



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:33 AM UTC

PDB ID : 1WQA / pdb_00001wqa
Title : Crystal Structure of Pyrococcus horikoshii phosphomannomutase/phosphoglucose mutase complexed with Mg²⁺
Authors : Kawamura, T.; Tsuge, M.; Watanabe, N.; Tanaka, I.
Deposited on : 2004-09-24
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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
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

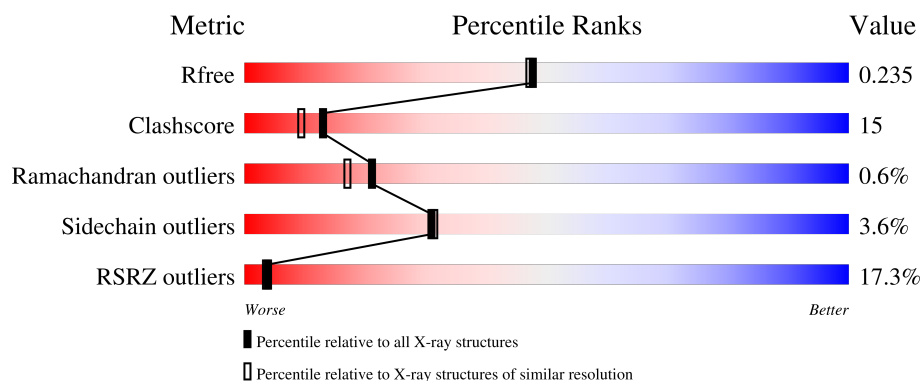
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	455	16% 70% 27% .
1	B	455	20% 71% 27% .
1	C	455	18% 73% 24% ..
1	D	455	15% 72% 26% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14766 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 phospho-sugar mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			
1	B	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			
1	C	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			
1	D	455	Total	C	N	O	S	0	0	0
			3512	2236	604	661	11			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

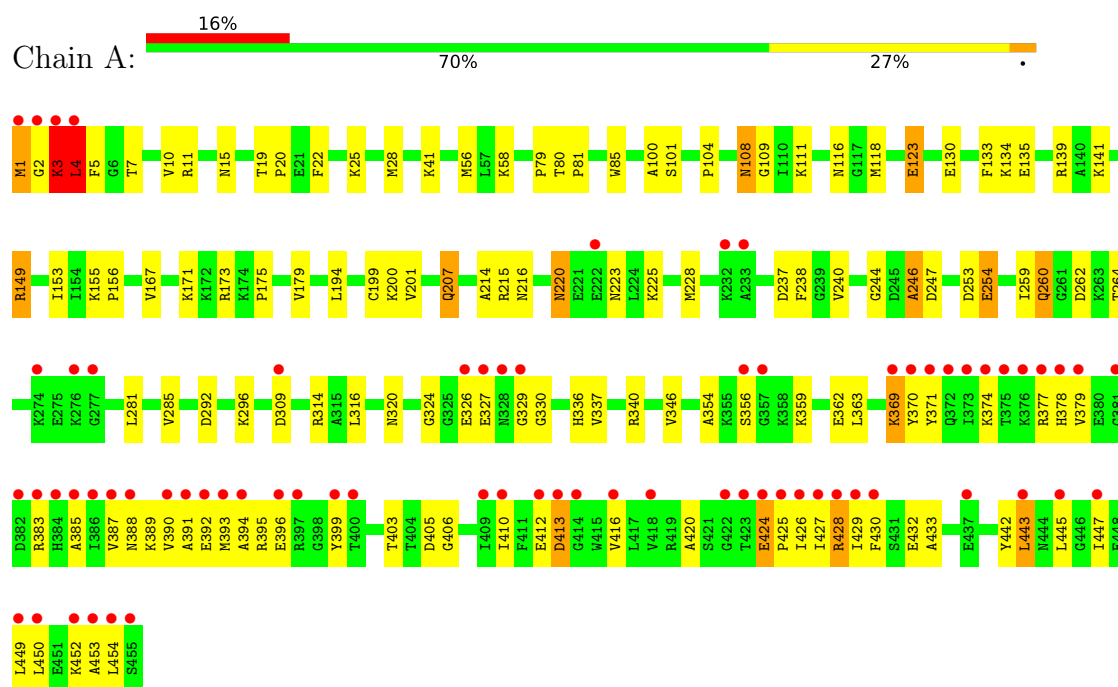
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	192	Total	O	0	0
			192	192		
3	C	186	Total	O	0	0
			186	186		
3	D	165	Total	O	0	0
			165	165		

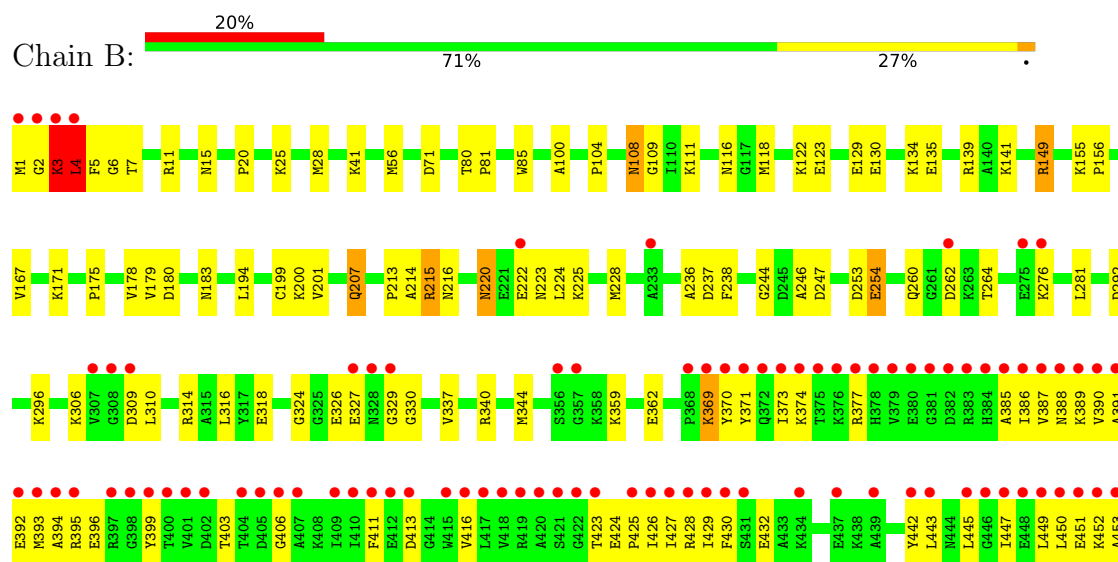
3 Residue-property plots [i](#)

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: phospho-sugar mutase

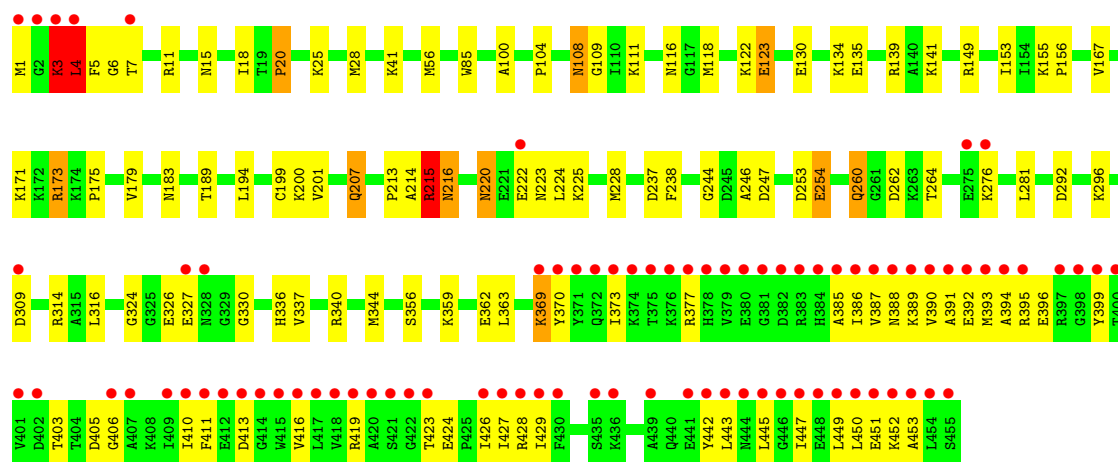
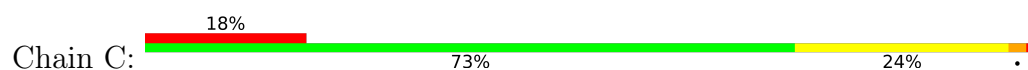


