450:THR:HG21	1.89	0.53
1:D:206:MET:HE2	1:D:206:MET:HA	1.91	0.53
1:A:141:GLU:HA	1:A:144:LEU:HD12	1.91	0.53
1:B:509:TRP:O	1:B:513:THR:HG23	2.09	0.53
1:C:262:THR:HG21	1:D:452:LYS:N	2.23	0.53
1:D:401:ILE:HG21	1:D:543:ILE:HG22	1.89	0.53
1:C:106:ASN:OD1	1:C:170:LYS:HD3	2.09	0.53
1:C:224:ARG:N	1:C:228:SER:OG	2.32	0.53
1:C:248:ILE:HG12	1:C:499:PHE:HE1	1.73	0.53
1:B:288:GLU:OE2	1:B:406:LYS:NZ	2.42	0.53
1:D:206:MET:HE1	1:D:240:PHE:CE1	2.44	0.53
1:B:348:THR:OG1	1:D:179:LYS:NZ	2.32	0.53
1:D:112:ARG:CZ	1:D:113:THR:HG23	2.33	0.53
1:C:436:VAL:O	1:C:445:MET:HA	2.08	0.52
1:C:286:PHE:O	1:C:404:ALA:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:NH1	1:D:301:ASN:O	2.42	0.52
1:B:257:VAL:HG21	1:B:498:ASN:HD22	1.74	0.52
1:C:167:ILE:HG22	1:C:171:GLU:OE1	2.10	0.52
1:C:413:VAL:HG12	1:C:440:GLN:HG2	1.92	0.52
1:B:264:ARG:HD2	1:B:274:TRP:CE2	2.45	0.52
1:B:409:GLU:HG2	1:B:410:GLN:HG2	1.92	0.52
1:C:437:ILE:HA	1:C:444:ALA:O	2.10	0.52
1:C:86:LYS:CD	1:C:129:TYR:HE1	2.23	0.52
1:D:133:LEU:HG	1:D:134:SER:H	1.76	0.51
1:C:206:MET:HA	1:C:206:MET:CE	2.38	0.51
1:C:371:ASP:HB3	1:C:374:VAL:HG23	1.93	0.51
1:C:349:LYS:HB2	1:C:524:ILE:HD11	1.93	0.51
1:A:155:ASP:OD1	1:A:155:ASP:N	2.44	0.51
1:A:429:ALA:O	1:A:463:THR:OG1	2.29	0.51
1:C:156:SER:OG	1:C:159:ASP:HB2	2.10	0.51
1:A:96:TYR:CD2	1:A:143:PHE:HB2	2.46	0.50
1:C:155:ASP:N	1:C:155:ASP:OD1	2.44	0.50
1:C:419:PHE:CE2	1:D:269:ILE:HD11	2.46	0.50
1:D:61:CYS:SG	1:D:63:VAL:HG22	2.51	0.50
1:D:222:PHE:CZ	1:D:247:ARG:HG2	2.47	0.50
1:D:431:GLN:CD	1:D:551:GLN:HB3	2.35	0.50
1:A:534:ARG:NH2	3:A:603:SO4:O4	2.43	0.50
1:A:457:SER:OG	1:A:462:GLN:NE2	2.32	0.50
1:B:72:LEU:HD23	1:B:105:VAL:HG23	1.94	0.50
1:C:127:MET:HE2	1:C:141:GLU:CD	2.36	0.50
1:D:224:ARG:HH22	1:D:301:ASN:CG	2.19	0.50
1:B:74:ILE:HD13	1:B:184:LEU:HB3	1.94	0.50
1:B:136:ARG:HD3	1:B:479:ARG:HD3	1.92	0.50
1:C:122:LYS:CB	1:C:144:LEU:HD23	2.42	0.50
1:A:503:ASP:O	1:A:507:VAL:HG23	2.10	0.50
1:C:134:SER:HA	1:C:137:GLY:HA3	1.93	0.50
1:D:322:MET:HE3	1:D:336:GLU:HB2	1.92	0.50
1:A:371:ASP:HB3	1:A:374:VAL:HG22	1.94	0.50
1:B:238:PRO:C	1:B:239:PHE:HD1	2.20	0.50
1:B:327:SER:OG	1:B:328:LEU:N	2.44	0.50
1:B:338:VAL:HG13	1:B:504:GLU:HB3	1.94	0.50
1:B:220:LYS:C	1:B:220:LYS:HD2	2.37	0.50
1:C:503:ASP:O	1:C:507:VAL:HG13	2.12	0.50
1:D:295:ARG:HE	1:D:298:TYR:HB2	1.76	0.49
1:D:191:PRO:HA	1:D:194:PHE:CD2	2.47	0.49
1:D:197:VAL:O	1:D:201:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HD21	1:B:415:ILE:HG21	1.94	0.49
1:A:242:GLU:OE1	1:A:247:ARG:NH2	2.45	0.49
1:C:201:ILE:HG22	1:C:206:MET:HE3	1.94	0.49
1:D:225:ASP:N	1:D:228:SER:OG	2.45	0.49
