



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:51 PM UTC

PDB ID : 3H45 / pdb_00003h45
Title : Glycerol Kinase H232E with Ethylene Glycol
Authors : Yeh, J.I.; Kettering, R.D.
Deposited on : 2009-04-17
Resolution : 2.65 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

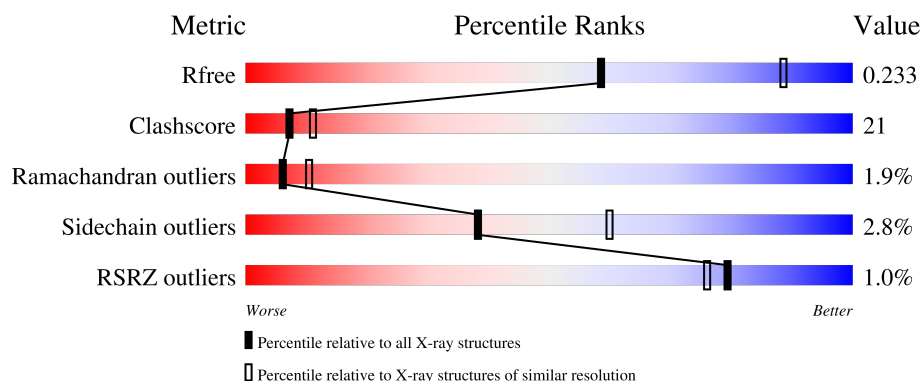
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	C	506	% 62% 34% ..
1	D	506	% 63% 31% 5% .
1	O	506	% 70% 26% ..
1	X	506	% 64% 32% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15832 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	499	Total	C	N	O	S	0	0	0
			3862	2447	642	759	14			
1	O	500	Total	C	N	O	S	0	0	0
			3875	2455	644	762	14			
1	C	500	Total	C	N	O	S	0	0	0
			3875	2455	644	762	14			
1	D	499	Total	C	N	O	S	0	0	0
			3870	2453	644	759	14			

There are 4 discrepancies between the modelled and reference sequences:

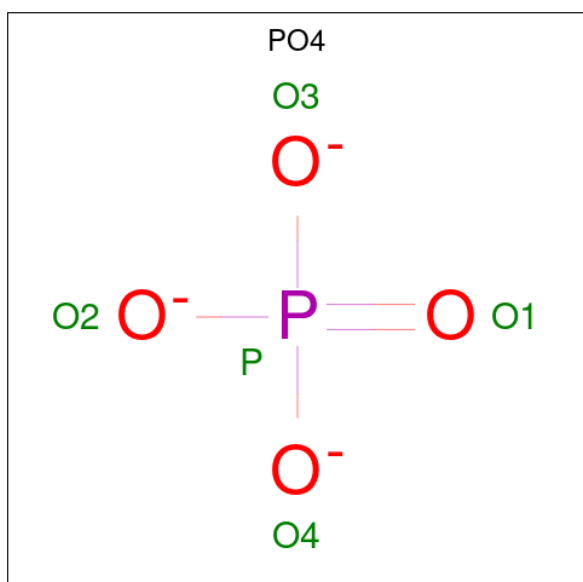
Chain	Residue	Modelled	Actual	Comment	Reference
X	232	GLU	HIS	engineered mutation	UNP O34153
O	232	GLU	HIS	engineered mutation	UNP O34153
C	232	GLU	HIS	engineered mutation	UNP O34153
D	232	GLU	HIS	engineered mutation	UNP O34153

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



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	1	Total O P 5 4 1	0	0
3	X	1	Total O P 5 4 1	0	0
3	X	1	Total O P 5 4 1	0	0
3	O	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

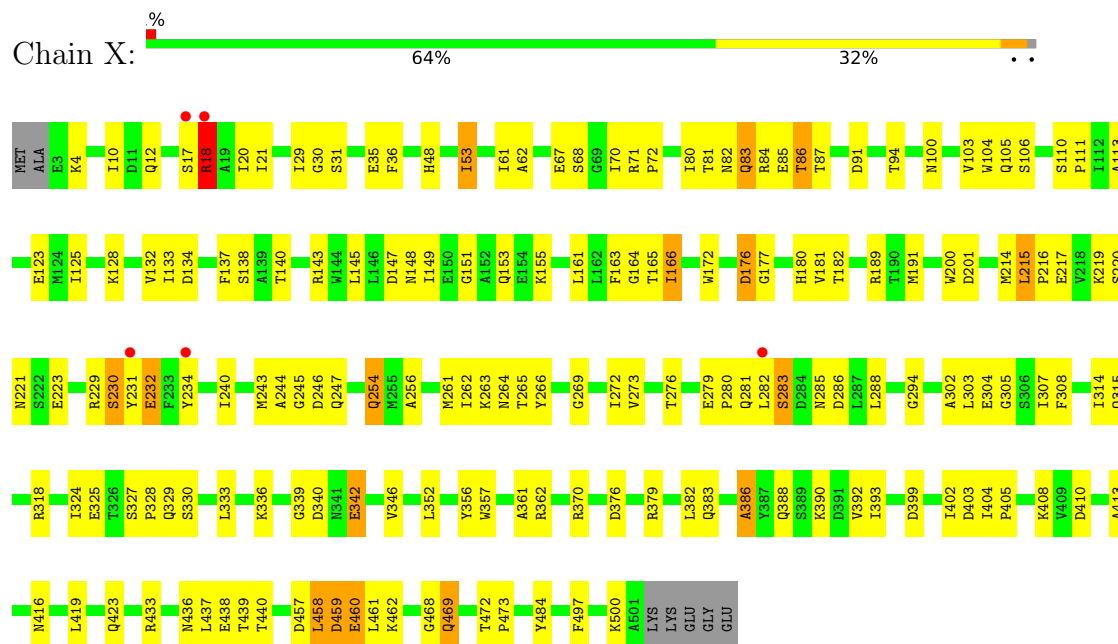
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	108	Total O 108 108	0	0
4	O	76	Total O 76 76	0	0
4	C	72	Total O 72 72	0	0
4	D	44	Total O 44 44	0	0

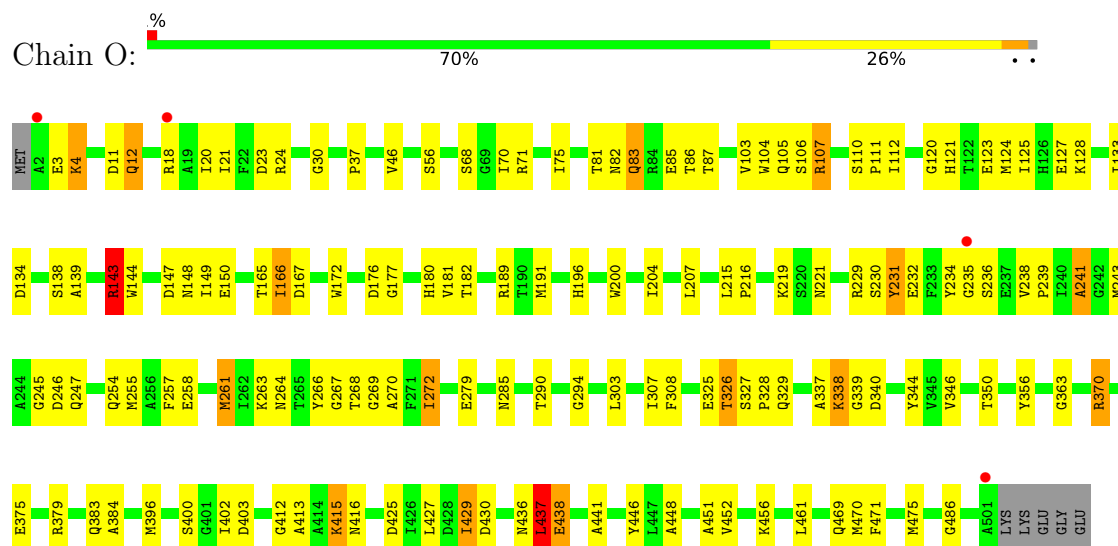
3 Residue-property plots [i](#)