- Molecule 1: phospho-sugar mutase

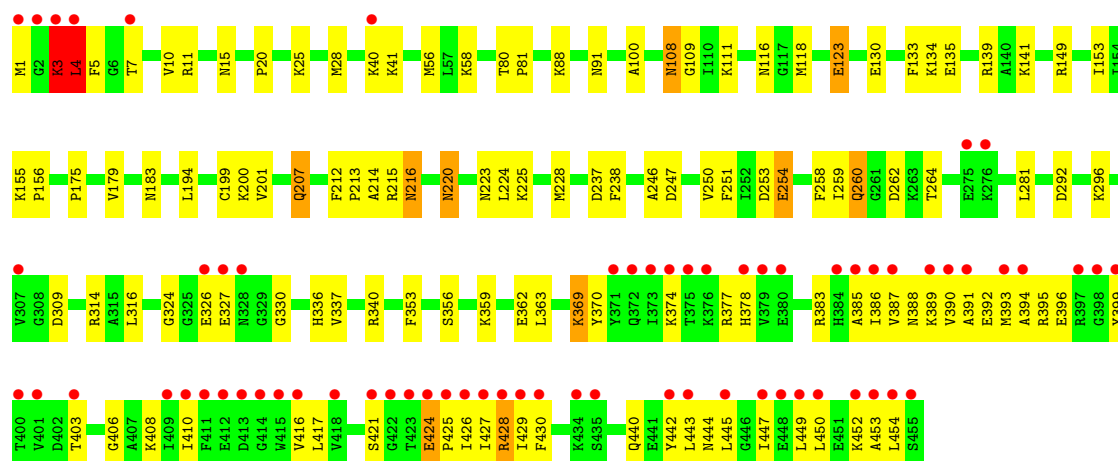
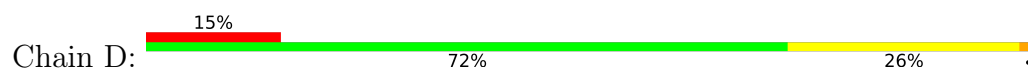




● Molecule 1: phospho-sugar mutase



● Molecule 1: phospho-sugar mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.65Å 137.92Å 98.41Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.00) 98.5 (50.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.236 0.210 , 0.235	Depositor DCC
R_{free} test set	6883 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14766	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	0/3570	0.98	15/4807 (0.3%)
1	B	0.66	1/3570 (0.0%)	0.96	12/4807 (0.2%)
1	C	0.64	1/3570 (0.0%)	0.98	16/4807 (0.3%)
1	D	0.59	0/3570	0.95	9/4807 (0.2%)
All	All	0.62	2/14280 (0.0%)	0.97	52/19228 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	344	MET	SD-CE	-5.15	1.66	1.79
1	C	344	MET	SD-CE	-5.04	1.67	1.79

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	LYS	N-CA-C	-12.03	90.19	108.00
1	A	3	LYS	N-CA-C	-7.70	95.07	108.08
1	A	2	GLY	N-CA-C	-7.37	95.72	113.18
1	D	3	LYS	N-CA-C	-7.26	95.33	110.80
1	C	4	LEU	N-CA-C	7.26	126.27	110.80
1	D	200	LYS	N-CA-C	-7.12	97.65	109.46
1	B	201	VAL	N-CA-C	7.01	117.92	108.11
1	A	200	LYS	N-CA-C	-6.96	97.91	109.46
1	B	200	LYS	N-CA-C	-6.93	97.96	109.46
1	D	246	ALA	N-CA-C	6.80	120.95	112.24
1	C	200	LYS	N-CA-C	-6.70	98.33	109.46
1	B	246	ALA	N-CA-C	6.70	120.79	111.74
1	A	4	LEU	N-CA-C	6.69	125.05	110.80
1	B	216	ASN	N-CA-C	-6.66	101.94	109.60
1	D	216	ASN	N-CA-C	-6.62	101.99	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	VAL	N-CA-C	6.58	117.32	108.11
1	A	216	ASN	N-CA-C	-6.55	101.32	109.64
1	B	247	ASP	N-CA-C	-6.42	104.48	112.90
1	A	141	LYS	N-CA-C	-6.34	102.16	110.53
1	B	3	LYS	N-CA-C	-6.26	98.22	108.67
1	C	247	ASP	N-CA-C	-6.25	104.72	112.90
1	A	201	VAL	N-CA-C	6.23	116.83	108.11
1	D	201	VAL	N-CA-C	6.22	116.83	108.11
1	C	246	ALA	N-CA-C	6.19	120.10	111.74
1	C	141	LYS	N-CA-C	-6.13	102.44	110.53
1	A	246	ALA	N-CA-C	6.12	120.08	112.24
1	A	5	PHE	N-CA-C	5.89	119.68	110.32
1	B	244	GLY	N-CA-C	5.88	119.76	112.64
1	C	18	ILE	N-CA-C	5.88	112.50	106.21
1	B	104	PRO	CA-C-N	5.88	126.29	119.47
1	B	104	PRO	C-N-CA	5.88	126.29	119.47
1	D	141	LYS	N-CA-C	-5.83	102.83	110.53
1	B	4	LEU	N-CA-C	5.71	122.97	110.80
1	A	104	PRO	CA-C-N	5.71	126.09	119.47
1	A	104	PRO	C-N-CA	5.71	126.09	119.47
1	C	244	GLY	N-CA-C	5.71	119.54	112.64
1	B	141	LYS	N-CA-C	-5.68	102.50	110.50
1	A	410	ILE	N-CA-C	5.59	116.79	108.23
1	C	189	THR	N-CA-C	5.59	119.61	112.12
1	D	4	LEU	N-CA-C	5.51	122.54	110.80
1	C	104	PRO	CA-C-N	5.41	125.74	119.47
1	C	104	PRO	C-N-CA	5.41	125.74	119.47
1	A	247	ASP	N-CA-C	-5.38	106.56	113.23
1	D	247	ASP	N-CA-C	-5.38	106.56	113.23
1	A	244	GLY	N-CA-C	5.28	119.03	112.64
1	C	20	PRO	N-CA-C	-5.27	106.34	113.40
1	C	5	PHE	N-CA-C	5.26	118.26	110.48
1	B	71	ASP	N-CA-C	-5.25	102.71	110.48
1	A	101	SER	N-CA-C	5.23	121.94	110.80
1	D	410	ILE	N-CA-C	5.17	115.54	107.99
1	C	216	ASN	N-CA-C	-5.15	103.68	109.60
1	C	410	ILE	N-CA-C	5.13	115.70	108.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3512	0	3590	111	0
1	B	3512	0	3590	116	0
1	C	3512	0	3590	101	0
1	D	3512	0	3591	99	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	171	0	0	8	0
3	B	192	0	0	8	0
3	C	186	0	0	4	0
3	D	165	0	0	3	0
All	All	14766	0	14361	427	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 15.