1:D:488:ILE:O	1:D:492:LEU:HD12	2.13	0.49
1:C:137:GLY:C	1:C:139:HIS:H	2.20	0.49
1:A:416:ARG:HG2	1:A:548:PHE:HZ	1.78	0.49
1:A:468:LEU:HG	1:B:469:ASP:O	2.12	0.49
1:A:487:LEU:HB3	1:A:499:PHE:CZ	2.47	0.49
1:B:119:GLU:OE2	1:B:122:LYS:NZ	2.38	0.49
1:A:174:PHE:CE2	1:A:176:GLY:HA3	2.48	0.49
1:B:184:LEU:HD12	1:B:215:ARG:O	2.13	0.49
1:B:440:GLN:HA	1:B:441:PRO:C	2.37	0.49
1:C:429:ALA:O	1:C:463:THR:OG1	2.24	0.49
1:A:120:LYS:NZ	1:A:124:GLU:OE2	2.43	0.49
1:A:285:THR:O	1:A:413:VAL:HA	2.12	0.49
1:D:118:VAL:HG21	1:D:149:TYR:HB2	1.95	0.49
1:D:357:TYR:CD1	1:D:368:TYR:HB2	2.48	0.49
1:D:534:ARG:NH2	1:D:537:LYS:HG2	2.27	0.49
1:C:331:GLU:HA	1:C:334:ARG:HG2	1.94	0.49
1:C:509:TRP:O	1:C:513:THR:OG1	2.29	0.49
1:D:222:PHE:O	1:D:229:SER:HB2	2.13	0.49
1:A:39:PHE:C	1:A:39:PHE:CD1	2.91	0.48
1:D:256:MET:HG3	1:D:443:GLU:HG3	1.94	0.48
1:D:306:ARG:CZ	1:D:516:LEU:HD22	2.43	0.48
1:D:507:VAL:O	1:D:511:ILE:HG13	2.13	0.48
1:D:77:PHE:HA	1:D:110:TYR:HB3	1.94	0.48
1:D:201:ILE:HG22	1:D:206:MET:HE3	1.95	0.48
1:D:226:THR:HA	1:D:509:TRP:HB3	1.95	0.48
1:D:431:GLN:CD	1:D:465:GLN:OE1	2.56	0.48
1:A:71:ALA:HB2	1:A:174:PHE:CG	2.49	0.48
1:B:337:LYS:NZ	1:B:497:THR:O	2.46	0.48
1:D:282:VAL:HG12	1:D:417:ILE:HD13	1.95	0.48
1:A:256:MET:HB2	1:A:439:ALA:HB2	1.95	0.48
1:C:174:PHE:CE2	1:C:176:GLY:HA3	2.48	0.48
1:C:248:ILE:HG23	1:C:487:LEU:CD1	2.43	0.48
1:D:317:LEU:HA	1:D:320:LEU:HD12	1.94	0.48
1:A:251:TYR:HB3	1:A:312:HIS:CE1	2.49	0.48
1:B:355:GLY:HA2	1:B:527:ILE:O	2.14	0.48
1:B:485:GLU:HA	1:B:488:ILE:HG22	1.95	0.48
1:C:115:VAL:HG21	1:C:121:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:PHE:O	1:D:404:ALA:HA	2.13	0.48
1:D:308:VAL:HG12	1:D:312:HIS:HD2	1.77	0.48
1:C:202:HIS:HA	1:C:206:MET:HG2	1.94	0.48
1:C:354:LEU:HD13	1:C:381:PRO:HB3	1.95	0.48
1:C:457:SER:HA	1:C:458:GLY:HA3	1.52	0.48
1:A:433:ASN:OD1	1:B:268:ARG:N	2.47	0.48
1:C:270:PHE:O	1:C:274:TRP:HB2	2.14	0.48
1:D:423:VAL:HG23	1:D:424:HIS:ND1	2.29	0.48
1:D:114:LYS:HG3	1:D:115:VAL:N	2.28	0.48
1:A:442:SER:O	1:A:442:SER:OG	2.30	0.47
1:C:437:ILE:HG12	1:C:445:MET:HG3	1.96	0.47
1:B:453:VAL:HG12	1:B:462:GLN:O	2.14	0.47
1:A:529:TYR:CD2	1:A:536:PRO:HD3	2.49	0.47
1:B:24:LEU:O	1:B:28:VAL:HG13	2.13	0.47
1:B:239:PHE:N	1:B:239:PHE:CD1	2.82	0.47
1:C:344:ILE:HB	1:C:511:ILE:HD13	1.96	0.47
1:A:514:PRO:O	1:A:518:GLN:HG3	2.14	0.47
1:B:75:ILE:HD13	1:B:185:PHE:CE1	2.50	0.47
1:B:208:GLN:HG3	4:B:1103:HOH:O	2.15	0.47
1:C:219:GLU:HG3	1:C:484:TYR:CE1	2.50	0.47
1:C:292:THR:HG21	1:C:368:TYR:HE2	1.79	0.47
1:B:86:LYS:HD3	1:B:129:TYR:CE1	2.50	0.47
1:D:206:MET:HE1	1:D:240:PHE:HE1	1.80	0.47
1:D:218:ILE:HG22	1:D:222:PHE:HE1	1.78	0.47