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

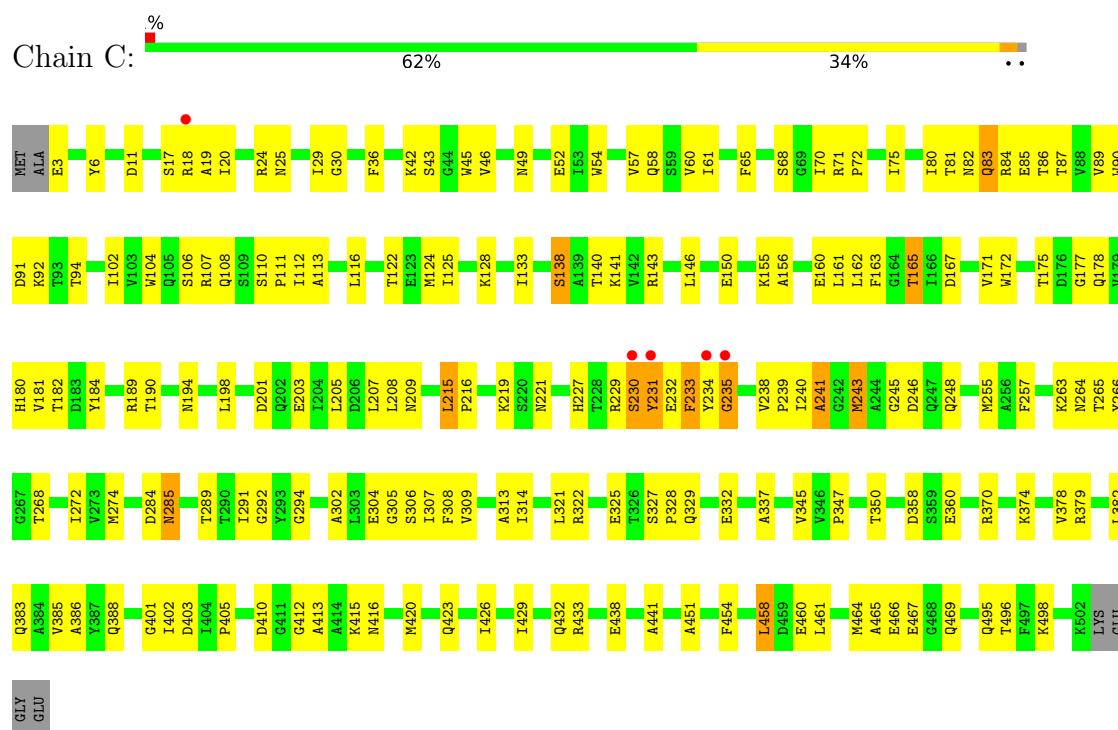
• Molecule 1: Glycerol kinase



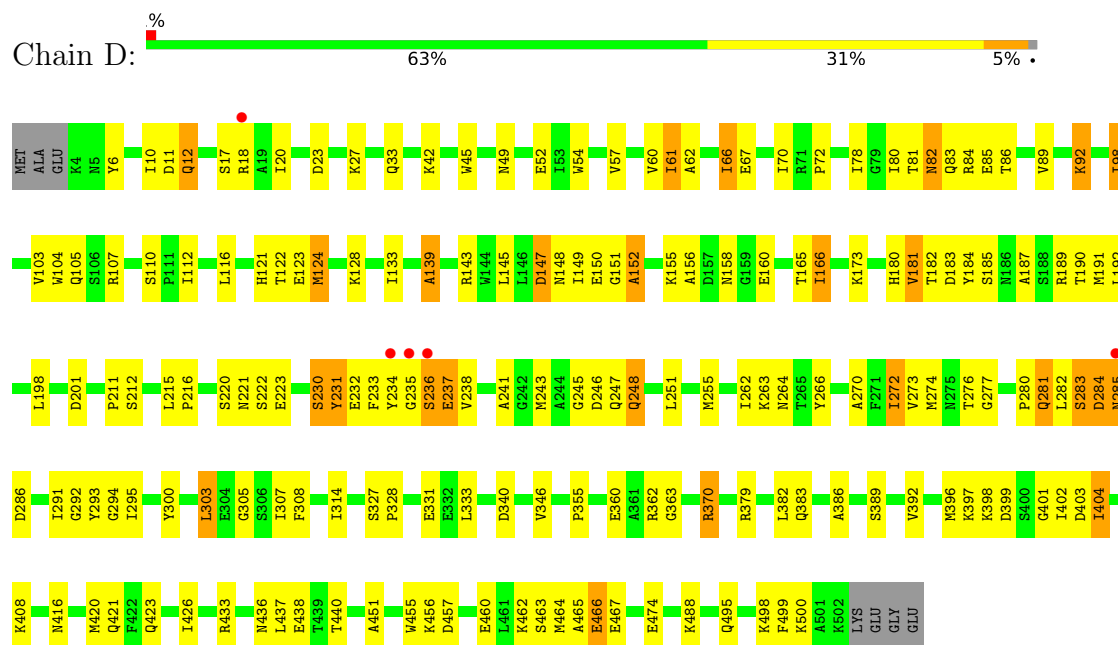
• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.61Å 105.19Å 114.31Å 90.00° 114.55° 90.00°	Depositor
Resolution (Å)	12.00 – 2.65 12.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.9 (12.00-2.65) 96.6 (12.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.251 0.219 , 0.233	Depositor DCC
R_{free} test set	3600 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: EDO, PO4

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	C	0.43	0/3955	0.97	19/5363 (0.4%)
1	D	0.41	0/3950	0.96	15/5355 (0.3%)
1	O	0.44	0/3955	0.95	17/5363 (0.3%)
1	X	0.46	0/3942	0.97	21/5347 (0.4%)
All	All	0.44	0/15802	0.96	72/21428 (0.3%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	SER	N-CA-C	8.42	120.08	111.07
1	C	29	ILE	N-CA-C	-7.89	104.83	113.43
1	X	215	LEU	N-CA-C	7.76	119.55	109.93
1	C	215	LEU	N-CA-C	7.49	119.08	109.65
1	C	245	GLY	N-CA-C	-7.12	102.95	112.14
1	X	240	ILE	N-CA-C	-7.09	96.95	107.51
1	C	165	THR	N-CA-C	-7.04	100.10	110.52
1	D	245	GLY	N-CA-C	-6.88	103.26	112.14
1	O	87	THR	N-CA-C	6.81	120.55	109.59
1	C	401	GLY	N-CA-C	-6.72	105.23	114.64
1	O	245	GLY	N-CA-C	-6.40	104.57	111.93
1	X	87	THR	N-CA-C	6.35	119.75	109.40
1	O	241	ALA	N-CA-C	6.33	120.63	112.41
1	O	165	THR	N-CA-C	-6.29	102.42	110.53
1	O	308	PHE	N-CA-C	6.28	118.64	111.11
1	D	401	GLY	N-CA-C	-6.22	106.17	114.25
1	O	83	GLN	N-CA-C	-6.19	100.49	109.59
1	X	82	ASN	N-CA-C	6.17	116.71	108.38
1	D	124	MET	N-CA-C	-6.16	104.20	111.03
1	X	53	ILE	N-CA-C	-6.12	104.54	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	ASN	N-CA-C	6.11	117.53	108.60
1	O	215	LEU	N-CA-C	6.10	117.50	109.93
1	D	281	GLN	N-CA-C	6.09	119.47	109.72
1	X	36	PHE	CA-C-N	6.08	127.43	119.84
1	X	36	PHE	C-N-CA	6.08	127.43	119.84
1	O	82	ASN	N-CA-C	6.07	118.40	109.24
1	D	398	LYS	N-CA-C	-6.04	104.62	111.14
1	X	106	SER	N-CA-C	6.01	119.18	110.28
1	X	245	GLY	N-CA-C	-5.96	104.38	111.36
1	C	306	SER	N-CA-C	5.93	118.62	109.07
1	X	29	ILE	N-CA-C	-5.91	107.51	113.47
1	O	56	SER	N-CA-C	-5.90	104.93	111.71
1	X	83	GLN	N-CA-C	-5.85	101.18	109.96
1	D	165	THR	N-CA-C	-5.82	103.03	110.53
1	C	235	GLY	N-CA-C	-5.78	105.78	112.83
1	O	356	TYR	N-CA-C	5.76	117.36	111.14
1	D	148	ASN	N-CA-C	5.72	119.96	112.92
1	C	215	LEU	CA-C-N	5.58	126.05	120.52
1	C	215	LEU	C-N-CA	5.58	126.05	120.52
1	X	269	GLY	N-CA-C	-5.58	102.79	112.06
1	C	268	THR	N-CA-C	-5.58	105.20	111.28
1	O	143	ARG	N-CA-C	-5.58	104.89	110.97
1	X	138	SER	N-CA-C	5.57	117.35	111.28
1	X	165	THR	N-CA-C	-5.50	102.76	110.35
1	X	346	VAL	CA-C-N	5.48	126.69	119.84
1	X	346	VAL	C-N-CA	5.48	126.69	119.84
1	D	61	ILE	N-CA-C	-5.46	105.18	110.42
1	C	82	ASN	N-CA-C	5.45	117.08	108.96
1	C	308	PHE	N-CA-C	5.44	116.89	111.07
1	X	399	ASP	N-CA-C	5.42	116.99	111.14
1	O	269	GLY	N-CA-C	-5.41	103.24	111.14
1	C	83	GLN	N-CA-C	-5.40	101.86	109.96
1	X	166	ILE	N-CA-C	5.38	116.11	110.62
1	D	181	VAL	N-CA-C	5.35	115.34	108.82
1	C	240	ILE	N-CA-C	-5.31	99.31	106.85
1	D	215	LEU	N-CA-C	5.27	117.35	110.08
1	C	36	PHE	CA-C-N	5.25	125.26	119.90
1	C	36	PHE	C-N-CA	5.25	125.26	119.90
1	X	308	PHE	N-CA-C	5.22	117.38	111.11
1	D	308	PHE	N-CA-C	5.20	117.62	111.33
1	O	120	GLY	N-CA-C	5.20	123.11	113.76
1	O	138	SER	N-CA-C	5.19	116.94	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	166	ILE	N-CA-C	5.16	118.28	111.17
1	D	238	VAL	N-CA-C	5.12	114.59	108.96
1	O	37	PRO	N-CA-C	5.11	119.23	111.15
1	O	200	TRP	N-CA-C	-5.10	102.83	110.23
1	D	467	GLU	CB-CA-C	-5.10	109.20	116.34
1	D	166	ILE	N-CA-C	5.09	116.42	110.62
1	X	386	ALA	N-CA-C	-5.07	105.75	111.28
1	X	254	GLN	N-CA-C	-5.05	106.89	113.16
1	C	241	ALA	N-CA-C	5.03	121.15	113.61
1	C	90	TRP	N-CA-C	5.03	116.83	109.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3875	0	3764	169	0
1	D	3870	0	3769	175	0
1	O	3875	0	3767	135	0
1	X	3862	0	3747	162	0
2	C	4	0	6	0	0
2	D	4	0	6	1	0
2	O	4	0	6	0	0
2	X	8	0	12	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	O	5	0	0	0	0
3	X	15	0	0	0	0
4	C	72	0	0	2	0
4	D	44	0	0	3	0
4	O	76	0	0	6	0
4	X	108	0	0	4	0
All	All	15832	0	15077	632	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 21.