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HA	1:A:3:LYS:CE	1.56	1.29
1:C:3:LYS:HE3	1:C:3:LYS:HA	1.24	1.15
1:A:416:VAL:HG22	1:A:442:TYR:HB3	1.39	0.99
1:D:416:VAL:HG22	1:D:442:TYR:HB3	1.45	0.98
1:A:3:LYS:HA	1:A:3:LYS:HE3	1.46	0.93
1:A:3:LYS:HA	1:A:3:LYS:HE2	1.48	0.93
1:C:3:LYS:HA	1:C:3:LYS:CE	1.98	0.91
1:C:3:LYS:HE3	1:C:3:LYS:CA	2.03	0.88
1:A:207:GLN:H	1:A:207:GLN:HE21	1.17	0.88
1:A:385:ALA:HA	1:A:388:ASN:HD22	1.39	0.87
1:C:416:VAL:HG22	1:C:442:TYR:HB3	1.58	0.86
1:B:416:VAL:HG22	1:B:442:TYR:HB3	1.58	0.86
1:D:207:GLN:H	1:D:207:GLN:HE21	1.20	0.86
1:B:207:GLN:H	1:B:207:GLN:HE21	1.24	0.84
1:C:207:GLN:H	1:C:207:GLN:HE21	1.22	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:ND2	1:B:223:ASN:H	1.78	0.81
1:D:385:ALA:HA	1:D:388:ASN:HD22	1.43	0.81
1:A:220:ASN:ND2	1:A:223:ASN:H	1.78	0.81
1:C:220:ASN:ND2	1:C:223:ASN:H	1.80	0.80
1:D:220:ASN:ND2	1:D:223:ASN:H	1.80	0.79
1:D:225:LYS:HA	1:D:228:MET:HE3	1.64	0.78
1:C:222:GLU:HG3	3:C:553:HOH:O	1.81	0.78
1:A:3:LYS:CE	1:A:3:LYS:CA	2.52	0.76
1:C:28:MET:HE1	1:C:139:ARG:NH1	1.99	0.76
1:C:385:ALA:HA	1:C:388:ASN:HD22	1.50	0.76
1:A:220:ASN:HD22	1:A:220:ASN:C	1.94	0.75
1:C:220:ASN:C	1:C:220:ASN:HD22	1.95	0.74
1:C:225:LYS:HA	1:C:228:MET:HE3	1.70	0.74
1:B:385:ALA:HA	1:B:388:ASN:HD22	1.51	0.73
1:D:220:ASN:C	1:D:220:ASN:HD22	1.94	0.73
1:B:220:ASN:C	1:B:220:ASN:HD22	1.96	0.73
1:B:122:LYS:HE2	1:B:314:ARG:HH22	1.53	0.73
1:C:429:ILE:HD11	1:C:450:LEU:HD12	1.69	0.73
1:A:225:LYS:HA	1:A:228:MET:HE3	1.70	0.72
1:B:1:MET:HE1	1:B:11:ARG:HD2	1.69	0.72
1:C:369:LYS:HD3	1:C:370:TYR:N	2.04	0.72
1:B:429:ILE:HD11	1:B:450:LEU:HD12	1.71	0.71
1:B:369:LYS:HD3	1:B:370:TYR:N	2.05	0.71
1:A:416:VAL:CG2	1:A:442:TYR:HB3	2.20	0.71
1:D:392:GLU:O	1:D:396:GLU:HG2	1.90	0.70
1:C:369:LYS:HD3	1:C:370:TYR:H	1.56	0.70
1:A:108:ASN:HD22	1:A:109:GLY:H	1.39	0.70
1:B:369:LYS:HD3	1:B:370:TYR:H	1.55	0.70
1:A:369:LYS:HD3	1:A:370:TYR:N	2.07	0.70
1:B:225:LYS:HA	1:B:228:MET:HE3	1.73	0.70
1:B:373:ILE:HB	1:B:443:LEU:HD12	1.75	0.69
1:B:108:ASN:HD22	1:B:109:GLY:H	1.38	0.69
1:B:393:MET:HE1	1:B:453:ALA:CB	2.22	0.69
1:D:416:VAL:CG2	1:D:442:TYR:HB3	2.21	0.69
1:D:1:MET:HE1	1:D:11:ARG:H	1.56	0.68
1:A:28:MET:HE1	1:A:139:ARG:NH1	2.09	0.68
1:B:3:LYS:HE3	1:B:3:LYS:HA	1.75	0.68
1:B:28:MET:HE1	1:B:139:ARG:NH1	2.07	0.68
1:D:369:LYS:HD3	1:D:370:TYR:N	2.09	0.68
1:D:220:ASN:HD21	1:D:223:ASN:H	1.42	0.68
1:C:108:ASN:HD22	1:C:109:GLY:H	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASN:HD21	1:B:223:ASN:H	1.41	0.67
1:B:306:LYS:HG3	3:B:532:HOH:O	1.95	0.67
1:D:316:LEU:HD11	1:D:324:GLY:HA3	1.77	0.66
1:A:369:LYS:HD3	1:A:370:TYR:H	1.60	0.66
1:A:220:ASN:HD21	1:A:223:ASN:H	1.42	0.66
1:C:122:LYS:HG2	1:C:314:ARG:HH12	1.60	0.66
1:D:369:LYS:HD3	1:D:370:TYR:H	1.61	0.66
1:B:222:GLU:HG3	3:B:644:HOH:O	1.95	0.65
1:C:1:MET:HE2	1:C:6:GLY:HA3	1.78	0.65
1:D:28:MET:HE1	1:D:139:ARG:NH1	2.11	0.65
1:D:108:ASN:HD22	1:D:109:GLY:H	1.44	0.65
1:D:377:ARG:HH12	1:D:447:ILE:HG23	1.62	0.65
1:A:392:GLU:O	1:A:396:GLU:HG2	1.96	0.64
1:D:326:GLU:HB2	1:D:327:GLU:OE1	1.98	0.63
1:A:207:GLN:HE21	1:A:207:GLN:N	1.95	0.63
1:B:1:MET:HE1	1:B:11:ARG:CD	2.28	0.62
1:A:374:LYS:HE3	1:A:430:PHE:CE2	2.34	0.62
1:C:220:ASN:HD21	1:C:223:ASN:H	1.45	0.62
1:C:292:ASP:O	1:C:296:LYS:HG2	2.00	0.62
1:D:207:GLN:HE21	1:D:207:GLN:N	1.96	0.62
1:A:326:GLU:HB2	1:A:327:GLU:OE1	2.00	0.62
1:C:393:MET:HE1	1:C:453:ALA:HB2	1.81	0.61
1:B:449:LEU:HD23	1:B:452:LYS:HD3	1.83	0.61
1:C:179:VAL:HG21	1:C:194:LEU:CD1	2.31	0.61
1:D:383:ARG:HH11	1:D:425:PRO:HA	1.65	0.61
1:B:393:MET:HE1	1:B:453:ALA:HB2	1.81	0.61
1:A:179:VAL:HG21	1:A:194:LEU:CD1	2.31	0.61
1:B:179:VAL:HG21	1:B:194:LEU:CD1	2.31	0.61
1:A:3:LYS:HG3	1:A:133:PHE:CZ	2.36	0.60
1:C:416:VAL:CG2	1:C:442:TYR:HB3	2.30	0.60
1:B:390:VAL:HG13	1:B:449:LEU:HB3	1.83	0.60
1:C:445:LEU:HD13	1:C:445:LEU:O	2.02	0.60
1:C:207:GLN:HE21	1:C:207:GLN:N	1.98	0.59
1:C:116:ASN:OD1	1:C:118:MET:HG2	2.02	0.59
1:B:326:GLU:HB2	1:B:327:GLU:OE1	2.01	0.59
1:A:3:LYS:HE3	1:A:3:LYS:CA	2.26	0.59
1:B:392:GLU:O	1:B:396:GLU:HG2	2.03	0.59
1:C:390:VAL:HG13	1:C:449:LEU:HB3	1.85	0.59
1:B:445:LEU:HD13	1:B:445:LEU:O	2.01	0.59
1:C:449:LEU:HD23	1:C:452:LYS:HD3	1.85	0.59
1:A:383:ARG:NH1	1:A:424:GLU:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:HE3	1:B:430:PHE:CZ	2.38	0.58
1:D:179:VAL:HG21	1:D:194:LEU:CD1	2.34	0.58
1:C:326:GLU:HB2	1:C:327:GLU:OE1	2.03	0.58
1:A:393:MET:HE1	1:A:453:ALA:HB2	1.86	0.58
1:C:130:GLU:CG	1:C:134:LYS:HE2	2.34	0.58
1:A:3:LYS:HE2	1:A:3:LYS:CA	2.27	0.58
1:B:20:PRO:HG3	1:B:56:MET:SD	2.44	0.58
1:B:292:ASP:O	1:B:296:LYS:HG2	2.03	0.58
1:C:393:MET:HE1	1:C:453:ALA:CB	2.35	0.57
1:C:392:GLU:O	1:C:396:GLU:HG2	2.04	0.57
1:B:122:LYS:HE2	1:B:314:ARG:NH2	2.19	0.57