1:D:461:ARG:O	1:D:463:THR:HG23	2.13	0.47
1:A:509:TRP:O	1:A:513:THR:HG23	2.15	0.47
1:C:306:ARG:NH2	1:C:516:LEU:HD22	2.28	0.47
1:D:292:THR:HG21	1:D:299:PHE:CD1	2.50	0.47
1:D:298:TYR:O	1:D:302:ILE:HG13	2.14	0.47
1:D:416:ARG:NE	1:D:434:GLU:OE2	2.34	0.47
1:A:38:GLN:OE1	1:B:472:TYR:HA	2.14	0.47
1:B:28:VAL:HG23	1:B:29:LEU:HG	1.95	0.47
1:B:127:MET:HE2	1:B:127:MET:HB3	1.76	0.47
1:B:357:TYR:HA	1:B:529:TYR:O	2.14	0.47
1:B:436:VAL:HG11	1:B:446:TYR:CZ	2.49	0.47
1:C:268:ARG:N	1:D:433:ASN:OD1	2.47	0.47
1:C:334:ARG:O	1:C:338:VAL:HG23	2.14	0.47
1:D:356:GLN:HB2	1:D:526:PRO:HB2	1.96	0.47
1:D:445:MET:HE3	1:D:470:LEU:HD21	1.95	0.47
1:D:459:ASP:C	1:D:460:LEU:HD12	2.40	0.47
1:D:224:ARG:NH2	1:D:301:ASN:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:O	1:A:147:ILE:HA	2.15	0.47
1:B:365:ILE:CD1	1:B:531:ALA:HB3	2.44	0.47
1:D:251:TYR:CD2	1:D:312:HIS:HB3	2.50	0.47
1:A:281:CYS:HG	1:A:548:PHE:HD1	1.62	0.46
1:C:63:VAL:C	1:C:67:GLN:HE22	2.23	0.46
1:C:251:TYR:CD2	1:C:312:HIS:HB3	2.50	0.46
1:A:457:SER:CB	1:A:462:GLN:HE22	2.27	0.46
1:C:249:ASP:O	1:C:251:TYR:N	2.48	0.46
1:D:415:ILE:HD11	1:D:417:ILE:HD11	1.96	0.46
1:D:415:ILE:HG12	1:D:416:ARG:N	2.30	0.46
1:A:254:LYS:HD3	1:A:490:ASP:OD2	2.16	0.46
1:A:323:GLU:CD	1:A:394:ARG:HE	2.22	0.46
1:D:75:ILE:HD13	1:D:185:PHE:CE1	2.51	0.46
1:B:197:VAL:O	1:B:201:ILE:HG12	2.15	0.46
1:B:387:ARG:CZ	1:B:399:PRO:HB3	2.46	0.46
1:C:257:VAL:HA	1:C:260:ILE:HD12	1.96	0.46
1:D:69:SER:O	1:D:177:PRO:HD2	2.15	0.46
1:A:64:LYS:HB3	1:A:67:GLN:CD	2.40	0.46
1:C:193:VAL:HG12	1:C:197:VAL:CG2	2.45	0.46
1:C:259:ASN:OD1	1:C:263:THR:OG1	2.27	0.46
1:D:191:PRO:HA	1:D:194:PHE:CE2	2.51	0.46
1:C:127:MET:HE2	1:C:141:GLU:OE1	2.15	0.46
1:D:281:CYS:SG	1:D:548:PHE:HD1	2.38	0.46
1:D:431:GLN:H	1:D:450:THR:HG21	1.81	0.46
1:C:78:GLY:O	1:C:81:GLY:N	2.49	0.46
1:D:242:GLU:OE1	1:D:247:ARG:NH2	2.48	0.46
1:A:207:PRO:HD3	1:A:214:VAL:HB	1.98	0.46
1:C:119:GLU:HG3	1:C:123:HIS:NE2	2.30	0.46
1:B:362:ASP:OD1	1:B:364:SER:OG	2.22	0.46
1:C:167:ILE:O	1:C:171:GLU:HG2	2.16	0.46
1:D:282:VAL:HG23	1:D:400:PHE:HA	1.97	0.46
1:D:453:VAL:O	1:D:455:GLY:N	2.47	0.46
1:D:462:GLN:OE1	1:D:462:GLN:HA	2.16	0.46
1:A:43:SER:O	1:A:47:LEU:HG	2.16	0.45
1:A:163:LEU:O	1:A:166:VAL:HG12	2.16	0.45
1:A:296:GLY:C	1:A:298:TYR:H	2.24	0.45
1:A:459:ASP:HB3	1:A:462:GLN:HG3	1.98	0.45
1:B:199:GLU:HB2	1:B:239:PHE:HE2	1.79	0.45
1:B:354:LEU:HD23	1:B:381:PRO:HG3	1.96	0.45
1:C:411:LYS:O	1:C:411:LYS:HG2	2.16	0.45
1:D:122:LYS:HZ3	1:D:147:ILE:HB	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:PHE:CE2	1:C:218:ILE:HB	2.51	0.45