All (632) 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:D:18:ARG:NH1	1:D:20:ILE:HD11	1.24	1.48
1:D:18:ARG:CZ	1:D:20:ILE:HD11	1.45	1.47
1:D:18:ARG:NH2	1:D:438:GLU:HB2	1.38	1.39
1:D:18:ARG:NH1	1:D:20:ILE:CD1	2.00	1.23
1:C:18:ARG:NH2	1:C:441:ALA:HB2	1.53	1.20
1:X:18:ARG:NH1	1:X:438:GLU:HG2	1.55	1.19
1:D:18:ARG:CZ	1:D:20:ILE:CD1	2.22	1.16
1:O:18:ARG:HH12	1:O:438:GLU:HG3	1.07	1.12
1:X:18:ARG:HG2	1:X:18:ARG:HH21	0.98	1.08
1:X:18:ARG:HH21	1:X:18:ARG:CG	1.70	1.05
1:O:18:ARG:NH1	1:O:438:GLU:HG3	1.74	1.02
1:X:18:ARG:NH2	1:X:20:ILE:HG12	1.73	1.02
1:X:18:ARG:HH22	1:X:20:ILE:HG12	1.25	1.00
1:C:18:ARG:HH12	1:C:438:GLU:HB3	1.26	1.00
1:D:18:ARG:HH22	1:D:438:GLU:CB	1.74	0.99
1:C:18:ARG:NH2	1:C:441:ALA:CB	2.25	0.98
1:C:18:ARG:HD2	1:C:20:ILE:HD11	1.46	0.98
1:D:18:ARG:NH2	1:D:438:GLU:CB	2.28	0.96
1:X:18:ARG:HH11	1:X:438:GLU:HG2	1.23	0.95
1:X:20:ILE:CD1	1:X:31:SER:HB2	1.97	0.94
1:X:20:ILE:CD1	1:X:31:SER:CB	2.45	0.94
1:C:18:ARG:HG2	1:C:20:ILE:CD1	1.99	0.91
1:X:20:ILE:HD12	1:X:31:SER:HB3	1.50	0.91
1:O:12:GLN:HE22	1:O:83:GLN:HE21	1.09	0.91
1:D:276:THR:HG22	1:D:281:GLN:HE21	1.36	0.91
1:C:18:ARG:NH1	1:C:438:GLU:HB3	1.84	0.91
1:O:326:THR:HG23	1:O:328:PRO:HD2	1.51	0.91
1:D:183:ASP:OD2	1:D:185:SER:HB3	1.71	0.90
1:X:18:ARG:HG2	1:X:18:ARG:NH2	1.65	0.89
1:C:18:ARG:CD	1:C:20:ILE:HD11	2.02	0.88
1:D:221:ASN:HD22	1:D:294:GLY:H	0.93	0.87
1:X:438:GLU:O	1:X:438:GLU:HG3	1.72	0.86
1:O:167:ASP:HB2	1:O:243:MET:HE2	1.56	0.86
1:X:254:GLN:HG2	1:X:439:THR:HG21	1.59	0.84
1:D:18:ARG:HH22	1:D:438:GLU:HB2	1.05	0.83
1:C:221:ASN:HD22	1:C:294:GLY:H	1.27	0.82
1:O:123:GLU:O	1:O:127:GLU:HG3	1.79	0.82
1:X:20:ILE:HD12	1:X:31:SER:CB	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:12:GLN:NE2	1:O:83:GLN:HE21	1.78	0.82
1:X:221:ASN:HD22	1:X:294:GLY:H	1.26	0.81
1:D:436:ASN:OD1	1:D:438:GLU:CD	2.25	0.80
1:D:221:ASN:ND2	1:D:294:GLY:H	1.76	0.80
1:C:18:ARG:CG	1:C:20:ILE:HD11	2.12	0.80
1:D:331:GLU:HG3	1:D:416:ASN:ND2	1.96	0.80
1:D:283:SER:CB	1:D:399:ASP:HB3	2.12	0.79
1:C:18:ARG:CZ	1:C:441:ALA:HB2	2.12	0.79
1:X:264:ASN:CG	1:X:272:ILE:HD13	2.07	0.79
1:C:18:ARG:CG	1:C:20:ILE:CD1	2.60	0.79
1:X:325:GLU:H	1:X:329:GLN:NE2	1.81	0.79
1:D:57:VAL:O	1:D:61:ILE:HG12	1.83	0.79
1:D:221:ASN:HD22	1:D:294:GLY:N	1.75	0.79
1:X:17:SER:O	1:X:18:ARG:HB2	1.82	0.78
1:X:459:ASP:C	1:X:461:LEU:H	1.90	0.77
1:X:18:ARG:NH2	1:X:20:ILE:CG1	2.48	0.76
1:C:18:ARG:HH22	1:C:441:ALA:H	1.32	0.76
1:O:12:GLN:HE22	1:O:83:GLN:NE2	1.83	0.76
1:C:433:ARG:HH21	1:C:469:GLN:HG2	1.51	0.76
1:O:437:LEU:N	1:O:437:LEU:HD23	2.01	0.76
1:X:266:TYR:HB3	1:X:413:ALA:HB3	1.66	0.76
1:X:48:HIS:HB3	1:X:53:ILE:HD11	1.67	0.75
1:C:307:ILE:HD12	1:C:388:GLN:CD	2.12	0.75
1:D:370:ARG:HH11	1:D:370:ARG:HB3	1.50	0.75
1:C:221:ASN:ND2	1:C:294:GLY:H	1.85	0.75
1:C:379:ARG:O	1:C:383:GLN:HG3	1.86	0.75
1:C:432:GLN:OE1	1:C:467:GLU:HG3	1.87	0.74
1:O:189:ARG:HH11	1:O:290:THR:HG21	1.51	0.74
1:D:314:ILE:HD11	1:D:382:LEU:HD23	1.70	0.73
1:O:327:SER:HB2	1:O:328:PRO:HD3	1.70	0.72
1:D:181:VAL:HG22	1:D:182:THR:H	1.54	0.72
1:X:18:ARG:HH11	1:X:438:GLU:CG	2.01	0.72
1:X:189:ARG:HH22	1:X:288:LEU:CD1	2.02	0.72
1:D:89:VAL:HB	1:D:98:ILE:HD12	1.72	0.72
1:X:18:ARG:NH1	1:X:20:ILE:HG13	2.04	0.72
1:C:231:TYR:HD2	1:C:232:GLU:N	1.87	0.71
1:O:437:LEU:HD23	1:O:437:LEU:H	1.55	0.71
1:C:433:ARG:NH2	1:C:469:GLN:HG2	2.06	0.71
1:X:189:ARG:NH2	1:X:288:LEU:HD13	2.04	0.70
1:D:18:ARG:HH22	1:D:438:GLU:CG	2.04	0.70
1:D:187:ALA:O	1:D:190:THR:HG22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:LYS:HD2	1:D:462:LYS:O	1.92	0.70
1:O:18:ARG:HH11	1:O:20:ILE:HD11	1.57	0.70
1:X:125:ILE:HD12	1:X:133:ILE:HG12	1.74	0.69
1:D:283:SER:HB3	1:D:399:ASP:HB3	1.73	0.69
1:D:82:ASN:HD22	1:D:166:ILE:HB	1.57	0.69
1:D:438:GLU:O	1:D:438:GLU:HG2	1.91	0.69
1:O:83:GLN:HG3	1:O:83:GLN:O	1.93	0.68
1:O:107:ARG:HH22	1:O:134:ASP:CG	2.01	0.68
1:C:18:ARG:HH22	1:C:441:ALA:CB	2.03	0.68
1:D:84:ARG:HD2	1:D:189:ARG:HD2	1.75	0.68
1:O:326:THR:HG22	1:O:329:GLN:H	1.57	0.68
1:C:92:LYS:HD3	4:C:559:HOH:O	1.94	0.68
1:O:257:PHE:N	1:O:261:MET:HE3	2.09	0.68
1:C:143:ARG:HH21	1:C:146:LEU:HB2	1.59	0.68
1:D:98:ILE:HD11	1:D:145:LEU:HD22	1.77	0.68
1:O:258:GLU:H	1:O:261:MET:CE	2.07	0.67
1:C:107:ARG:HG2	1:C:107:ARG:HH11	1.59	0.67
1:C:234:TYR:CG	1:D:234:TYR:HB2	2.30	0.67
1:X:18:ARG:NH1	1:X:438:GLU:CG	2.47	0.67
1:X:340:ASP:HB2	1:X:342:GLU:OE1	1.94	0.67
1:C:124:MET:HE1	1:C:207:LEU:HD22	1.76	0.67
1:O:263:LYS:HD2	1:O:263:LYS:C	2.20	0.67
1:D:85:GLU:OE2	1:D:189:ARG:HD3	1.94	0.67
1:C:412:GLY:O	1:C:415:LYS:HG2	1.95	0.67
1:X:327:SER:HB2	1:X:328:PRO:HD3	1.76	0.66
1:O:176:ASP:HB3	1:O:229:ARG:HD2	1.77	0.66
1:O:326:THR:HG23	1:O:328:PRO:CD	2.23	0.66
1:O:402:ILE:HG22	1:O:403:ASP:N	2.08	0.66
1:D:151:GLY:O	1:D:155:LYS:HG3	1.95	0.66
1:C:18:ARG:CD	1:C:20:ILE:CD1	2.72	0.66
1:D:248:GLN:H	1:D:248:GLN:HE21	1.44	0.66
1:C:19:ALA:C	1:C:20:ILE:HD12	2.20	0.66
1:X:325:GLU:H	1:X:329:GLN:HE22	1.41	0.66
1:C:143:ARG:HH12	1:C:209:ASN:HB3	1.61	0.66
1:D:263:LYS:HD2	1:D:263:LYS:C	2.21	0.66
1:C:112:ILE:HD13	1:C:143:ARG:HG3	1.77	0.65
1:X:458:LEU:O	1:X:462:LYS:HE2	1.97	0.65
1:X:189:ARG:HH22	1:X:288:LEU:HD13	1.60	0.65
1:O:221:ASN:HD22	1:O:294:GLY:H	1.45	0.65
1:O:189:ARG:NH1	1:O:290:THR:HG21	2.12	0.64
1:O:12:GLN:HE21	1:O:166:ILE:HG21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:TYR:HB2	1:D:234:TYR:CE1	2.32	0.64
1:C:266:TYR:HB3	1:C:413:ALA:HB3	1.78	0.64
1:O:139:ALA:HB3	1:O:191:MET:HE2	1.80	0.64
1:X:143:ARG:NH1	1:X:147:ASP:OD1	2.30	0.64
1:D:23:ASP:OD2	1:D:27:LYS:HB3	1.98	0.64
1:X:221:ASN:ND2	1:X:294:GLY:H	1.96	0.64
1:X:181:VAL:HG13	1:X:243:MET:HE1	1.78	0.64
1:O:272:ILE:HD12	1:O:272:ILE:N	2.13	0.64
1:D:379:ARG:O	1:D:383:GLN:HG3	1.98	0.64
1:D:18:ARG:NH1	1:D:20:ILE:HD13	2.10	0.63
1:O:266:TYR:HB3	1:O:413:ALA:HB3	1.79	0.63
1:O:338:LYS:H	1:O:338:LYS:HD2	1.64	0.63
1:X:217:GLU:OE2	1:X:219:LYS:HE3	1.99	0.62
1:X:315:GLN:HE21	1:X:318:ARG:HH22	1.45	0.62
1:O:258:GLU:HG2	1:O:261:MET:HE2	1.81	0.62
1:D:84:ARG:HD3	1:D:248:GLN:HE22	1.64	0.62
1:C:325:GLU:H	1:C:329:GLN:NE2	1.96	0.62
1:X:20:ILE:HD11	1:X:31:SER:HB2	1.80	0.62
1:X:263:LYS:HD2	1:X:263:LYS:C	2.24	0.62
1:O:85:GLU:HB2	1:O:104:TRP:HB3	1.81	0.62
1:C:85:GLU:OE2	1:C:189:ARG:HD2	1.99	0.62
1:D:112:ILE:HD12	1:D:112:ILE:H	1.63	0.62
1:D:235:GLY:O	1:D:237:GLU:N	2.32	0.62
1:X:457:ASP:C	1:X:459:ASP:H	2.07	0.62
1:X:468:GLY:O	1:X:469:GLN:HB2	2.00	0.62
1:C:18:ARG:HH12	1:C:438:GLU:CB	2.07	0.62
1:D:143:ARG:O	1:D:147:ASP:HB2	2.00	0.62
1:O:258:GLU:H	1:O:261:MET:HE3	1.65	0.61
1:C:172:TRP:CE2	1:C:177:GLY:HA2	2.35	0.61
1:D:18:ARG:CZ	1:D:438:GLU:HB2	2.26	0.61
1:C:181:VAL:HG22	1:C:182:THR:N	2.14	0.61
1:D:283:SER:OG	1:D:399:ASP:HB3	1.99	0.61
1:D:122:THR:HG22	1:D:123:GLU:N	2.16	0.61
1:O:18:ARG:NH2	1:O:438:GLU:HB2	2.17	0.60
1:X:20:ILE:HD13	1:X:31:SER:CB	2.30	0.60
1:C:18:ARG:HH22	1:C:441:ALA:N	1.98	0.60