1:B:330:GLY:HA3	1:B:340:ARG:HD3	1.87	0.57
1:B:374:LYS:HE3	1:B:430:PHE:CE2	2.40	0.57
1:B:416:VAL:CG2	1:B:442:TYR:HB3	2.31	0.57
1:D:1:MET:HE1	1:D:11:ARG:N	2.20	0.56
1:D:426:ILE:HG22	1:D:427:ILE:N	2.20	0.56
1:B:391:ALA:O	1:B:395:ARG:HG3	2.05	0.56
1:A:314:ARG:NH1	3:A:521:HOH:O	2.38	0.56
1:B:130:GLU:CG	1:B:134:LYS:HE2	2.35	0.56
1:B:390:VAL:HA	1:B:393:MET:HE3	1.86	0.56
1:C:391:ALA:O	1:C:395:ARG:HG3	2.06	0.56
1:D:330:GLY:HA3	1:D:340:ARG:HD3	1.88	0.56
1:A:377:ARG:HH12	1:A:447:ILE:HG23	1.71	0.56
1:A:130:GLU:CG	1:A:134:LYS:HE2	2.36	0.55
1:C:122:LYS:HE2	1:C:314:ARG:HH22	1.72	0.55
1:D:123:GLU:CD	1:D:123:GLU:H	2.13	0.55
1:D:281:LEU:C	1:D:281:LEU:HD23	2.31	0.55
1:B:1:MET:O	1:B:5:PHE:O	2.25	0.55
1:A:118:MET:HE1	1:A:314:ARG:HA	1.89	0.54
1:A:330:GLY:HA3	1:A:340:ARG:HD3	1.88	0.54
1:B:393:MET:HE1	1:B:453:ALA:HA	1.88	0.54
1:C:427:ILE:HG23	1:C:427:ILE:O	2.07	0.54
1:A:123:GLU:CD	1:A:123:GLU:H	2.14	0.54
1:D:130:GLU:CG	1:D:134:LYS:HE2	2.37	0.54
1:C:390:VAL:HA	1:C:393:MET:HE3	1.88	0.54
1:D:394:ALA:O	1:D:399:TYR:HB2	2.07	0.54
1:B:155:LYS:HB3	1:B:156:PRO:HD3	1.88	0.54
1:C:175:PRO:HG2	1:C:199:CYS:SG	2.48	0.54
1:C:11:ARG:HH22	1:C:111:LYS:NZ	2.06	0.53
1:D:387:VAL:HG22	1:D:427:ILE:HD11	1.89	0.53
1:D:391:ALA:O	1:D:395:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ALA:O	1:A:389:LYS:HG3	2.08	0.53
1:B:149:ARG:NH2	3:B:546:HOH:O	2.33	0.53
1:B:41:LYS:HB2	1:B:41:LYS:NZ	2.23	0.53
1:A:316:LEU:HD11	1:A:324:GLY:HA3	1.90	0.53
1:D:1:MET:HE1	1:D:10:VAL:HA	1.90	0.53
1:D:25:LYS:HE3	1:D:135:GLU:HG2	1.91	0.53
1:B:207:GLN:HE21	1:B:207:GLN:N	2.02	0.53
1:B:123:GLU:H	1:B:123:GLU:CD	2.16	0.53
1:D:3:LYS:HG2	1:D:133:PHE:CE2	2.44	0.53
1:A:281:LEU:C	1:A:281:LEU:HD23	2.33	0.53
1:A:412:GLU:HG3	1:A:413:ASP:N	2.24	0.53
1:C:11:ARG:HH22	1:C:111:LYS:HZ1	1.57	0.53
1:D:427:ILE:HG23	1:D:427:ILE:O	2.09	0.52
1:A:292:ASP:O	1:A:296:LYS:HG2	2.09	0.52
1:D:383:ARG:NH1	1:D:425:PRO:HA	2.25	0.52
1:D:359:LYS:HB2	1:D:362:GLU:HG3	1.92	0.52
1:B:423:THR:HB	1:B:424:GLU:OE1	2.09	0.52
1:A:20:PRO:HG3	1:A:56:MET:SD	2.50	0.52
1:B:377:ARG:HH12	1:B:447:ILE:HG23	1.75	0.52
1:D:393:MET:HE1	1:D:453:ALA:HB2	1.91	0.52
1:B:393:MET:HE1	1:B:453:ALA:CA	2.40	0.52
1:C:41:LYS:HB2	1:C:41:LYS:NZ	2.24	0.52
1:D:20:PRO:HG3	1:D:56:MET:SD	2.49	0.52
1:B:373:ILE:CB	1:B:443:LEU:HD12	2.40	0.51
1:C:253:ASP:HB2	1:C:254:GLU:OE1	2.10	0.51
1:D:383:ARG:HD2	1:D:426:ILE:O	2.10	0.51
1:C:130:GLU:HG2	1:C:134:LYS:HE2	1.91	0.51
1:D:116:ASN:OD1	1:D:118:MET:HG2	2.11	0.51
1:D:207:GLN:H	1:D:207:GLN:NE2	1.99	0.51
1:D:214:ALA:O	1:D:215:ARG:HB3	2.10	0.51
1:B:130:GLU:HG2	1:B:134:LYS:HE2	1.92	0.51
1:B:427:ILE:HG23	1:B:427:ILE:O	2.09	0.51
1:C:330:GLY:HA3	1:C:340:ARG:HD3	1.92	0.51
1:D:108:ASN:HD22	1:D:109:GLY:N	2.09	0.51
1:B:1:MET:O	1:B:2:GLY:C	2.54	0.51
1:B:4:LEU:HD12	1:B:5:PHE:CE1	2.45	0.51
1:A:108:ASN:HD22	1:A:109:GLY:N	2.07	0.51
1:A:387:VAL:HG22	1:A:427:ILE:HD11	1.93	0.51
1:B:403:THR:HA	1:B:406:GLY:O	2.11	0.51
1:D:118:MET:HE1	1:D:314:ARG:HA	1.92	0.51
1:C:445:LEU:HD13	1:C:445:LEU:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLN:HB3	1:A:262:ASP:OD1	2.12	0.50
1:B:426:ILE:HG22	1:B:427:ILE:N	2.27	0.50
1:A:25:LYS:HE3	1:A:135:GLU:HG2	1.93	0.50
1:A:428:ARG:HB3	1:A:430:PHE:HE1	1.76	0.50
1:B:413:ASP:HB3	1:B:442:TYR:OH	2.12	0.50
1:C:1:MET:O	1:C:3:LYS:O	2.29	0.50
1:D:1:MET:HE1	1:D:11:ARG:HD2	1.93	0.50
1:B:445:LEU:HD13	1:B:445:LEU:C	2.37	0.50
1:A:254:GLU:CG	3:A:512:HOH:O	2.59	0.50
1:C:1:MET:C	1:C:3:LYS:O	2.55	0.50
1:C:276:LYS:NZ	3:C:614:HOH:O	2.44	0.50
1:C:423:THR:HB	1:C:424:GLU:OE1	2.12	0.50
1:D:108:ASN:ND2	1:D:109:GLY:H	2.09	0.50
1:D:383:ARG:NH1	1:D:424:GLU:O	2.43	0.50
1:B:359:LYS:HB2	1:B:362:GLU:HG3	1.94	0.49
1:D:1:MET:CE	1:D:11:ARG:HD2	2.41	0.49
1:A:130:GLU:HG2	1:A:134:LYS:HE2	1.93	0.49
1:A:429:ILE:HD11	1:A:450:LEU:HD12	1.93	0.49
1:B:100:ALA:HB2	1:B:108:ASN:HA	1.94	0.49
1:B:11:ARG:HH22	1:B:111:LYS:NZ	2.10	0.49
1:B:108:ASN:HD22	1:B:109:GLY:N	2.08	0.49
1:B:377:ARG:O	1:B:427:ILE:HG22	2.13	0.49
1:B:387:VAL:HG22	1:B:427:ILE:HD11	1.93	0.49
1:D:374:LYS:HE3	1:D:430:PHE:CE2	2.47	0.49
1:A:116:ASN:OD1	1:A:118:MET:HG2	2.12	0.49
1:A:427:ILE:HG23	1:A:427:ILE:O	2.11	0.49
1:C:426:ILE:HG22	1:C:427:ILE:N	2.27	0.49
1:B:116:ASN:OD1	1:B:118:MET:HG2	2.12	0.49
1:B:122:LYS:CE	1:B:314:ARG:HH22	2.24	0.49
1:C:260:GLN:HB3	1:C:262:ASP:OD1	2.13	0.49
1:D:91:ASN:HB3	3:D:619:HOH:O	2.12	0.49
1:D:260:GLN:HB3	1:D:262:ASP:OD1	2.11	0.49
1:D:393:MET:HE1	1:D:453:ALA:CB	2.43	0.49
1:C:377:ARG:O	1:C:427:ILE:HG22	2.13	0.49
1:C:20:PRO:HG3	1:C:56:MET:SD	2.52	0.48
1:C:450:LEU:O	1:C:453:ALA:HB3	2.13	0.48
1:B:399:TYR:HE1	1:B:445:LEU:HD21	1.78	0.48
1:A:450:LEU:HD23	1:A:454:LEU:HD13	1.95	0.48
1:B:281:LEU:C	1:B:281:LEU:HD23	2.38	0.48
1:D:11:ARG:HH22	1:D:111:LYS:NZ	2.10	0.48