1:D:311:ASN:OD1	1:D:311:ASN:N	2.43	0.45
1:D:385:VAL:HG22	1:D:403:LYS:HG3	1.99	0.45
1:B:270:PHE:HA	1:B:273:VAL:HG12	1.98	0.45
1:C:440:GLN:HB2	1:C:441:PRO:HA	1.99	0.45
1:D:347:ILE:HD13	1:D:386:MET:CE	2.44	0.45
1:A:412:TYR:CA	1:A:440:GLN:HE22	2.23	0.45
1:C:67:GLN:HG3	1:C:102:PRO:HA	1.99	0.45
1:C:345:GLU:HG3	1:C:346:PRO:HD2	1.97	0.45
1:D:419:PHE:O	1:D:432:ARG:HB3	2.16	0.45
1:B:250:HIS:HA	1:B:487:LEU:HD12	1.98	0.45
1:C:252:LEU:HA	1:C:257:VAL:HG21	1.98	0.45
1:B:264:ARG:HD2	1:B:274:TRP:CD2	2.51	0.45
1:B:464:HIS:ND1	1:B:464:HIS:C	2.75	0.45
1:B:409:GLU:OE1	1:B:534:ARG:HA	2.17	0.45
1:B:106:ASN:HD22	1:B:170:LYS:CD	2.19	0.45
1:B:507:VAL:O	1:B:511:ILE:HG13	2.17	0.45
1:D:284:ILE:HG22	1:D:313:LEU:HD13	1.99	0.45
1:A:75:ILE:HD13	1:A:185:PHE:CE2	2.52	0.45
1:D:429:ALA:HB2	1:D:461:ARG:HG2	1.98	0.45
1:C:257:VAL:O	1:C:319:LEU:HD13	2.17	0.44
1:D:362:ASP:HB2	1:D:364:SER:HB2	1.99	0.44
1:C:107:ILE:HB	1:C:147:ILE:HD12	1.99	0.44
1:C:456:LEU:O	1:C:457:SER:C	2.60	0.44
1:A:315:GLN:OE1	1:A:337:LYS:NZ	2.39	0.44
1:B:122:LYS:HB3	1:B:144:LEU:HD13	2.00	0.44
1:B:309:MET:CE	1:B:384:ALA:HB3	2.47	0.44
1:C:195:ALA:HA	1:C:236:LEU:HD11	1.99	0.44
1:D:356:GLN:HA	1:D:382:THR:OG1	2.17	0.44
1:A:452:LYS:HD2	1:B:258:GLN:HG3	1.99	0.44
1:A:132:ASN:O	1:A:134:SER:N	2.43	0.44
1:A:287:LYS:HB2	1:A:412:TYR:H	1.82	0.44
1:A:475:ARG:HG2	1:A:477:ASP:H	1.82	0.44
1:B:481:PRO:HA	1:B:485:GLU:OE2	2.18	0.44
1:C:168:ARG:NH1	1:C:208:GLN:OE1	2.51	0.44
1:C:183:ARG:CZ	1:C:207:PRO:HA	2.47	0.44
1:D:91:ALA:CB	1:D:485:GLU:HG2	2.48	0.44
1:D:285:THR:HG22	1:D:287:LYS:HG3	2.00	0.44
1:D:459:ASP:O	1:D:461:ARG:N	2.51	0.44
1:B:306:ARG:CZ	1:B:516:LEU:HD22	2.47	0.44
1:A:357:TYR:CE1	1:A:368:TYR:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:THR:OG1	1:B:514:PRO:HD3	2.17	0.44
1:C:181:GLY:O	1:C:212:GLY:HA3	2.18	0.44
1:C:251:TYR:CD1	1:C:254:LYS:HD2	2.53	0.44
1:A:89:PHE:HA	1:A:92:LEU:HD12	2.00	0.44
1:B:77:PHE:O	1:B:188:ALA:HB3	2.18	0.44
1:C:163:LEU:O	1:C:166:VAL:HG22	2.18	0.44
1:D:278:ASN:C	1:D:420:ARG:HG3	2.43	0.44
1:A:120:LYS:HG3	1:A:124:GLU:OE2	2.18	0.43
1:A:274:TRP:HA	1:A:279:ILE:HD11	2.00	0.43
1:D:164:ASP:O	1:D:168:ARG:HG3	2.18	0.43
1:A:20:ILE:O	1:A:23:VAL:HG22	2.17	0.43
1:A:219:GLU:CD	1:A:250:HIS:HE2	2.27	0.43
1:A:299:PHE:HE1	1:A:303:GLY:C	2.26	0.43
1:A:331:GLU:OE1	1:A:501:ARG:NH1	2.48	0.43
1:A:354:LEU:HB2	1:A:526:PRO:CA	2.45	0.43
1:B:239:PHE:HD1	1:B:239:PHE:N	2.17	0.43
1:B:416:ARG:HH11	1:B:434:GLU:CD	2.26	0.43
1:C:503:ASP:OD1	1:C:503:ASP:N	2.50	0.43
1:D:292:THR:O	1:D:295:ARG:N	2.47	0.43
1:C:292:THR:HG21	1:C:368:TYR:CE2	2.53	0.43
1:D:201:ILE:HG22	1:D:206:MET:CE	2.48	0.43