1:C:337:ALA:HB3	1:C:379:ARG:NH1	2.17	0.60
1:D:72:PRO:HG2	1:D:234:TYR:CE1	2.37	0.60
1:D:457:ASP:HB2	4:D:544:HOH:O	2.02	0.59
1:O:103:VAL:HG12	1:O:105:GLN:H	1.68	0.59
1:C:307:ILE:HD12	1:C:388:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG12	1:D:105:GLN:H	1.68	0.59
1:O:124:MET:HE1	1:O:204:ILE:HG12	1.85	0.59
1:C:143:ARG:NH1	1:C:209:ASN:HB3	2.18	0.59
1:C:162:LEU:HD22	1:C:180:HIS:CE1	2.37	0.59
1:O:107:ARG:HD2	1:O:350:THR:HB	1.83	0.59
1:O:384:ALA:HB3	4:O:509:HOH:O	2.03	0.59
1:D:18:ARG:HH11	1:D:20:ILE:HD11	1.54	0.58
1:O:221:ASN:ND2	1:O:294:GLY:H	2.00	0.58
1:O:338:LYS:HD2	1:O:338:LYS:N	2.19	0.58
1:C:155:LYS:O	1:C:160:GLU:HB3	2.03	0.58
1:C:231:TYR:CD2	1:C:232:GLU:N	2.70	0.58
1:X:18:ARG:CG	1:X:18:ARG:NH2	2.41	0.58
1:X:181:VAL:HG22	1:X:182:THR:H	1.69	0.58
1:C:289:THR:HG23	4:C:577:HOH:O	2.04	0.58
1:O:326:THR:HG22	1:O:329:GLN:N	2.18	0.58
1:O:3:GLU:HG3	1:O:4:LYS:N	2.19	0.58
1:C:178:GLN:NE2	1:C:229:ARG:HH11	2.02	0.58
1:D:18:ARG:NE	1:D:20:ILE:HD11	2.12	0.58
1:X:72:PRO:HB2	1:X:234:TYR:O	2.04	0.58
1:C:18:ARG:NH1	1:C:438:GLU:CB	2.61	0.58
1:C:107:ARG:HD2	1:C:350:THR:O	2.04	0.58
1:X:234:TYR:CE1	1:O:231:TYR:HA	2.39	0.57
1:X:263:LYS:HD2	1:X:264:ASN:N	2.19	0.57
1:O:402:ILE:HG22	1:O:403:ASP:H	1.68	0.57
1:D:262:ILE:HD11	1:D:272:ILE:HG22	1.86	0.57
1:C:3:GLU:HA	1:C:3:GLU:OE2	2.04	0.57
1:C:382:LEU:O	1:C:385:VAL:HG12	2.03	0.57
1:C:24:ARG:O	1:C:464:MET:HE1	2.03	0.57
1:O:438:GLU:O	1:O:438:GLU:HG2	2.05	0.57
1:C:272:ILE:HD12	1:C:272:ILE:N	2.20	0.57
1:D:12:GLN:HE22	1:D:83:GLN:HE21	1.51	0.57
1:X:181:VAL:HG22	1:X:182:THR:N	2.20	0.57
1:D:143:ARG:HD2	1:D:147:ASP:OD1	2.03	0.57
1:D:327:SER:HB2	1:D:328:PRO:HD3	1.85	0.57
1:D:284:ASP:C	1:D:286:ASP:H	2.13	0.56
1:C:181:VAL:CG2	1:C:219:LYS:HG3	2.35	0.56
1:C:314:ILE:HD11	1:C:382:LEU:CD2	2.35	0.56
1:O:229:ARG:HD3	1:O:231:TYR:OH	2.06	0.56
1:C:11:ASP:HA	1:C:81:THR:HG23	1.87	0.56
1:X:80:ILE:O	1:X:243:MET:HA	2.05	0.56
1:X:265:THR:HG23	1:X:410:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:LYS:O	1:C:378:VAL:HG23	2.05	0.56
1:X:180:HIS:CE1	1:X:216:PRO:HB3	2.40	0.56
1:O:370:ARG:HH11	1:O:370:ARG:HB3	1.70	0.56
1:D:181:VAL:HG22	1:D:182:THR:N	2.19	0.56
1:O:290:THR:HG22	4:O:508:HOH:O	2.05	0.56
1:C:18:ARG:HG2	1:C:20:ILE:HD12	1.87	0.56
1:D:198:LEU:N	1:D:198:LEU:HD22	2.21	0.56
1:C:309:VAL:HG12	1:C:313:ALA:HB2	1.87	0.56
1:X:18:ARG:CZ	1:X:20:ILE:CG1	2.84	0.55
1:C:263:LYS:HD2	1:C:263:LYS:C	2.30	0.55
1:D:122:THR:HG22	1:D:123:GLU:H	1.70	0.55
1:D:18:ARG:CZ	1:D:20:ILE:HD12	2.30	0.55
1:X:81:THR:OG1	1:X:246:ASP:HA	2.05	0.55
1:O:18:ARG:NH1	1:O:20:ILE:HD11	2.22	0.55
1:D:286:ASP:HB3	1:D:355:PRO:HB2	1.88	0.55
1:O:121:HIS:CD2	1:O:207:LEU:HD21	2.42	0.55
1:X:12:GLN:HE21	1:X:166:ILE:HG21	1.72	0.55
1:X:18:ARG:HH12	1:X:20:ILE:HG13	1.68	0.55
1:O:180:HIS:CE1	1:O:216:PRO:HB3	2.42	0.55
1:C:184:TYR:HB3	1:C:291:ILE:HG21	1.89	0.55
1:O:279:GLU:HB2	4:O:569:HOH:O	2.07	0.55
1:X:81:THR:HA	1:X:244:ALA:O	2.07	0.54
1:X:113:ALA:HB2	1:X:140:THR:HG21	1.89	0.54
1:C:458:LEU:HD12	1:C:461:LEU:HD12	1.90	0.54
1:D:122:THR:O	1:D:123:GLU:HB3	2.06	0.54
1:X:305:GLY:HA3	1:X:392:VAL:HG11	1.89	0.54
1:O:125:ILE:HG13	1:O:133:ILE:HD11	1.88	0.54
1:X:234:TYR:CD2	1:O:234:TYR:HA	2.41	0.54
1:C:18:ARG:HD2	1:C:20:ILE:CD1	2.31	0.54
1:X:276:THR:HG23	1:X:302:ALA:HA	1.90	0.54
1:X:459:ASP:C	1:X:461:LEU:N	2.59	0.54
1:X:18:ARG:HH12	1:X:438:GLU:HG2	1.65	0.54
1:X:282:LEU:O	1:X:283:SER:HB3	2.07	0.54
1:C:57:VAL:O	1:C:61:ILE:HG13	2.07	0.54
1:D:181:VAL:HG13	1:D:243:MET:HE1	1.90	0.54
1:X:125:ILE:HD12	1:X:133:ILE:CG1	2.38	0.54
1:C:466:GLU:O	1:C:467:GLU:HB3	2.07	0.54
1:D:455:TRP:HE1	1:D:464:MET:HE1	1.72	0.54
1:X:151:GLY:O	1:X:155:LYS:HG3	2.08	0.53
1:O:70:ILE:HG22	1:O:71:ARG:N	2.21	0.53
1:X:132:VAL:O	1:X:191:MET:HE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:246:ASP:OD1	1:O:247:GLN:N	2.41	0.53
1:X:282:LEU:N	1:X:282:LEU:HD12	2.23	0.53
1:C:128:LYS:HZ1	1:C:203:GLU:CD	2.15	0.53
1:X:172:TRP:CE2	1:X:177:GLY:HA2	2.44	0.53
1:D:158:ASN:ND2	1:D:160:GLU:HG2	2.23	0.53
1:X:30:GLY:HA2	1:X:67:GLU:OE1	2.08	0.53
1:X:103:VAL:HG12	1:X:105:GLN:H	1.73	0.53
1:O:437:LEU:N	1:O:437:LEU:CD2	2.72	0.53
1:O:436:ASN:OD1	1:O:438:GLU:OE1	2.27	0.53
1:X:85:GLU:O	1:X:86:THR:C	2.52	0.53
1:C:107:ARG:HG2	1:C:107:ARG:NH1	2.24	0.53
1:O:427:LEU:HB3	1:O:429:ILE:HG23	1.89	0.53
1:O:448:ALA:O	1:O:452:VAL:HG22	2.09	0.53
1:D:276:THR:HG21	4:D:550:HOH:O	2.09	0.52
1:X:393:ILE:HG23	1:X:404:ILE:HD12	1.90	0.52
1:O:124:MET:HE1	1:O:204:ILE:CG1	2.39	0.52
1:O:257:PHE:H	1:O:261:MET:HE3	1.73	0.52
1:C:138:SER:HB2	1:C:190:THR:HA	1.92	0.52
1:O:438:GLU:CD	1:O:438:GLU:H	2.17	0.52
1:O:346:VAL:O	1:O:363:GLY:HA2	2.10	0.52
1:D:128:LYS:HD3	1:D:201:ASP:CG	2.34	0.52
1:O:181:VAL:HG22	1:O:182:THR:H	1.75	0.52
1:C:116:LEU:HD21	1:C:208:LEU:HD21	1.92	0.52
1:C:255:MET:HE1	1:C:465:ALA:HA	1.91	0.52
1:O:437:LEU:H	1:O:437:LEU:CD2	2.22	0.52
1:O:30:GLY:HA3	1:O:68:SER:HB3	1.90	0.52
1:C:81:THR:OG1	1:C:246:ASP:HA	2.10	0.52
1:C:180:HIS:CD2	1:C:216:PRO:HB3	2.44	0.52
1:X:103:VAL:HG12	1:X:104:TRP:N	2.25	0.51
1:X:110:SER:OG	1:X:111:PRO:HD3	2.10	0.51
1:O:167:ASP:HB2	1:O:243:MET:CE	2.35	0.51
1:O:326:THR:O	1:O:329:GLN:HB3	2.10	0.51
1:C:18:ARG:NH2	1:C:441:ALA:H	2.06	0.51
1:D:84:ARG:H	2:D:1003:EDO:H21	1.75	0.51
1:O:172:TRP:CE2	1:O:177:GLY:HA2	2.45	0.51
1:D:18:ARG:HH12	1:D:438:GLU:HG3	1.76	0.51
1:D:433:ARG:HD2	1:D:437:LEU:HD21	1.90	0.51
1:X:149:ILE:HD12	1:X:149:ILE:N	2.24	0.51
1:C:65:PHE:HE1	1:C:75:ILE:HD11	1.75	0.51
1:C:234:TYR:HB3	1:D:234:TYR:CB	2.40	0.51
1:D:272:ILE:HD13	1:D:272:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:81:THR:OG1	1:O:246:ASP:HA	2.10	0.51
1:C:495:GLN:O	1:C:498:LYS:NZ	2.44	0.51
1:D:92:LYS:NZ	1:D:92:LYS:HB3	2.25	0.51
1:X:230:SER:O	1:X:231:TYR:HB2	2.11	0.51
1:X:457:ASP:O	1:X:459:ASP:N	2.44	0.51
1:O:400:SER:C	1:O:402:ILE:H	2.19	0.51
1:C:181:VAL:HG22	1:C:182:THR:H	1.74	0.51
1:C:255:MET:HA	1:C:257:PHE:CZ	2.45	0.51
1:C:263:LYS:HD2	1:C:264:ASN:N	2.26	0.51
1:X:137:PHE:HD2	1:X:191:MET:CE	2.24	0.51
1:X:148:ASN:C	1:X:149:ILE:HD12	2.35	0.51
1:C:189:ARG:HH22	1:C:304:GLU:CD	2.19	0.51
1:O:402:ILE:CG2	1:O:403:ASP:N	2.74	0.51
1:C:25:ASN:HA	1:C:464:MET:CE	2.41	0.51
1:D:305:GLY:HA3	1:D:392:VAL:HG11	1.93	0.51
1:D:54:TRP:CD1	1:D:173:LYS:HE2	2.46	0.51
1:D:182:THR:HA	1:D:243:MET:HE3	1.92	0.51
1:X:189:ARG:HH22	1:X:288:LEU:HD12	1.73	0.50
1:C:83:GLN:HG3	1:C:83:GLN:O	2.11	0.50
1:C:102:ILE:HB	1:C:141:LYS:HD3	1.93	0.50
1:D:277:GLY:O	1:D:300:TYR:HA	2.11	0.50
1:D:62:ALA:HB2	1:D:232:GLU:OE2	2.11	0.50
1:D:83:GLN:O	1:D:83:GLN:HG3	2.12	0.50
1:D:180:HIS:CD2	1:D:216:PRO:HB3	2.46	0.50
1:D:262:ILE:HD11	1:D:272:ILE:CG2	2.42	0.50
1:X:85:GLU:OE2	1:X:189:ARG:HD3	2.11	0.50
1:X:137:PHE:HD2	1:X:191:MET:HE3	1.76	0.50
1:D:103:VAL:HG12	1:D:104:TRP:N	2.26	0.50
1:O:124:MET:HE3	1:O:128:LYS:HD2	1.93	0.50
1:O:230:SER:C	1:O:232:GLU:H	2.20	0.50
1:C:314:ILE:HD11	1:C:382:LEU:HD23	1.94	0.50