1:D:386:ILE:O	1:D:390:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:O	1:B:228:MET:HG3	2.13	0.48
1:A:383:ARG:HH11	1:A:425:PRO:HA	1.78	0.48
1:B:399:TYR:CE1	1:B:445:LEU:HD21	2.48	0.48
1:A:220:ASN:ND2	1:A:220:ASN:C	2.64	0.48
1:D:155:LYS:HB3	1:D:156:PRO:HD3	1.96	0.48
1:A:108:ASN:ND2	1:A:109:GLY:H	2.08	0.48
1:A:443:LEU:HD22	1:A:447:ILE:HD11	1.96	0.48
1:B:254:GLU:OE1	1:B:254:GLU:N	2.47	0.48
1:B:253:ASP:HB2	1:B:254:GLU:OE1	2.14	0.48
1:C:399:TYR:CE1	1:C:445:LEU:HD21	2.49	0.48
1:C:413:ASP:HB3	1:C:442:TYR:OH	2.14	0.48
1:D:417:LEU:HB3	1:D:430:PHE:HB2	1.95	0.48
1:B:175:PRO:HG2	1:B:199:CYS:SG	2.54	0.47
1:A:80:THR:HB	1:A:81:PRO:HD3	1.95	0.47
1:C:377:ARG:HH12	1:C:447:ILE:HG23	1.80	0.47
1:C:399:TYR:HE1	1:C:445:LEU:HD21	1.79	0.47
1:A:285:VAL:HG21	1:A:405:ASP:HB3	1.97	0.47
1:C:281:LEU:C	1:C:281:LEU:HD23	2.40	0.47
1:D:251:PHE:CD2	1:D:264:THR:HG21	2.50	0.47
1:B:394:ALA:O	1:B:399:TYR:HB2	2.14	0.47
1:A:426:ILE:HG22	1:A:427:ILE:N	2.28	0.47
1:C:214:ALA:O	1:C:215:ARG:HB3	2.14	0.47
1:C:394:ALA:O	1:C:399:TYR:HB2	2.14	0.47
1:C:429:ILE:HD11	1:C:450:LEU:CD1	2.42	0.47
1:D:100:ALA:HB2	1:D:108:ASN:HA	1.97	0.47
1:A:155:LYS:HB3	1:A:156:PRO:HD3	1.97	0.47
1:A:253:ASP:HB2	1:A:254:GLU:OE1	2.15	0.47
1:B:447:ILE:O	1:B:451:GLU:HG3	2.14	0.47
1:A:11:ARG:HH22	1:A:111:LYS:NZ	2.12	0.46
1:A:237:ASP:O	1:A:238:PHE:HB3	2.15	0.46
1:B:254:GLU:CG	3:B:476:HOH:O	2.63	0.46
1:D:292:ASP:O	1:D:296:LYS:HG2	2.14	0.46
1:B:108:ASN:ND2	1:B:109:GLY:H	2.10	0.46
1:C:220:ASN:ND2	1:C:220:ASN:C	2.65	0.46
1:D:428:ARG:HB3	1:D:430:PHE:HE1	1.79	0.46
1:A:327:GLU:H	1:A:327:GLU:CD	2.19	0.46
1:A:383:ARG:NH1	1:A:425:PRO:HA	2.29	0.46
1:B:443:LEU:HD23	1:B:443:LEU:O	2.15	0.46
1:C:123:GLU:CD	1:C:123:GLU:H	2.22	0.46
1:C:155:LYS:HB3	1:C:156:PRO:HD3	1.97	0.46
1:C:108:ASN:HD22	1:C:109:GLY:N	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:NH2	3:A:625:HOH:O	2.48	0.46
1:D:356:SER:CB	1:D:363:LEU:HD21	2.46	0.46
1:A:320:ASN:HB2	3:A:594:HOH:O	2.15	0.46
1:D:336:HIS:CD2	1:D:337:VAL:HG22	2.51	0.46
1:D:429:ILE:HD11	1:D:450:LEU:HD12	1.98	0.46
1:B:85:TRP:HB2	1:B:337:VAL:HG11	1.98	0.46
1:B:167:VAL:CG1	1:B:171:LYS:HE3	2.46	0.45
1:C:254:GLU:CG	3:C:568:HOH:O	2.63	0.45
1:B:100:ALA:HB2	1:B:108:ASN:CA	2.47	0.45
1:D:88:LYS:HE3	3:D:485:HOH:O	2.15	0.45
1:D:449:LEU:HA	1:D:452:LYS:HG2	1.98	0.45
1:C:100:ALA:HB2	1:C:108:ASN:CA	2.46	0.45
1:D:215:ARG:HG2	1:D:216:ASN:O	2.15	0.45
1:D:237:ASP:O	1:D:238:PHE:HB3	2.16	0.45
1:D:377:ARG:HH22	1:D:447:ILE:HD13	1.81	0.45
1:A:254:GLU:OE1	1:A:254:GLU:N	2.50	0.45
1:A:336:HIS:CD2	1:A:337:VAL:HG22	2.51	0.45
1:A:393:MET:HE1	1:A:453:ALA:CB	2.46	0.45
1:D:100:ALA:HB2	1:D:108:ASN:CA	2.46	0.45
1:A:330:GLY:CA	1:A:340:ARG:HD3	2.47	0.45
1:B:11:ARG:NH2	3:B:570:HOH:O	2.33	0.45
1:A:175:PRO:HG2	1:A:199:CYS:SG	2.57	0.45
1:A:254:GLU:HG2	3:A:512:HOH:O	2.17	0.45
1:D:40:LYS:HD2	3:D:598:HOH:O	2.16	0.45
1:A:254:GLU:HG3	3:A:512:HOH:O	2.17	0.45
1:A:359:LYS:HB2	1:A:362:GLU:HG3	1.98	0.45
1:D:80:THR:HB	1:D:81:PRO:HD3	1.98	0.45
1:A:445:LEU:HD13	1:A:445:LEU:O	2.16	0.45
1:C:25:LYS:HE3	1:C:135:GLU:HG2	1.99	0.45
1:C:403:THR:HA	1:C:406:GLY:O	2.17	0.45
1:D:259:ILE:HD12	1:D:259:ILE:N	2.32	0.45
1:D:330:GLY:CA	1:D:340:ARG:HD3	2.46	0.45
1:A:371:TYR:O	1:A:432:GLU:HA	2.17	0.44
1:C:85:TRP:HB2	1:C:337:VAL:HG11	1.99	0.44
1:B:183:ASN:CG	1:B:213:PRO:HD2	2.42	0.44
1:D:377:ARG:HH12	1:D:447:ILE:CG2	2.28	0.44
1:C:183:ASN:CG	1:C:213:PRO:HD2	2.42	0.44
1:A:41:LYS:NZ	1:A:41:LYS:HB2	2.32	0.44
1:B:122:LYS:HG2	1:B:314:ARG:HH12	1.83	0.44
1:B:429:ILE:HD11	1:B:450:LEU:CD1	2.43	0.44
1:D:253:ASP:HB2	1:D:254:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:THR:HA	1:D:406:GLY:O	2.17	0.44
1:B:180:ASP:CG	1:B:215:ARG:HH22	2.25	0.44
1:B:183:ASN:OD1	1:B:213:PRO:HD2	2.17	0.44
1:C:254:GLU:OE1	1:C:254:GLU:N	2.50	0.44
1:C:387:VAL:HG22	1:C:427:ILE:HD11	2.00	0.44
1:A:7:THR:HB	1:A:309:ASP:HB2	2.00	0.44
1:A:149:ARG:NH2	3:A:602:HOH:O	2.45	0.44
1:B:214:ALA:O	1:B:215:ARG:HB3	2.18	0.44
1:A:445:LEU:HD13	1:A:445:LEU:C	2.43	0.44
1:B:260:GLN:HB3	1:B:262:ASP:OD1	2.17	0.44
1:C:336:HIS:CD2	1:C:337:VAL:HG22	2.53	0.44
1:A:100:ALA:HB2	1:A:108:ASN:CA	2.48	0.44
1:A:173:ARG:HG3	1:A:354:ALA:HA	2.00	0.44
1:B:329:GLY:O	1:B:330:GLY:C	2.61	0.44
1:B:443:LEU:HD23	1:B:443:LEU:C	2.43	0.44
1:B:377:ARG:HH12	1:B:447:ILE:CG2	2.31	0.43
1:C:108:ASN:ND2	1:C:109:GLY:H	2.12	0.43
1:C:377:ARG:HH22	1:C:447:ILE:HD13	1.83	0.43
1:D:421:SER:HB3	1:D:424:GLU:O	2.18	0.43
1:B:237:ASP:O	1:B:238:PHE:HB3	2.18	0.43
1:C:316:LEU:HD11	1:C:324:GLY:HA3	1.99	0.43
1:A:11:ARG:NH1	3:A:614:HOH:O	2.51	0.43
1:D:1:MET:CE	1:D:10:VAL:HA	2.48	0.43
1:A:19:THR:HB	1:A:20:PRO:CD	2.49	0.43
1:A:100:ALA:HB2	1:A:108:ASN:HA	1.99	0.43
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.83	0.43