1:D:459:ASP:C	1:D:461:ARG:H	2.26	0.43
1:A:33:PRO:C	1:A:35:ASP:N	2.75	0.43
1:A:322:MET:HE3	1:A:336:GLU:HB2	2.01	0.43
1:B:336:GLU:HA	1:B:339:SER:OG	2.18	0.43
1:D:119:GLU:HA	1:D:122:LYS:HD2	2.00	0.43
1:D:259:ASN:OD1	1:D:262:THR:HB	2.18	0.43
1:A:24:LEU:O	1:A:28:VAL:HG12	2.17	0.43
1:C:487:LEU:HD23	1:C:487:LEU:HA	1.66	0.43
1:A:328:LEU:HD21	1:B:425:PRO:HG2	2.01	0.43
1:A:355:GLY:C	1:A:526:PRO:HB2	2.43	0.43
1:B:199:GLU:CG	1:B:203:LYS:HE3	2.49	0.43
1:B:409:GLU:HG2	1:B:410:GLN:N	2.32	0.43
1:C:390:ILE:HD12	1:C:400:PHE:CZ	2.54	0.43
1:C:464:HIS:O	1:C:464:HIS:ND1	2.52	0.43
1:D:118:VAL:CG2	1:D:149:TYR:HB2	2.48	0.43
1:A:284:ILE:HG12	1:A:415:ILE:HD13	2.00	0.43
1:A:191:PRO:HA	1:A:194:PHE:CD2	2.54	0.43
1:A:453:VAL:HG12	1:A:462:GLN:O	2.18	0.43
1:B:71:ALA:HB2	1:B:174:PHE:CG	2.54	0.43
1:B:77:PHE:HA	1:B:110:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLY:HA2	1:C:208:GLN:NE2	2.33	0.43
1:C:219:GLU:HG2	1:C:248:ILE:HB	2.00	0.43
1:C:484:TYR:HA	1:C:487:LEU:HB2	2.00	0.43
1:A:123:HIS:O	1:A:127:MET:HE2	2.19	0.42
1:A:187:LEU:HD12	1:A:218:ILE:HG22	2.00	0.42
1:A:471:THR:HG21	1:B:452:LYS:HZ3	1.84	0.42
1:C:268:ARG:NH1	1:D:420:ARG:HB2	2.33	0.42
1:A:68:LYS:O	1:A:69:SER:C	2.56	0.42
1:C:249:ASP:C	1:C:251:TYR:H	2.27	0.42
1:A:299:PHE:O	1:A:299:PHE:HD1	2.03	0.42
1:A:432:ARG:NH1	2:A:601:EDO:O1	2.40	0.42
1:C:320:LEU:HD11	1:C:415:ILE:HD13	2.00	0.42
1:A:292:THR:HG22	1:A:299:PHE:HD2	1.83	0.42
1:A:336:GLU:CA	1:A:339:SER:HB3	2.47	0.42
1:B:334:ARG:HD3	1:B:496:SER:O	2.20	0.42
1:C:93:PHE:CD2	1:C:130:PHE:HD2	2.37	0.42
1:C:183:ARG:HH11	1:C:183:ARG:HD2	1.54	0.42
1:D:357:TYR:HA	1:D:529:TYR:O	2.19	0.42
1:B:469:ASP:OD1	1:B:471:THR:HG23	2.19	0.42
1:D:462:GLN:H	1:D:462:GLN:HG2	1.44	0.42
1:C:289:THR:HG22	1:C:408:VAL:O	2.19	0.42
1:D:529:TYR:CD1	1:D:536:PRO:HD3	2.54	0.42
1:A:513:THR:OG1	1:A:514:PRO:HD3	2.20	0.42
1:B:23:VAL:HG12	1:B:127:MET:SD	2.59	0.42
1:C:360:SER:OG	1:C:362:ASP:HB3	2.20	0.42
1:D:63:VAL:HG13	1:D:99:GLY:O	2.20	0.42
1:D:274:TRP:O	1:D:394:ARG:NH1	2.49	0.42
1:D:292:THR:C	1:D:294:GLY:H	2.27	0.42
1:D:356:GLN:OE1	1:D:369:LEU:HD11	2.20	0.42
1:B:85:LYS:HG3	1:B:86:LYS:HG2	2.02	0.42
1:C:63:VAL:CG1	1:C:99:GLY:O	2.67	0.42
1:C:515:LEU:O	1:C:519:ILE:HG13	2.19	0.42
1:B:258:GLN:O	1:B:262:THR:HB	2.20	0.42
1:B:338:VAL:HG11	1:B:503:ASP:CG	2.43	0.42
1:C:249:ASP:C	1:C:251:TYR:N	2.78	0.42
1:D:140:ALA:O	1:D:144:LEU:HD12	2.20	0.42
1:D:429:ALA:HB1	1:D:461:ARG:O	2.20	0.42
1:A:191:PRO:HG3	1:A:221:PRO:HG2	2.02	0.42
1:A:334:ARG:NH1	1:A:496:SER:HB3	2.34	0.42
1:B:346:PRO:HG2	1:D:210:VAL:O	2.20	0.42