1:C:49:ASN:HB3	1:C:52:GLU:HB2	1.92	0.50
1:C:70:ILE:HG22	1:C:71:ARG:N	2.25	0.50
1:O:325:GLU:H	1:O:329:GLN:NE2	2.10	0.50
1:C:231:TYR:CD2	1:C:231:TYR:C	2.90	0.50
1:D:18:ARG:NH2	1:D:20:ILE:CD1	2.71	0.50
1:D:230:SER:C	1:D:232:GLU:H	2.20	0.50
1:X:18:ARG:HH21	1:X:18:ARG:CB	2.24	0.50
1:O:110:SER:OG	1:O:111:PRO:HD3	2.12	0.50
1:D:11:ASP:HA	1:D:81:THR:HG22	1.94	0.50
1:D:466:GLU:CD	1:D:466:GLU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:155:LYS:HE3	1:X:161:LEU:HD21	1.94	0.49
1:C:72:PRO:HB2	1:C:235:GLY:HA3	1.94	0.49
1:C:265:THR:HG23	1:C:410:ASP:OD1	2.11	0.49
1:D:150:GLU:C	1:D:152:ALA:H	2.20	0.49
1:X:10:ILE:CD1	1:X:61:ILE:HD11	2.42	0.49
1:O:181:VAL:HG22	1:O:182:THR:N	2.27	0.49
1:O:238:VAL:HG13	1:O:239:PRO:HD2	1.94	0.49
1:D:89:VAL:HB	1:D:98:ILE:CD1	2.41	0.49
1:C:18:ARG:NH2	1:C:441:ALA:N	2.60	0.49
1:D:303:LEU:HD13	1:D:396:MET:HG3	1.93	0.49
1:O:18:ARG:HH22	1:O:438:GLU:HB2	1.77	0.49
1:X:163:PHE:CG	1:X:164:GLY:N	2.81	0.49
1:C:128:LYS:HD3	1:C:201:ASP:CG	2.37	0.49
1:D:12:GLN:HE22	1:D:83:GLN:NE2	2.10	0.49
1:D:85:GLU:HB2	1:D:104:TRP:HB3	1.93	0.49
1:X:70:ILE:HG22	1:X:71:ARG:N	2.27	0.49
1:X:315:GLN:HE21	1:X:318:ARG:NH2	2.10	0.49
1:X:315:GLN:HG3	1:X:318:ARG:NH2	2.28	0.49
1:C:46:VAL:H	1:C:106:SER:HB2	1.78	0.49
1:C:182:THR:HA	1:C:243:MET:HE1	1.94	0.49
1:X:405:PRO:HD2	4:X:538:HOH:O	2.12	0.48
1:D:116:LEU:HB2	1:D:133:ILE:HG21	1.95	0.48
1:D:248:GLN:H	1:D:248:GLN:NE2	2.07	0.48
1:D:221:ASN:ND2	1:D:293:TYR:HA	2.28	0.48
1:X:18:ARG:HH22	1:X:20:ILE:CG1	2.10	0.48
1:O:263:LYS:HD2	1:O:264:ASN:N	2.28	0.48
1:O:379:ARG:O	1:O:383:GLN:HG3	2.14	0.48
1:C:87:THR:HG23	1:C:163:PHE:CE1	2.48	0.48
1:C:171:VAL:HG21	1:C:243:MET:SD	2.53	0.48
1:C:181:VAL:HG23	1:C:219:LYS:HG3	1.94	0.48
1:D:82:ASN:HD22	1:D:166:ILE:CB	2.25	0.48
1:O:21:ILE:HG21	1:O:70:ILE:HD12	1.95	0.48
1:D:180:HIS:NE2	1:D:216:PRO:HB3	2.28	0.48
1:C:85:GLU:O	1:C:86:THR:C	2.57	0.48
1:D:402:ILE:HG22	1:D:403:ASP:N	2.28	0.48
1:X:125:ILE:HD12	1:X:133:ILE:CD1	2.43	0.48
1:X:231:TYR:O	1:X:232:GLU:CB	2.60	0.48
1:X:264:ASN:CG	1:X:272:ILE:CD1	2.85	0.48
1:O:254:GLN:O	1:O:255:MET:HB2	2.13	0.48
1:C:386:ALA:HA	1:C:423:GLN:HE22	1.79	0.48
1:D:231:TYR:CD1	1:D:231:TYR:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LYS:O	1:D:45:TRP:HB2	2.14	0.48
1:D:241:ALA:HB1	1:D:451:ALA:CB	2.43	0.48
1:X:62:ALA:HB2	1:X:232:GLU:OE1	2.13	0.48
1:X:145:LEU:O	1:X:149:ILE:HD13	2.13	0.48
1:X:282:LEU:O	1:X:283:SER:CB	2.62	0.48
1:O:18:ARG:NH2	1:O:441:ALA:HB2	2.29	0.48
1:D:276:THR:HG21	1:D:281:GLN:HG3	1.96	0.48
1:X:305:GLY:HA3	1:X:392:VAL:CG1	2.44	0.48
1:C:386:ALA:HA	1:C:423:GLN:NE2	2.28	0.48
1:D:49:ASN:CG	1:D:52:GLU:HG3	2.39	0.48
1:D:235:GLY:O	1:D:236:SER:C	2.57	0.48
1:D:282:LEU:O	1:D:283:SER:O	2.31	0.48
1:X:18:ARG:CZ	1:X:20:ILE:HG13	2.44	0.47
1:O:337:ALA:HA	1:O:375:GLU:HB3	1.96	0.47
1:D:112:ILE:HD12	1:D:112:ILE:N	2.29	0.47
1:D:184:TYR:HB3	1:D:291:ILE:HG21	1.95	0.47
1:O:85:GLU:O	1:O:86:THR:C	2.56	0.47
1:C:128:LYS:O	1:C:194:ASN:HA	2.14	0.47
1:D:122:THR:O	1:D:124:MET:N	2.39	0.47
1:D:421:GLN:NE2	1:D:474:GLU:HG2	2.29	0.47
1:X:134:ASP:H	1:X:191:MET:HE1	1.78	0.47
1:O:107:ARG:NH2	1:O:134:ASP:OD2	2.48	0.47
1:O:258:GLU:CB	1:O:261:MET:HE2	2.45	0.47
1:D:420:MET:HA	1:D:420:MET:HE2	1.97	0.47
1:X:128:LYS:HD3	1:X:201:ASP:CG	2.39	0.47
1:X:279:GLU:CD	1:X:279:GLU:N	2.72	0.47
1:C:113:ALA:HB2	1:C:140:THR:HG21	1.96	0.47
1:C:11:ASP:HA	1:C:81:THR:CG2	2.45	0.47
1:D:17:SER:O	1:D:33:GLN:HA	2.14	0.47
1:D:156:ALA:HB1	1:D:211:PRO:HG3	1.96	0.47
1:X:457:ASP:C	1:X:459:ASP:N	2.73	0.47
1:C:180:HIS:CE1	1:C:216:PRO:HB3	2.49	0.47
1:D:255:MET:HE1	1:D:465:ALA:HB2	1.97	0.47
1:C:180:HIS:NE2	1:C:216:PRO:HB3	2.30	0.47
1:C:248:GLN:HG2	1:C:292:GLY:O	2.15	0.47
1:X:70:ILE:CG2	1:X:71:ARG:N	2.78	0.47
1:O:18:ARG:NH1	1:O:20:ILE:HG13	2.29	0.47
1:C:24:ARG:HA	1:C:454:PHE:CE2	2.50	0.47
1:D:284:ASP:O	1:D:285:ASN:CG	2.58	0.47
1:C:178:GLN:HB2	1:C:229:ARG:NH1	2.30	0.46
1:C:416:ASN:C	1:C:416:ASN:HD22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:HIS:C	1:D:122:THR:O	2.54	0.46
1:X:200:TRP:CD2	1:X:215:LEU:HD13	2.51	0.46
1:O:30:GLY:CA	1:O:68:SER:HB3	2.46	0.46
1:O:402:ILE:CG2	1:O:403:ASP:H	2.28	0.46
1:C:110:SER:N	1:C:111:PRO:CD	2.79	0.46
1:O:258:GLU:H	1:O:261:MET:HE2	1.79	0.46
1:O:446:TYR:HB3	1:O:461:LEU:HD21	1.96	0.46
1:C:327:SER:HB2	1:C:328:PRO:HD3	1.96	0.46
1:D:180:HIS:CE1	1:D:216:PRO:HB3	2.50	0.46
1:D:222:SER:O	1:D:223:GLU:HB3	2.15	0.46
1:D:264:ASN:ND2	1:D:266:TYR:CZ	2.84	0.46
1:O:46:VAL:H	1:O:106:SER:HB2	1.80	0.46
1:O:232:GLU:OE2	1:O:232:GLU:HA	2.15	0.46
1:D:386:ALA:O	1:D:389:SER:HB2	2.15	0.46
1:X:84:ARG:H	2:X:1000:EDO:H11	1.80	0.46
1:X:231:TYR:O	1:X:232:GLU:HB2	2.14	0.46
1:D:331:GLU:HG3	1:D:416:ASN:HD21	1.77	0.46
1:C:162:LEU:HD22	1:C:180:HIS:ND1	2.31	0.46
1:D:360:GLU:HB2	1:D:498:LYS:CE	2.45	0.46
1:X:497:PHE:CD1	1:X:497:PHE:C	2.94	0.46
1:D:112:ILE:H	1:D:112:ILE:CD1	2.29	0.46
1:C:112:ILE:HD13	1:C:143:ARG:CG	2.44	0.46
1:D:248:GLN:O	1:D:251:LEU:HB3	2.16	0.46
1:D:460:GLU:O	1:D:463:SER:HB2	2.15	0.46
1:X:282:LEU:HD12	1:X:282:LEU:H	1.81	0.46
1:O:258:GLU:CG	1:O:261:MET:HE2	2.46	0.46
1:D:143:ARG:CD	1:D:147:ASP:OD1	2.62	0.46
1:X:307:ILE:HD13	1:X:388:GLN:HB3	1.98	0.46
1:D:276:THR:CG2	1:D:281:GLN:HE21	2.17	0.46
1:C:420:MET:HE2	1:C:420:MET:HA	1.98	0.45
1:D:10:ILE:CD1	1:D:61:ILE:HD11	2.45	0.45
1:D:12:GLN:NE2	1:D:83:GLN:HE21	2.14	0.45
1:D:283:SER:O	1:D:284:ASP:HB2	2.16	0.45
1:X:379:ARG:O	1:X:383:GLN:HG3	2.16	0.45
1:D:274:MET:HE2	1:D:303:LEU:HD12	1.98	0.45
1:X:285:ASN:O	1:X:286:ASP:HB2	2.16	0.45
1:O:272:ILE:N	1:O:272:ILE:CD1	2.80	0.45
1:D:220:SER:HB2	1:D:294:GLY:O	2.16	0.45
1:O:429:ILE:HG12	1:O:430:ASP:N	2.31	0.45
1:C:143:ARG:NH2	1:C:146:LEU:HB2	2.31	0.45
1:D:263:LYS:HA	1:D:408:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:236:SER:N	4:O:554:HOH:O	2.36	0.45
1:O:264:ASN:ND2	1:O:266:TYR:CZ	2.85	0.45
1:O:18:ARG:HD2	1:O:20:ILE:HD11	1.99	0.45
1:C:25:ASN:HA	1:C:464:MET:HE2	1.99	0.45
1:C:128:LYS:NZ	1:C:203:GLU:CD	2.75	0.45
1:C:358:ASP:C	1:C:358:ASP:OD1	2.60	0.45
1:X:176:ASP:OD2	1:X:229:ARG:NH1	2.49	0.45
1:C:18:ARG:HG2	1:C:20:ILE:HD13	1.94	0.45
1:D:49:ASN:HB3	1:D:52:GLU:HG3	1.98	0.45
1:X:81:THR:HG21	1:X:440:THR:HG22	1.98	0.45
1:X:85:GLU:HB2	1:X:104:TRP:HB3	1.98	0.45
1:X:497:PHE:C	1:X:497:PHE:HD1	2.25	0.45
1:C:17:SER:O	1:C:60:VAL:HG11	2.17	0.45
1:C:54:TRP:O	1:C:58:GLN:HG3	2.17	0.45
1:D:145:LEU:O	1:D:149:ILE:HG12	2.17	0.45
1:D:284:ASP:O	1:D:286:ASP:N	2.34	0.45
1:O:176:ASP:CB	1:O:229:ARG:HD2	2.47	0.44
1:O:425:ASP:HB3	1:O:475:MET:CB	2.46	0.44
1:O:469:GLN:HG3	1:O:471:PHE:CE2	2.52	0.44
1:C:329:GLN:HA	1:C:332:GLU:OE2	2.18	0.44
1:D:6:TYR:CE2	1:D:70:ILE:HD12	2.52	0.44
1:D:85:GLU:O	1:D:86:THR:C	2.60	0.44
1:X:123:GLU:H	1:X:123:GLU:CD	2.25	0.44
1:X:137:PHE:CD2	1:X:191:MET:HE3	2.52	0.44
1:D:190:THR:HG23	1:D:192:LEU:H	1.83	0.44