1:A:391:ALA:O	1:A:395:ARG:HG3	2.19	0.43
1:B:371:TYR:O	1:B:432:GLU:HA	2.18	0.43
1:C:122:LYS:HG2	1:C:314:ARG:NH1	2.31	0.43
1:C:237:ASP:O	1:C:238:PHE:HB3	2.19	0.43
1:D:130:GLU:HG2	1:D:134:LYS:HE2	1.99	0.43
1:A:4:LEU:HD21	1:A:22:PHE:CE1	2.53	0.43
1:B:118:MET:HE1	1:B:314:ARG:HA	2.00	0.43
1:C:183:ASN:OD1	1:C:213:PRO:HD2	2.18	0.43
1:C:447:ILE:O	1:C:451:GLU:HG3	2.18	0.43
1:B:411:PHE:HE1	1:B:416:VAL:HG23	1.84	0.43
1:C:373:ILE:HB	1:C:443:LEU:HD12	2.00	0.43
1:B:374:LYS:HG2	1:B:430:PHE:CD2	2.54	0.43
1:D:58:LYS:HE2	1:D:58:LYS:HB3	1.79	0.43
1:D:445:LEU:HD13	1:D:445:LEU:O	2.17	0.43
1:B:7:THR:HB	1:B:309:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:PHE:HE1	1:C:416:VAL:HG23	1.84	0.43
1:D:1:MET:O	1:D:5:PHE:O	2.36	0.42
1:D:175:PRO:HG2	1:D:199:CYS:SG	2.59	0.42
1:D:395:ARG:HH21	1:D:403:THR:HG23	1.84	0.42
1:A:413:ASP:OD1	1:A:433:ALA:HB1	2.20	0.42
1:B:377:ARG:HH22	1:B:447:ILE:HD13	1.83	0.42
1:C:443:LEU:O	1:C:443:LEU:HD23	2.18	0.42
1:D:385:ALA:O	1:D:389:LYS:HG3	2.19	0.42
1:A:58:LYS:HE2	1:A:58:LYS:HB3	1.80	0.42
1:B:122:LYS:HE2	1:B:314:ARG:HH12	1.84	0.42
1:C:100:ALA:HB2	1:C:108:ASN:HA	2.01	0.42
1:A:85:TRP:HB2	1:A:337:VAL:HG11	2.02	0.42
1:A:374:LYS:HG2	1:A:430:PHE:CD2	2.54	0.42
1:A:390:VAL:HG13	1:A:449:LEU:HB3	2.02	0.42
1:B:310:LEU:O	1:B:314:ARG:HG3	2.19	0.42
1:D:408:LYS:HA	1:D:416:VAL:O	2.19	0.42
1:A:378:HIS:ND1	1:A:378:HIS:C	2.78	0.42
1:D:224:LEU:O	1:D:228:MET:HG3	2.20	0.42
1:B:80:THR:HB	1:B:81:PRO:HD3	2.01	0.42
1:B:178:VAL:HG23	1:B:236:ALA:CB	2.49	0.42
1:C:7:THR:HB	1:C:309:ASP:HB2	2.02	0.42
1:C:215:ARG:O	1:C:216:ASN:C	2.63	0.42
1:A:167:VAL:CG1	1:A:171:LYS:HE3	2.50	0.42
1:B:276:LYS:NZ	3:B:537:HOH:O	2.50	0.42
1:C:443:LEU:HD23	1:C:443:LEU:C	2.45	0.42
1:A:79:PRO:HB3	1:A:246:ALA:HB3	2.02	0.41
1:C:173:ARG:HD2	1:C:173:ARG:O	2.19	0.41
1:A:383:ARG:HG2	1:A:420:ALA:HB1	2.02	0.41
1:B:178:VAL:HG23	1:B:236:ALA:HB2	2.02	0.41
1:D:179:VAL:HG21	1:D:194:LEU:HD12	2.01	0.41
1:D:183:ASN:OD1	1:D:213:PRO:HD2	2.20	0.41
1:A:259:ILE:HD12	1:A:259:ILE:N	2.35	0.41
1:A:449:LEU:HA	1:A:452:LYS:HG2	2.03	0.41
1:B:25:LYS:HE3	1:B:135:GLU:HG2	2.02	0.41
1:B:316:LEU:HD11	1:B:324:GLY:HA3	2.02	0.41
1:D:212:PHE:N	1:D:213:PRO:HD3	2.36	0.41
1:A:153:ILE:C	1:A:156:PRO:HD2	2.45	0.41
1:B:1:MET:HE2	1:B:6:GLY:HA3	2.02	0.41
1:B:449:LEU:O	1:B:453:ALA:HB2	2.20	0.41
1:C:179:VAL:HG21	1:C:194:LEU:HD11	2.01	0.41
1:D:41:LYS:HB2	1:D:41:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD13	1:A:4:LEU:C	2.45	0.41
1:B:254:GLU:HG3	3:B:476:HOH:O	2.21	0.41
1:B:449:LEU:HA	1:B:452:LYS:HG2	2.02	0.41
1:C:385:ALA:O	1:C:389:LYS:HG3	2.21	0.41
1:C:449:LEU:HA	1:C:452:LYS:HG2	2.02	0.41
1:A:1:MET:SD	1:A:10:VAL:HG23	2.61	0.41
1:B:220:ASN:ND2	1:B:220:ASN:C	2.67	0.41
1:C:28:MET:HE3	3:C:459:HOH:O	2.20	0.41
1:C:405:ASP:OD1	1:C:419:ARG:NH1	2.54	0.41
1:D:250:VAL:HG11	1:D:258:PHE:CE1	2.55	0.41
1:D:454:LEU:C	1:D:454:LEU:HD12	2.46	0.41
1:A:403:THR:HA	1:A:406:GLY:O	2.20	0.41
1:C:167:VAL:CG1	1:C:171:LYS:HE3	2.51	0.41
1:C:330:GLY:CA	1:C:340:ARG:HD3	2.51	0.41
1:D:7:THR:HB	1:D:309:ASP:HB2	2.02	0.41
1:D:378:HIS:ND1	1:D:378:HIS:C	2.79	0.41
1:A:240:VAL:HG11	1:A:346:VAL:HG21	2.03	0.41
1:C:359:LYS:HB2	1:C:362:GLU:HG3	2.02	0.41
1:D:153:ILE:C	1:D:156:PRO:HD2	2.46	0.41
1:A:80:THR:N	1:A:81:PRO:CD	2.83	0.41
1:A:356:SER:CB	1:A:363:LEU:HD21	2.51	0.41
1:B:4:LEU:HB3	1:B:129:GLU:HG2	2.02	0.41
1:C:153:ILE:C	1:C:156:PRO:HD2	2.46	0.41
1:C:224:LEU:O	1:C:228:MET:HG3	2.21	0.41
1:C:356:SER:CB	1:C:363:LEU:HD21	2.51	0.41
1:A:19:THR:HB	1:A:20:PRO:HD2	2.03	0.41
1:B:318:GLU:OE1	1:B:318:GLU:HA	2.21	0.41
1:B:424:GLU:HA	1:B:425:PRO:HD3	1.89	0.41
1:C:207:GLN:H	1:C:207:GLN:NE2	2.01	0.41
1:B:385:ALA:O	1:B:389:LYS:HG3	2.22	0.40
1:C:386:ILE:O	1:C:390:VAL:HG23	2.21	0.40
1:A:214:ALA:O	1:A:215:ARG:HB3	2.20	0.40
1:B:386:ILE:O	1:B:390:VAL:HG23	2.21	0.40
1:A:3:LYS:HG3	1:A:133:PHE:CE2	2.56	0.40
1:D:220:ASN:ND2	1:D:220:ASN:C	2.65	0.40
1:A:329:GLY:O	1:A:330:GLY:C	2.62	0.40
1:A:379:VAL:HG21	1:A:427:ILE:HG21	2.03	0.40
1:A:383:ARG:HD2	1:A:426:ILE:O	2.22	0.40
1:B:254:GLU:HG2	3:B:476:HOH:O	2.21	0.40
1:D:175:PRO:HB3	1:D:353:PHE:CE2	2.56	0.40
1:D:426:ILE:CG2	1:D:427:ILE:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ALA:O	1:A:399:TYR:HB2	2.20	0.40
1:D:440:GLN:HG3	1:D:444:ASN:HD21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/455 (100%)	431 (95%)	20 (4%)	2 (0%)	30	27
1	B	453/455 (100%)	425 (94%)	26 (6%)	2 (0%)	30	27
1	C	453/455 (100%)	428 (94%)	22 (5%)	3 (1%)	18	14
1	D	453/455 (100%)	429 (95%)	21 (5%)	3 (1%)	18	14
All	All	1812/1820 (100%)	1713 (94%)	89 (5%)	10 (1%)	21	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	LEU
1	D	428	ARG
1	B	4	LEU
1	D	3	LYS
1	A	428	ARG
1	B	428	ARG
1	C	428	ARG
1	A	4	LEU
1	D	4	LEU
1	C	215	ARG