1:C:225:ASP:HB2	1:C:513:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD23	1:A:87:LYS:HB2	2.01	0.41
1:C:137:GLY:C	1:C:139:HIS:N	2.77	0.41
1:C:248:ILE:HG23	1:C:487:LEU:HD12	2.00	0.41
1:D:156:SER:HB3	1:D:159:ASP:HB2	2.02	0.41
1:B:74:ILE:CD1	1:B:184:LEU:HD23	2.50	0.41
1:B:292:THR:O	1:B:292:THR:OG1	2.37	0.41
1:C:468:LEU:HD12	1:D:468:LEU:CB	2.48	0.41
1:A:311:ASN:OD1	1:A:312:HIS:N	2.53	0.41
1:B:91:ALA:O	1:B:95:LEU:HD22	2.20	0.41
1:C:259:ASN:HB2	1:D:452:LYS:HZ2	1.85	0.41
1:D:132:ASN:HA	1:D:135:GLU:OE1	2.21	0.41
1:A:191:PRO:HG3	1:A:221:PRO:O	2.20	0.41
1:A:336:GLU:C	1:A:339:SER:HB3	2.46	0.41
1:B:248:ILE:HD12	1:B:499:PHE:CE2	2.53	0.41
1:B:338:VAL:CG1	1:B:504:GLU:HB3	2.50	0.41
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.73	0.41
1:C:320:LEU:HD21	1:C:415:ILE:HD13	2.02	0.41
1:C:341:LEU:HA	1:C:344:ILE:HD12	2.03	0.41
1:C:362:ASP:OD2	1:C:362:ASP:C	2.63	0.41
1:D:256:MET:HG3	1:D:443:GLU:HG2	2.02	0.41
1:B:406:LYS:NZ	4:B:1104:HOH:O	2.54	0.41
1:C:183:ARG:HB2	1:C:214:VAL:HG23	2.02	0.41
1:C:202:HIS:CG	1:C:239:PHE:HD1	2.38	0.41
1:C:265:PHE:HB3	1:D:425:PRO:CD	2.50	0.41
1:A:225:ASP:N	1:A:228:SER:OG	2.54	0.41
1:B:215:ARG:NH1	1:B:491:ALA:O	2.54	0.41
1:B:447:VAL:HG23	1:B:470:LEU:CD1	2.48	0.41
1:C:256:MET:HA	1:C:259:ASN:HB2	2.02	0.41
1:C:482:ASP:C	1:C:485:GLU:OE1	2.64	0.41
1:A:127:MET:HE2	1:A:127:MET:HB3	1.92	0.41
1:B:226:THR:N	1:B:513:THR:HG21	2.36	0.41
1:B:345:GLU:OE2	1:D:70:ARG:NH1	2.47	0.41
1:C:180:GLY:HA2	1:C:208:GLN:CD	2.46	0.41
1:C:246:TYR:HD2	1:C:499:PHE:CD2	2.39	0.41
1:D:347:ILE:HD11	1:D:388:LEU:HD22	2.02	0.41
1:D:431:GLN:NE2	1:D:465:GLN:OE1	2.54	0.41
1:D:456:LEU:O	1:D:458:GLY:N	2.50	0.41
1:A:13:TYR:O	1:A:13:TYR:CG	2.74	0.41
1:B:202:HIS:ND1	1:B:206:MET:HE2	2.36	0.41
1:B:332:CYS:HA	1:B:335:ASP:HB2	2.03	0.41
1:B:513:THR:HA	1:B:516:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:MET:SD	1:C:384:ALA:HB3	2.61	0.41
1:D:242:GLU:CD	1:D:502:LYS:HB2	2.46	0.41
1:A:250:HIS:H	1:A:250:HIS:CD2	2.39	0.40
1:B:36:ILE:HG22	1:B:40:ILE:HD11	2.03	0.40
1:C:117:ASP:OD1	1:C:120:LYS:HG3	2.21	0.40
1:C:456:LEU:HD23	1:D:489:ASN:ND2	2.36	0.40
1:B:12:ALA:HB1	1:B:15:ALA:H	1.86	0.40
1:D:279:ILE:HA	1:D:419:PHE:HA	2.03	0.40
1:A:14:VAL:HA	1:A:17:VAL:HB	2.04	0.40
1:A:45:LEU:O	1:A:48:GLN:HG2	2.22	0.40
1:C:183:ARG:HB2	1:C:214:VAL:HA	2.03	0.40
1:A:421:ASP:HB2	1:A:432:ARG:NH1	2.35	0.40
1:A:479:ARG:HD2	1:A:479:ARG:HA	1.87	0.40
1:D:122:LYS:NZ	1:D:147:ILE:O	2.46	0.40
1:A:14:VAL:HA	1:A:17:VAL:H	1.85	0.40
1:A:160:PHE:CE2	1:A:201:ILE:HG13	2.51	0.40
1:A:431:GLN:HB3	1:A:549:LYS:NZ	2.37	0.40
1:B:283:GLN:OE1	1:B:285:THR:OG1	2.39	0.40
1:B:469:ASP:C	1:B:470:LEU:HD12	2.46	0.40