1:X:433:ARG:HH21	1:X:469:GLN:NE2	2.16	0.44
1:O:241:ALA:HB1	1:O:451:ALA:HB3	1.99	0.44
1:C:234:TYR:O	1:C:235:GLY:C	2.59	0.44
1:C:345:VAL:O	1:C:347:PRO:HD3	2.17	0.44
1:X:200:TRP:CG	1:X:215:LEU:HD13	2.53	0.44
1:C:266:TYR:CE2	1:C:420:MET:HE1	2.52	0.44
1:X:10:ILE:HD13	1:X:61:ILE:HD11	1.99	0.44
1:X:91:ASP:HB3	1:X:94:THR:OG1	2.18	0.44
1:C:458:LEU:O	1:C:461:LEU:HB2	2.18	0.44
1:C:175:THR:HG22	1:C:227:HIS:O	2.18	0.44
1:C:18:ARG:HH11	1:C:438:GLU:CD	2.25	0.44
1:X:433:ARG:CG	1:X:437:LEU:HD21	2.47	0.44
1:D:270:ALA:HB3	1:D:307:ILE:HB	2.00	0.44
1:X:336:LYS:HB3	1:X:336:LYS:HE2	1.79	0.43
1:C:42:LYS:O	1:C:43:SER:C	2.60	0.43
1:D:81:THR:HG21	1:D:440:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:SER:HB3	1:D:295:ILE:HG13	2.01	0.43
1:D:360:GLU:HB2	1:D:498:LYS:HE2	2.00	0.43
1:D:389:SER:HB2	1:D:423:GLN:HE22	1.83	0.43
1:X:390:LYS:HD3	1:X:484:TYR:CD1	2.53	0.43
1:X:459:ASP:O	1:X:461:LEU:N	2.50	0.43
1:D:346:VAL:O	1:D:363:GLY:HA2	2.18	0.43
1:C:205:LEU:HD11	1:C:215:LEU:HD11	2.00	0.43
1:C:403:ASP:O	1:C:405:PRO:HD3	2.17	0.43
1:C:231:TYR:HD2	1:C:232:GLU:H	1.64	0.43
1:X:246:ASP:OD1	1:X:247:GLN:N	2.50	0.43
1:C:6:TYR:CE2	1:C:70:ILE:HD12	2.54	0.43
1:O:70:ILE:CG2	1:O:71:ARG:N	2.82	0.43
1:D:18:ARG:NH2	1:D:20:ILE:HD12	2.33	0.43
1:D:263:LYS:HE3	1:D:273:VAL:HB	2.00	0.43
1:X:339:GLY:HA3	1:X:376:ASP:OD1	2.18	0.43
1:D:107:ARG:O	1:D:110:SER:HB2	2.19	0.43
1:X:21:ILE:HG21	1:X:70:ILE:HD12	1.99	0.43
1:X:30:GLY:HA3	1:X:68:SER:HB3	2.01	0.43
1:C:58:GLN:HB3	1:D:66:ILE:HD12	1.99	0.43
1:C:124:MET:HE3	1:C:125:ILE:HD13	2.00	0.43
1:C:266:TYR:CB	1:C:413:ALA:HB3	2.47	0.43
1:C:360:GLU:HB2	1:C:498:LYS:CE	2.49	0.43
1:X:143:ARG:NH2	1:X:153:GLN:NE2	2.66	0.43
1:O:258:GLU:HB2	1:O:261:MET:HE2	2.01	0.43
1:C:30:GLY:HA3	1:C:68:SER:HB3	2.01	0.43
1:C:321:LEU:O	1:C:322:ARG:HB2	2.18	0.43
1:D:284:ASP:C	1:D:285:ASN:CG	2.87	0.43
1:O:235:GLY:HA2	4:O:554:HOH:O	2.19	0.43
1:X:48:HIS:HB3	1:X:53:ILE:CD1	2.41	0.42
1:X:234:TYR:CD1	1:O:231:TYR:HA	2.54	0.42
1:O:412:GLY:O	1:O:415:LYS:HG3	2.19	0.42
1:C:402:ILE:O	1:C:403:ASP:C	2.62	0.42
1:D:78:ILE:HD11	1:D:233:PHE:CE1	2.53	0.42
1:D:86:THR:HG23	1:D:103:VAL:HA	2.01	0.42
1:D:191:MET:O	1:D:192:LEU:HD23	2.19	0.42
1:D:436:ASN:OD1	1:D:438:GLU:OE2	2.37	0.42
1:X:128:LYS:HD3	1:X:201:ASP:OD2	2.19	0.42
1:X:263:LYS:HA	1:X:408:LYS:O	2.18	0.42
1:O:270:ALA:HB3	1:O:307:ILE:HB	2.01	0.42
1:C:181:VAL:CG2	1:C:182:THR:N	2.80	0.42
1:C:233:PHE:C	1:C:235:GLY:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:HA	1:D:60:VAL:HG22	2.01	0.42
1:D:139:ALA:HB3	1:D:191:MET:HE2	2.00	0.42
1:D:276:THR:CG2	1:D:281:GLN:HG3	2.49	0.42
1:D:284:ASP:C	1:D:286:ASP:N	2.77	0.42
1:X:356:TYR:O	1:X:357:TRP:C	2.62	0.42
1:X:416:ASN:HB3	1:X:419:LEU:HB3	2.01	0.42
1:C:46:VAL:O	1:C:106:SER:HB2	2.19	0.42
1:C:124:MET:HE3	1:C:125:ILE:CD1	2.49	0.42
1:D:173:LYS:NZ	4:D:518:HOH:O	2.52	0.42
1:X:220:SER:OG	1:X:223:GLU:OE1	2.34	0.42
1:X:402:ILE:HG22	1:X:403:ASP:N	2.34	0.42
1:O:18:ARG:NH1	1:O:20:ILE:CD1	2.82	0.42
1:O:23:ASP:C	1:O:23:ASP:OD1	2.62	0.42
1:O:75:ILE:CG2	1:O:238:VAL:HG11	2.49	0.42
1:C:255:MET:HE1	1:C:465:ALA:CA	2.49	0.42
1:C:230:SER:HB3	1:C:231:TYR:H	1.63	0.42
1:D:246:ASP:OD1	1:D:247:GLN:N	2.52	0.42
1:X:324:ILE:HG22	1:X:333:LEU:CD1	2.49	0.42
1:O:438:GLU:OE1	1:O:438:GLU:N	2.46	0.42
1:C:122:THR:HA	1:C:133:ILE:CD1	2.49	0.42
1:D:62:ALA:O	1:D:66:ILE:HG12	2.19	0.42
1:D:122:THR:N	1:D:133:ILE:HD11	2.35	0.42
1:D:248:GLN:HG2	1:D:292:GLY:O	2.20	0.42
1:X:500:LYS:CB	4:X:617:HOH:O	2.67	0.42
1:O:267:GLY:O	1:O:268:THR:C	2.62	0.42
1:O:425:ASP:HB3	1:O:475:MET:HB2	2.02	0.42
1:C:255:MET:HE1	1:C:465:ALA:CB	2.50	0.42
1:X:256:ALA:HA	1:X:261:MET:HE2	2.01	0.42
1:O:149:ILE:N	1:O:149:ILE:CD1	2.83	0.42
1:C:91:ASP:OD2	1:C:94:THR:HG23	2.20	0.42
1:D:92:LYS:HB3	1:D:92:LYS:HZ3	1.85	0.42
1:X:20:ILE:CD1	1:X:31:SER:HB3	2.18	0.42
1:X:262:ILE:HD11	1:X:272:ILE:CG2	2.50	0.42
1:O:325:GLU:H	1:O:329:GLN:HE22	1.68	0.42
1:C:231:TYR:O	1:C:234:TYR:HB2	2.20	0.42
1:C:274:MET:O	1:C:302:ALA:HA	2.20	0.42
1:C:232:GLU:C	1:C:234:TYR:H	2.28	0.41
1:C:284:ASP:O	1:C:285:ASN:C	2.63	0.41
1:X:20:ILE:HD13	1:X:31:SER:HA	2.02	0.41
1:X:361:ALA:O	1:X:362:ARG:NH1	2.43	0.41
1:O:18:ARG:HH11	1:O:20:ILE:CD1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:143:ARG:NH1	1:O:147:ASP:OD1	2.38	0.41
1:O:258:GLU:HB2	1:O:261:MET:HG3	2.01	0.41
1:C:238:VAL:HA	1:C:239:PRO:HD3	1.86	0.41
1:D:11:ASP:HA	1:D:81:THR:CG2	2.50	0.41
1:D:495:GLN:O	1:D:498:LYS:NZ	2.37	0.41
1:X:83:GLN:O	1:X:83:GLN:HG3	2.20	0.41
1:X:180:HIS:NE2	1:X:216:PRO:HB3	2.34	0.41
1:X:352:LEU:HB3	1:X:356:TYR:HB2	2.03	0.41
1:O:303:LEU:HB3	1:O:396:MET:HE2	2.02	0.41
1:C:45:TRP:CE2	1:C:108:GLN:HB2	2.55	0.41
1:X:243:MET:O	1:X:244:ALA:HB2	2.21	0.41
1:X:500:LYS:HA	4:X:520:HOH:O	2.20	0.41
1:O:112:ILE:HD13	1:O:143:ARG:HB3	2.02	0.41
1:C:156:ALA:HB2	1:C:161:LEU:HD12	2.03	0.41
1:X:404:ILE:HA	4:X:538:HOH:O	2.20	0.41
1:O:144:TRP:O	1:O:148:ASN:ND2	2.53	0.41
1:C:309:VAL:CG1	1:C:313:ALA:HB2	2.49	0.41
1:D:397:LYS:HB2	1:D:402:ILE:O	2.20	0.41
1:X:273:VAL:HG22	1:X:304:GLU:HG3	2.02	0.41
1:X:433:ARG:HD2	1:X:437:LEU:HD21	2.03	0.41
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.98	0.41
1:X:460:GLU:O	1:X:460:GLU:HG2	2.20	0.41
1:O:172:TRP:CD2	1:O:177:GLY:HA2	2.55	0.41
1:C:89:VAL:HA	1:C:162:LEU:O	2.20	0.41
1:C:234:TYR:CB	1:D:234:TYR:HB2	2.50	0.41
1:X:232:GLU:C	1:X:234:TYR:H	2.28	0.41
1:X:264:ASN:OD1	1:X:272:ILE:HD13	2.20	0.41
1:X:314:ILE:HD11	1:X:382:LEU:HD23	2.02	0.41
1:X:330:SER:HB3	1:X:382:LEU:HD11	2.03	0.41
1:C:18:ARG:CZ	1:C:441:ALA:CB	2.85	0.41
1:C:80:ILE:O	1:C:243:MET:HA	2.21	0.41
1:C:122:THR:HA	1:C:133:ILE:HD11	2.02	0.41
1:X:386:ALA:HA	1:X:423:GLN:NE2	2.35	0.41
1:O:24:ARG:HE	1:O:24:ARG:HB2	1.64	0.41
1:O:181:VAL:HG21	1:O:219:LYS:HD2	2.03	0.41
1:O:344:TYR:CZ	1:O:486:GLY:HA3	2.56	0.41
1:C:20:ILE:HD12	1:C:20:ILE:N	2.36	0.41
1:C:165:THR:OG1	1:C:167:ASP:OD1	2.28	0.41
1:C:426:ILE:HD13	1:C:426:ILE:HA	1.93	0.41
1:D:80:ILE:O	1:D:243:MET:HA	2.21	0.41
1:D:83:GLN:HA	1:D:246:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:THR:C	1:D:124:MET:H	2.27	0.41
1:C:85:GLU:HB2	1:C:104:TRP:HB3	2.04	0.40
1:C:234:TYR:CB	1:D:234:TYR:CB	2.99	0.40
1:C:416:ASN:C	1:C:416:ASN:ND2	2.79	0.40
1:D:262:ILE:HG21	1:D:404:ILE:CG2	2.50	0.40
1:O:11:ASP:HA	1:O:81:THR:HG23	2.03	0.40
1:O:107:ARG:NH2	1:O:134:ASP:CG	2.76	0.40
1:O:110:SER:N	1:O:111:PRO:CD	2.85	0.40
1:O:196:HIS:HE1	4:O:546:HOH:O	2.03	0.40
1:C:84:ARG:C	1:C:85:GLU:OE1	2.64	0.40
1:C:304:GLU:HG2	1:C:305:GLY:N	2.36	0.40
1:D:10:ILE:HD12	1:D:80:ILE:CD1	2.51	0.40
1:X:161:LEU:HB2	1:X:214:MET:HE3	2.02	0.40
1:X:472:THR:HG23	1:X:473:PRO:HD2	2.03	0.40
1:O:229:ARG:O	1:O:232:GLU:HB2	2.21	0.40
1:D:436:ASN:OD1	1:D:438:GLU:CG	2.69	0.40
1:O:266:TYR:CB	1:O:413:ALA:HB3	2.47	0.40
1:C:241:ALA:HB1	1:C:451:ALA:HB3	2.03	0.40
1:D:362:ARG:HA	1:D:362:ARG:HD3	1.93	0.40
1:D:386:ALA:HA	1:D:423:GLN:NE2	2.37	0.40