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	368/368 (100%)	352 (96%)	16 (4%)	26	25
1	B	368/368 (100%)	357 (97%)	11 (3%)	36	38
1	C	368/368 (100%)	354 (96%)	14 (4%)	29	29
1	D	368/368 (100%)	356 (97%)	12 (3%)	33	34
All	All	1472/1472 (100%)	1419 (96%)	53 (4%)	31	31

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	4	LEU
1	A	15	ASN
1	A	108	ASN
1	A	123	GLU
1	A	149	ARG
1	A	207	GLN
1	A	220	ASN
1	A	254	GLU
1	A	260	GLN
1	A	264	THR
1	A	369	LYS
1	A	413	ASP
1	A	424	GLU
1	A	443	LEU
1	B	3	LYS
1	B	4	LEU
1	B	15	ASN
1	B	108	ASN
1	B	149	ARG
1	B	207	GLN
1	B	215	ARG
1	B	220	ASN

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Mol	Chain	Res	Type
1	B	254	GLU
1	B	264	THR
1	B	369	LYS
1	C	3	LYS
1	C	4	LEU
1	C	15	ASN
1	C	108	ASN
1	C	123	GLU
1	C	149	ARG
1	C	173	ARG
1	C	207	GLN
1	C	215	ARG
1	C	220	ASN
1	C	254	GLU
1	C	260	GLN
1	C	264	THR
1	C	369	LYS
1	D	4	LEU
1	D	15	ASN
1	D	108	ASN
1	D	123	GLU
1	D	149	ARG
1	D	207	GLN
1	D	220	ASN
1	D	254	GLU
1	D	260	GLN
1	D	369	LYS
1	D	424	GLU
1	D	443	LEU