1:C:465:GLN:HE21	1:C:465:GLN:HB3	1.58	0.40
1:D:219:GLU:OE2	1:D:484:TYR:OH	2.21	0.40
1:D:261:ILE:HD13	1:D:333:ILE:HD13	2.03	0.40
1:D:290:ILE:HA	1:D:290:ILE:HD12	1.82	0.40

All (2) 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:A:112:ARG:NH1	1:C:159:ASP:OD1[2_646]	1.93	0.27
1:A:175:LYS:NZ	1:A:526:PRO:O[1_545]	2.16	0.04

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	526/562 (94%)	488 (93%)	34 (6%)	4 (1%)	16	44
1	B	519/562 (92%)	493 (95%)	26 (5%)	0	100	100
1	C	479/562 (85%)	451 (94%)	27 (6%)	1 (0%)	43	72
1	D	481/562 (86%)	457 (95%)	24 (5%)	0	100	100
All	All	2005/2248 (89%)	1889 (94%)	111 (6%)	5 (0%)	43	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	A	376	GLU
1	C	443	GLU
1	A	33	PRO
1	A	34	ASP

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	454/482 (94%)	430 (95%)	24 (5%)	20	52
1	B	449/482 (93%)	438 (98%)	11 (2%)	43	77
1	C	412/482 (86%)	395 (96%)	17 (4%)	27	62
1	D	414/482 (86%)	396 (96%)	18 (4%)	26	60
All	All	1729/1928 (90%)	1659 (96%)	70 (4%)	28	63

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	36	ILE
1	A	46	SER
1	A	64	LYS

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Mol	Chain	Res	Type
1	A	67	GLN
1	A	114	LYS
1	A	124	GLU
1	A	133	LEU
1	A	142	ASP
1	A	148	SER
1	A	197	VAL
1	A	234	GLN
1	A	264	ARG
1	A	269	ILE
1	A	282	VAL
1	A	292	THR
1	A	295	ARG
1	A	315	GLN
1	A	339	SER
1	A	385	VAL
1	A	436	VAL
1	A	462	GLN
1	A	463	THR
1	A	468	LEU
1	B	14	VAL
1	B	18	ASP
1	B	63	VAL
1	B	67	GLN
1	B	125	THR
1	B	228	SER
1	B	315	GLN
1	B	431	GLN
1	B	442	SER
1	B	460	LEU
1	B	464	HIS
1	C	67	GLN
1	C	69	SER
1	C	82	ASP
1	C	87	LYS
1	C	118	VAL
1	C	131	SER
1	C	196	SER
1	C	200	SER
1	C	210	VAL
1	C	229	SER
1	C	308	VAL

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Mol	Chain	Res	Type
1	C	334	ARG
1	C	348	THR
1	C	411	LYS
1	C	464	HIS
1	C	468	LEU
1	C	470	LEU
1	D	64	LYS
1	D	80	SER
1	D	87	LYS
1	D	113	THR
1	D	281	CYS
1	D	289	THR
1	D	293	GLU
1	D	360	SER
1	D	376	GLU
1	D	409	GLU
1	D	415	ILE
1	D	452	LYS
1	D	460	LEU
1	D	462	GLN
1	D	470	LEU
1	D	471	THR
1	D	485	GLU
1	D	552	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	278	ASN
1	A	356	GLN
1	A	418	GLN
1	A	440	GLN
1	A	462	GLN
1	A	489	ASN
1	A	545	ASN
1	B	106	ASN
1	B	234	GLN
1	B	244	GLN
1	B	275	ASN
1	B	278	ASN
1	B	312	HIS

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Mol	Chain	Res	Type
1	B	315	GLN
1	B	410	GLN
1	B	440	GLN
1	C	67	GLN
1	C	495	ASN
1	D	234	GLN
1	D	250	HIS
1	D	258	GLN
1	D	259	ASN
1	D	418	GLN
1	D	440	GLN
1	D	489	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	D	601	-	3,3,3	0.43	0	2,2,2	0.41	0