There are no symmetry-related clashes.

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	C	498/506 (98%)	465 (93%)	29 (6%)	4 (1%)	16	27
1	D	497/506 (98%)	450 (90%)	32 (6%)	15 (3%)	3	5
1	O	498/506 (98%)	462 (93%)	29 (6%)	7 (1%)	9	14
1	X	497/506 (98%)	452 (91%)	33 (7%)	12 (2%)	4	7
All	All	1990/2024 (98%)	1829 (92%)	123 (6%)	38 (2%)	6	10

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	232	GLU
1	X	281	GLN
1	O	285	ASN
1	C	230	SER
1	D	230	SER
1	D	236	SER
1	D	237	GLU
1	D	283	SER
1	D	499	PHE
1	X	18	ARG
1	X	230	SER
1	X	458	LEU
1	X	469	GLN
1	O	4	LYS
1	O	416	ASN
1	O	437	LEU
1	X	4	LYS
1	X	283	SER
1	X	460	GLU
1	O	339	GLY
1	O	456	LYS
1	C	285	ASN
1	D	284	ASP
1	D	285	ASN
1	D	500	LYS
1	O	231	TYR
1	C	150	GLU
1	C	233	PHE
1	D	212	SER
1	D	231	TYR
1	D	456	LYS
1	X	86	THR
1	X	176	ASP
1	D	139	ALA
1	D	152	ALA
1	X	280	PRO
1	D	66	ILE
1	D	280	PRO