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

Mol	Chain	Res	Type
1	A	15	ASN
1	A	108	ASN
1	A	207	GLN
1	A	220	ASN
1	A	223	ASN
1	A	289	ASN
1	A	388	ASN
1	A	444	ASN
1	B	15	ASN

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Mol	Chain	Res	Type
1	B	108	ASN
1	B	207	GLN
1	B	220	ASN
1	B	223	ASN
1	B	260	GLN
1	B	372	GLN
1	B	388	ASN
1	C	15	ASN
1	C	108	ASN
1	C	207	GLN
1	C	220	ASN
1	C	223	ASN
1	C	260	GLN
1	C	289	ASN
1	C	388	ASN
1	D	15	ASN
1	D	103	ASN
1	D	108	ASN
1	D	207	GLN
1	D	220	ASN
1	D	223	ASN
1	D	242	GLN
1	D	289	ASN
1	D	388	ASN
1	D	444	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	455/455 (100%)	0.52	71 (15%) 5 4	13, 29, 73, 89	0
1	B	455/455 (100%)	0.76	92 (20%) 3 2	11, 27, 88, 100	0
1	C	455/455 (100%)	0.70	84 (18%) 3 3	12, 28, 87, 99	0
1	D	455/455 (100%)	0.61	68 (14%) 5 5	13, 30, 82, 100	0
All	All	1820/1820 (100%)	0.65	315 (17%) 4 3	11, 28, 84, 100	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	ILE	8.2
1	C	450	LEU	7.2
1	C	427	ILE	6.8
1	C	379	VAL	6.4
1	B	379	VAL	6.3
1	B	1	MET	6.3
1	B	426	ILE	6.3
1	B	450	LEU	6.0
1	B	449	LEU	6.0
1	B	394	ALA	5.6
1	B	447	ILE	5.6
1	B	416	VAL	5.5
1	C	373	ILE	5.5
1	B	430	PHE	5.3
1	A	427	ILE	5.3
1	C	1	MET	5.2
1	D	427	ILE	5.2
1	C	387	VAL	5.2
1	B	401	VAL	5.2
1	B	453	ALA	5.1
1	B	454	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	418	VAL	5.1
1	D	1	MET	5.1
1	B	409	ILE	5.0
1	A	379	VAL	5.0
1	C	449	LEU	5.0
1	A	413	ASP	4.8
1	B	386	ILE	4.8
1	C	390	VAL	4.8
1	B	446	GLY	4.7
1	B	378	HIS	4.7
1	D	450	LEU	4.7
1	C	399	TYR	4.7
1	C	430	PHE	4.7
1	B	390	VAL	4.6
1	C	426	ILE	4.6
1	B	387	VAL	4.6
1	C	443	LEU	4.6
1	B	425	PRO	4.5
1	B	375	THR	4.5
1	C	375	THR	4.5
1	C	377	ARG	4.5
1	B	2	GLY	4.5
1	B	442	TYR	4.4
1	C	384	HIS	4.4
1	D	387	VAL	4.4
1	C	400	THR	4.4
1	C	401	VAL	4.4
1	C	385	ALA	4.3
1	D	327	GLU	4.3
1	B	377	ARG	4.3
1	D	449	LEU	4.2
1	B	406	GLY	4.2
1	C	398	GLY	4.2
1	B	429	ILE	4.2
1	D	3	LYS	4.2
1	C	442	TYR	4.2
1	B	398	GLY	4.2
1	B	399	TYR	4.2
1	C	454	LEU	4.2
1	A	386	ILE	4.1
1	D	386	ILE	4.1
1	C	452	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	454	LEU	4.1
1	A	426	ILE	4.1
1	B	385	ALA	4.1
1	D	416	VAL	4.1
1	D	430	PHE	4.1
1	B	391	ALA	4.0
1	D	426	ILE	4.0
1	C	378	HIS	4.0
1	B	388	ASN	3.9
1	B	3	LYS	3.9
1	B	411	PHE	3.9
1	C	453	ALA	3.9
1	C	397	ARG	3.9
1	A	4	LEU	3.9
1	C	222	GLU	3.9
1	A	329	GLY	3.8
1	A	410	ILE	3.8
1	A	445	LEU	3.8
1	C	429	ILE	3.8
1	C	445	LEU	3.8
1	C	455	SER	3.8
1	C	402	ASP	3.8
1	B	373	ILE	3.7
1	C	394	ALA	3.7
1	A	1	MET	3.7
1	C	413	ASP	3.7
1	D	413	ASP	3.7
1	A	452	LYS	3.7
1	C	327	GLU	3.7
1	D	425	PRO	3.7
1	B	397	ARG	3.7
1	D	394	ALA	3.7
1	A	391	ALA	3.6
1	C	439	ALA	3.6
1	A	450	LEU	3.6
1	C	383	ARG	3.6
1	D	410	ILE	3.6
1	C	7	THR	3.6
1	B	371	TYR	3.6
1	A	378	HIS	3.6
1	C	416	VAL	3.6
1	C	386	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	371	TYR	3.6
1	B	455	SER	3.6
1	C	391	ALA	3.5
1	A	2	GLY	3.5
1	C	2	GLY	3.5
1	D	390	VAL	3.5
1	B	448	GLU	3.5
1	D	375	THR	3.4
1	A	430	PHE	3.4
1	A	454	LEU	3.4
1	B	423	THR	3.4
1	D	442	TYR	3.4
1	B	307	VAL	3.4
1	B	445	LEU	3.3
1	C	395	ARG	3.3
1	A	373	ILE	3.3
1	D	445	LEU	3.3
1	C	428	ARG	3.3
1	C	376	LYS	3.3
1	C	418	VAL	3.3
1	B	327	GLU	3.3
1	D	411	PHE	3.3
1	A	390	VAL	3.2
1	D	379	VAL	3.2
1	A	327	GLU	3.2
1	A	399	TYR	3.2
1	C	410	ILE	3.2
1	A	414	GLY	3.2
1	B	407	ALA	3.2
1	C	388	ASN	3.2
1	B	421	SER	3.2
1	D	400	THR	3.2
1	C	372	GLN	3.2
1	C	420	ALA	3.1
1	D	409	ILE	3.1
1	B	415	TRP	3.1
1	B	443	LEU	3.1
1	C	448	GLU	3.1
1	D	424	GLU	3.1
1	A	3	LYS	3.1
1	D	374	LYS	3.1
1	C	411	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	7	THR	3.1
1	D	414	GLY	3.1
1	C	389	LYS	3.1
1	D	399	TYR	3.1
1	B	428	ARG	3.1
1	B	384	HIS	3.1
1	A	387	VAL	3.1
1	B	452	LYS	3.1
1	B	4	LEU	3.1
1	C	371	TYR	3.0
1	B	400	THR	3.0
1	D	378	HIS	3.0
1	B	376	LYS	3.0
1	A	375	THR	3.0
1	D	415	TRP	3.0
1	B	420	ALA	3.0
1	B	410	ILE	3.0
1	C	447	ILE	3.0
1	B	413	ASP	3.0
1	D	384	HIS	3.0
1	C	421	SER	3.0
1	B	380	GLU	3.0
1	A	429	ILE	3.0
1	B	329	GLY	3.0
1	A	425	PRO	3.0
1	D	452	LYS	3.0
1	C	412	GLU	2.9
1	A	394	ALA	2.9
1	C	409	ILE	2.9
1	A	383	ARG	2.9
1	A	449	LEU	2.9
1	D	2	GLY	2.9
1	B	405	ASP	2.9
1	A	447	ILE	2.9
1	B	383	ARG	2.9
1	A	416	VAL	2.8
1	D	429	ILE	2.8
1	C	3	LYS	2.8
1	B	395	ARG	2.8
1	A	422	GLY	2.8
1	B	308	GLY	2.8
1	C	328	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	328	ASN	2.8
1	B	402	ASP	2.8
1	B	422	GLY	2.8
1	D	418	VAL	2.8
1	A	376	LYS	2.8
1	C	374	LYS	2.8
1	A	328	ASN	2.8
1	B	417	LEU	2.8
1	A	418	VAL	2.8
1	D	373	ILE	2.8
1	B	393	MET	2.7
1	C	275	GLU	2.7
1	C	309	ASP	2.7
1	B	451	GLU	2.7
1	A	357	GLY	2.7
1	C	422	GLY	2.7
1	D	391	ALA	2.7
1	A	393	MET	2.7
1	D	401	VAL	2.7
1	D	376	LYS	2.7
1	B	381	GLY	2.7
1	C	441	GLU	2.6
1	D	385	ALA	2.6
1	B	309	ASP	2.6
1	A	232	LYS	2.6
1	A	372	GLN	2.6
1	C	393	MET	2.6
1	B	374	LYS	2.6
1	A	371	TYR	2.6
1	B	328	ASN	2.6
1	A	233	ALA	2.6
1	D	448	GLU	2.6
1	D	423	THR	2.6
1	C	4	LEU	2.6
1	A	396	GLU	2.5
1	A	400	THR	2.5
1	B	404	THR	2.5
1	D	453	ALA	2.5
1	B	222	GLU	2.5
1	B	412	GLU	2.5
1	D	398	GLY	2.5
1	A	384	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	434	LYS	2.5
1	B	419	ARG	2.5
1	C	451	GLU	2.5
1	D	435	SER	2.5
1	D	397	ARG	2.5
1	C	370	TYR	2.5
1	A	369	LYS	2.5
1	C	276	LYS	2.5
1	C	369	LYS	2.5
1	B	262	ASP	2.4
1	B	431	SER	2.4
1	D	455	SER	2.4
1	A	453	ALA	2.4
1	D	4	LEU	2.4
1	C	414	GLY	2.4
1	B	356	SER	2.4
1	A	423	THR	2.4
1	D	40	LYS	2.4
1	C	444	ASN	2.4
1	A	412	GLU	2.4
1	A	409	ILE	2.4
1	D	447	ILE	2.4
1	A	356	SER	2.4
1	B	370	TYR	2.4
1	C	417	LEU	2.4
1	D	443	LEU	2.4
1	C	446	GLY	2.4
1	A	309	ASP	2.4
1	C	407	ALA	2.3
1	D	412	GLU	2.3
1	A	377	ARG	2.3
1	A	392	GLU	2.3
1	C	380	GLU	2.3
1	D	393	MET	2.3
1	B	437	GLU	2.3
1	C	415	TRP	2.3
1	D	422	GLY	2.3
1	D	276	LYS	2.3
1	C	435	SER	2.3
1	D	428	ARG	2.3
1	A	381	GLY	2.3
1	C	381	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	406	GLY	2.3
1	B	275	GLU	2.2
1	A	397	ARG	2.2
1	B	434	LYS	2.2
1	A	382	ASP	2.2
1	A	276	LYS	2.2
1	B	389	LYS	2.2
1	A	385	ALA	2.2
1	C	392	GLU	2.2
1	A	277	GLY	2.2
1	B	392	GLU	2.2
1	C	419	ARG	2.2
1	A	374	LYS	2.2
1	B	368	PRO	2.1
1	C	423	THR	2.2
1	A	326	GLU	2.1
1	A	424	GLU	2.1
1	B	372	GLN	2.1
1	B	276	LYS	2.1
1	A	388	ASN	2.1
1	A	222	GLU	2.1
1	C	382	ASP	2.1
1	D	380	GLU	2.1
1	A	455	SER	2.1
1	D	372	GLN	2.1
1	D	403	THR	2.1
1	A	428	ARG	2.1
1	B	357	GLY	2.1
1	B	439	ALA	2.1
1	A	443	LEU	2.1
1	A	437	GLU	2.1
1	D	275	GLU	2.1
1	B	382	ASP	2.0
1	C	436	LYS	2.0
1	D	307	VAL	2.0
1	D	326	GLU	2.0
1	D	421	SER	2.0
1	B	233	ALA	2.0
1	A	274	LYS	2.0
1	B	369	LYS	2.0
1	D	389	LYS	2.0
1	A	370	TYR	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	MG	D	456	1/1	0.91	0.09	34,34,34,34	0
2	MG	A	456	1/1	0.92	0.06	32,32,32,32	0
2	MG	C	456	1/1	0.96	0.04	29,29,29,29	0
2	MG	B	456	1/1	0.96	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.