3	SO4	B	1004	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	601	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	A	602	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	B	1002	-	3,3,3	0.45	0	2,2,2	0.43	0
3	SO4	C	604	-	4,4,4	0.26	0	6,6,6	0.18	0
2	EDO	C	601	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	C	603	-	3,3,3	0.44	0	2,2,2	0.37	0
3	SO4	A	603	-	4,4,4	0.25	0	6,6,6	0.04	0
2	EDO	B	1001	-	3,3,3	0.43	0	2,2,2	0.33	0
2	EDO	B	1003	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	C	602	-	3,3,3	0.44	0	2,2,2	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	601	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	B	1002	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	B	1001	-	-	0/1/1/1	-
2	EDO	B	1003	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	EDO	O1-C1-C2-O2
2	A	601	EDO	O1-C1-C2-O2
2	B	1003	EDO	O1-C1-C2-O2
2	C	603	EDO	O1-C1-C2-O2
2	B	1002	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EDO	1	0
2	A	602	EDO	1	0
3	A	603	SO4	1	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	530/562 (94%)	-0.04	5 (0%) 81 74	49, 80, 140, 204	0
1	B	525/562 (93%)	-0.01	6 (1%) 78 70	48, 81, 140, 199	0
1	C	483/562 (85%)	0.15	12 (2%) 58 48	51, 88, 149, 199	0
1	D	485/562 (86%)	0.11	8 (1%) 70 61	60, 87, 132, 179	0
All	All	2023/2248 (89%)	0.05	31 (1%) 72 63	48, 85, 140, 204	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	ALA	4.6
1	C	89	PHE	3.6
1	B	45	LEU	3.5
1	B	72	LEU	3.0
1	D	539	ALA	2.9
1	C	67	GLN	2.8
1	A	12	ALA	2.7
1	B	13	TYR	2.7
1	D	470	LEU	2.6
1	C	133	LEU	2.6
1	D	89	PHE	2.5
1	C	100	LEU	2.5
1	A	498	ASN	2.4
1	D	524	ILE	2.4
1	D	472	TYR	2.4
1	D	134	SER	2.3
1	A	458	GLY	2.3
1	C	213	TRP	2.3
1	B	67	GLN	2.3
1	C	482	ASP	2.2
1	A	280	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	79	ALA	2.2
1	D	456	LEU	2.2
1	C	365	ILE	2.2
1	C	147	ILE	2.2
1	C	194	PHE	2.1
1	C	207	PRO	2.1
1	C	143	PHE	2.0
1	C	183	ARG	2.0
1	B	214	VAL	2.0
1	B	338	VAL	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($\text{\AA}^2$)	Q<0.9
2	EDO	C	602	4/4	0.70	0.19	89,90,102,110	0
2	EDO	C	601	4/4	0.75	0.11	113,117,119,128	0
2	EDO	A	602	4/4	0.75	0.13	65,77,78,83	0
2	EDO	D	601	4/4	0.76	0.26	81,87,88,107	0
3	SO4	B	1004	5/5	0.77	0.08	115,119,122,140	0
2	EDO	B	1001	4/4	0.79	0.12	64,72,80,91	0
2	EDO	B	1002	4/4	0.80	0.20	50,59,67,71	0
3	SO4	A	603	5/5	0.82	0.08	109,111,130,142	0
3	SO4	C	604	5/5	0.83	0.14	97,108,124,130	0
2	EDO	C	603	4/4	0.84	0.10	83,109,111,114	0
2	EDO	A	601	4/4	0.87	0.11	79,96,97,107	0
2	EDO	B	1003	4/4	0.92	0.13	69,73,73,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.