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	C	404/410 (98%)	396 (98%)	8 (2%)	48	69
1	D	404/410 (98%)	390 (96%)	14 (4%)	32	52
1	O	404/410 (98%)	389 (96%)	15 (4%)	30	50
1	X	402/410 (98%)	394 (98%)	8 (2%)	48	69
All	All	1614/1640 (98%)	1569 (97%)	45 (3%)	38	60

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	18	ARG
1	X	35	GLU
1	X	100	ASN
1	X	303	LEU
1	X	342	GLU
1	X	370	ARG
1	X	436	ASN
1	X	459	ASP
1	O	12	GLN
1	O	107	ARG
1	O	143	ARG
1	O	150	GLU
1	O	261	MET
1	O	272	ILE
1	O	326	THR
1	O	338	LYS
1	O	340	ASP
1	O	370	ARG
1	O	415	LYS
1	O	429	ILE
1	O	437	LEU
1	O	438	GLU
1	O	470	MET
1	C	198	LEU

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Mol	Chain	Res	Type
1	C	231	TYR
1	C	243	MET
1	C	370	ARG
1	C	429	ILE
1	C	458	LEU
1	C	460	GLU
1	C	496	THR
1	D	12	GLN
1	D	67	GLU
1	D	92	LYS
1	D	98	ILE
1	D	147	ASP
1	D	248	GLN
1	D	272	ILE
1	D	303	LEU
1	D	340	ASP
1	D	370	ARG
1	D	404	ILE
1	D	426	ILE
1	D	466	GLU
1	D	488	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	12	GLN
1	X	83	GLN
1	X	96	GLN
1	X	100	ASN
1	X	121	HIS
1	X	126	HIS
1	X	148	ASN
1	X	153	GLN
1	X	178	GLN
1	X	180	HIS
1	X	209	ASN
1	X	221	ASN
1	X	264	ASN
1	X	315	GLN
1	X	329	GLN
1	X	423	GLN
1	X	432	GLN

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Mol	Chain	Res	Type
1	O	12	GLN
1	O	96	GLN
1	O	148	ASN
1	O	178	GLN
1	O	180	HIS
1	O	196	HIS
1	O	209	ASN
1	O	221	ASN
1	O	264	ASN
1	O	383	GLN
1	O	423	GLN
1	O	495	GLN
1	C	5	ASN
1	C	115	GLN
1	C	121	HIS
1	C	126	HIS
1	C	158	ASN
1	C	178	GLN
1	C	209	ASN
1	C	221	ASN
1	C	254	GLN
1	C	264	ASN
1	C	285	ASN
1	C	315	GLN
1	C	329	GLN
1	C	383	GLN
1	C	416	ASN
1	C	423	GLN
1	C	482	ASN
1	D	12	GLN
1	D	38	GLN
1	D	82	ASN
1	D	83	GLN
1	D	126	HIS
1	D	158	ASN
1	D	180	HIS
1	D	186	ASN
1	D	209	ASN
1	D	221	ASN
1	D	248	GLN
1	D	264	ASN
1	D	281	GLN

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Mol	Chain	Res	Type
1	D	423	GLN
1	D	432	GLN

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 ⓘ

11 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
3	PO4	C	507	-	4,4,4	1.60	0	6,6,6	0.46	0
3	PO4	X	508	-	4,4,4	1.56	0	6,6,6	0.47	0
3	PO4	X	510	-	4,4,4	1.45	0	6,6,6	0.49	0
2	EDO	X	507	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	D	1003	-	3,3,3	0.55	0	2,2,2	0.32	0
3	PO4	X	509	-	4,4,4	1.46	0	6,6,6	0.47	0
3	PO4	D	507	-	4,4,4	1.63	0	6,6,6	0.49	0
2	EDO	X	1000	-	3,3,3	0.59	0	2,2,2	0.29	0
2	EDO	O	1001	-	3,3,3	0.65	0	2,2,2	0.32	0
3	PO4	O	507	-	4,4,4	1.62	0	6,6,6	0.45	0
2	EDO	C	1002	-	3,3,3	0.53	0	2,2,2	0.29	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	X	507	-	-	1/1/1/1	-
2	EDO	D	1003	-	-	1/1/1/1	-
2	EDO	X	1000	-	-	1/1/1/1	-
2	EDO	O	1001	-	-	1/1/1/1	-
2	EDO	C	1002	-	-	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	X	507	EDO	O1-C1-C2-O2
2	C	1002	EDO	O1-C1-C2-O2
2	X	1000	EDO	O1-C1-C2-O2
2	O	1001	EDO	O1-C1-C2-O2
2	D	1003	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1003	EDO	1	0
2	X	1000	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	500/506 (98%)	-0.56	5 (1%) 79 76	22, 36, 62, 88	0
1	D	499/506 (98%)	-0.36	5 (1%) 79 76	26, 44, 73, 100	0
1	O	500/506 (98%)	-0.60	4 (0%) 82 79	21, 33, 60, 84	0
1	X	499/506 (98%)	-0.57	5 (1%) 79 76	19, 33, 63, 82	0
All	All	1998/2024 (98%)	-0.52	19 (0%) 79 76	19, 37, 65, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	231	TYR	4.3
1	X	18	ARG	3.8
1	C	234	TYR	3.4
1	D	236	SER	3.4
1	C	18	ARG	3.4
1	D	234	TYR	3.3
1	C	231	TYR	3.2
1	D	18	ARG	3.0
1	X	234	TYR	2.9
1	D	285	ASN	2.9
1	O	235	GLY	2.8
1	C	230	SER	2.8
1	C	235	GLY	2.7
1	D	235	GLY	2.6
1	X	282	LEU	2.4
1	O	18	ARG	2.4
1	O	501	ALA	2.1
1	X	17	SER	2.0
1	O	2	ALA	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
3	PO4	X	510	5/5	0.79	0.17	57,59,68,72	0
2	EDO	X	507	4/4	0.82	0.11	50,67,68,69	0
3	PO4	X	509	5/5	0.86	0.18	52,56,74,75	0
2	EDO	X	1000	4/4	0.89	0.12	27,28,34,36	0
2	EDO	O	1001	4/4	0.89	0.10	22,22,23,27	0
2	EDO	D	1003	4/4	0.90	0.08	29,37,39,44	0
3	PO4	D	507	5/5	0.92	0.07	50,56,60,63	0
3	PO4	C	507	5/5	0.93	0.08	38,42,50,50	0
3	PO4	X	508	5/5	0.93	0.08	58,59,64,66	0
2	EDO	C	1002	4/4	0.95	0.07	20,22,22,28	0
3	PO4	O	507	5/5	0.95	0.06	42,44,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.