



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 2F7L / pdb_00002f7l
Title : Crystal structure of Sulfolobus tokodaii phosphomannomutase/phosphoglucose mutase
Authors : Kawamura, T.; Sakai, N.; Akutsu, J.; Zhang, Z.; Watanabe, N.; Kawarabayashi, Y.; Tanaka, I.
Deposited on : 2005-12-01
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

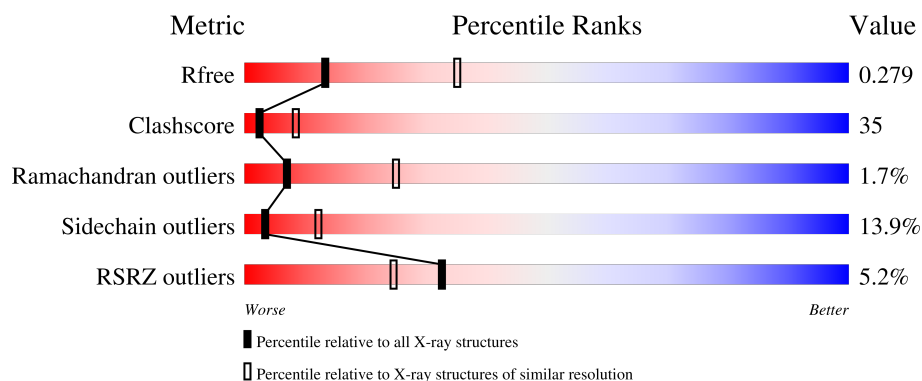
1 Overall quality at a glance

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	455	51% 38% 11% .
1	B	455	9% 41% 47% 11% .

2 Entry composition [i](#)

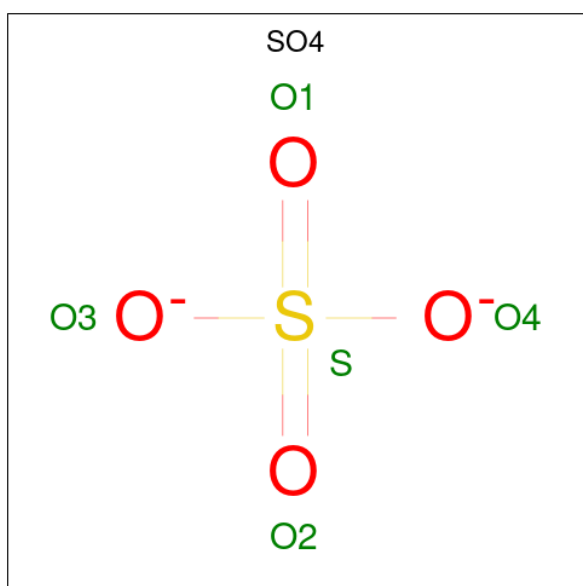
There are 3 unique types of molecules in this entry. The entry contains 7113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 455aa long hypothetical phospho-sugar mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3531	2259	589	674	9			
1	B	455	Total	C	N	O	S	0	0	0
			3531	2259	589	674	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		

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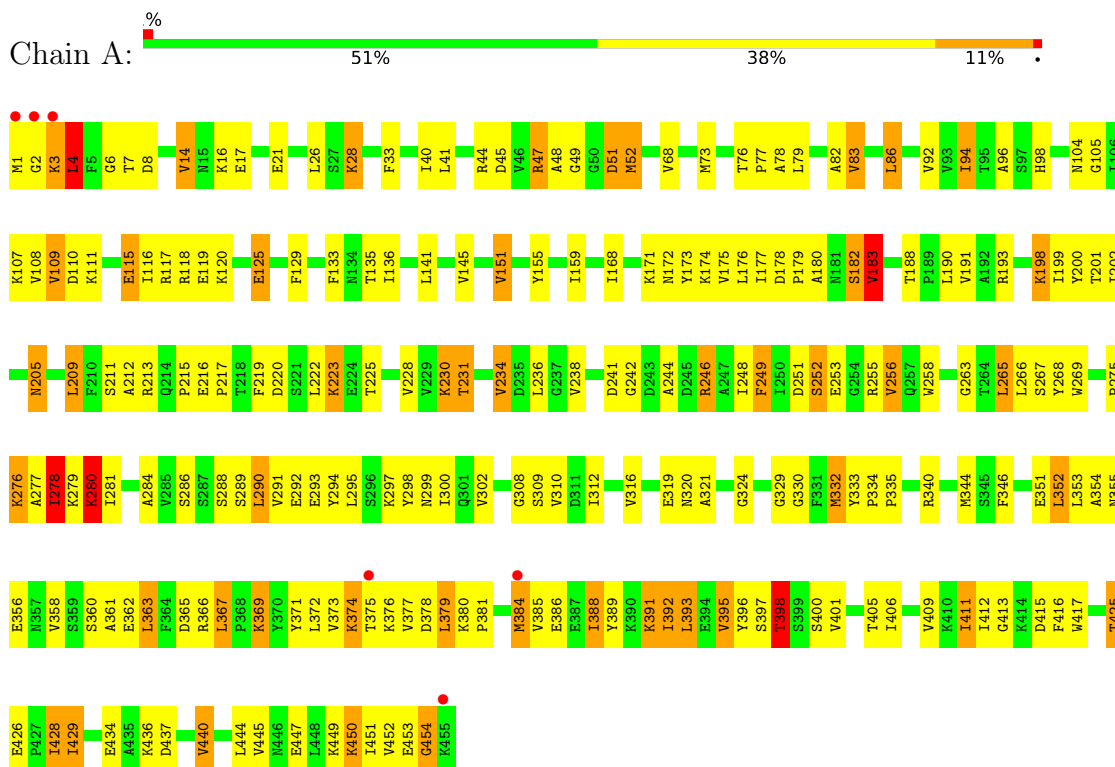
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	12	Total	O	0	0
			12	12		

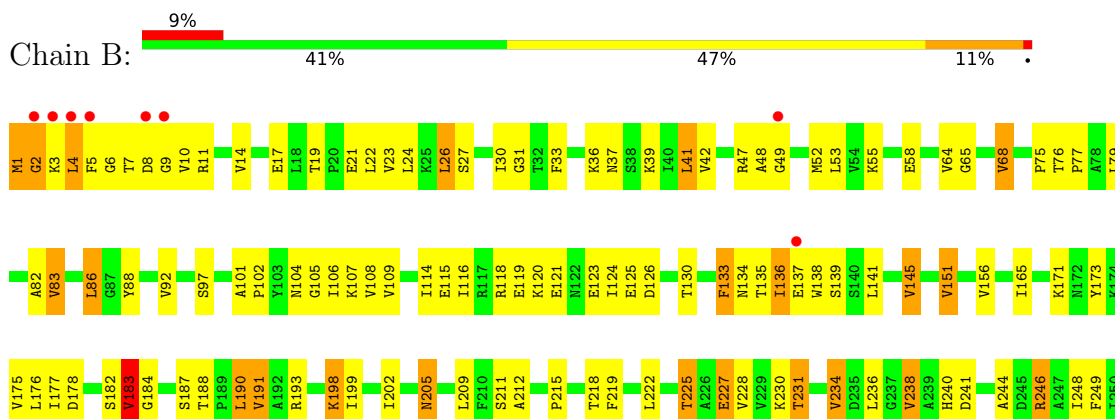
3 Residue-property plots [i](#)

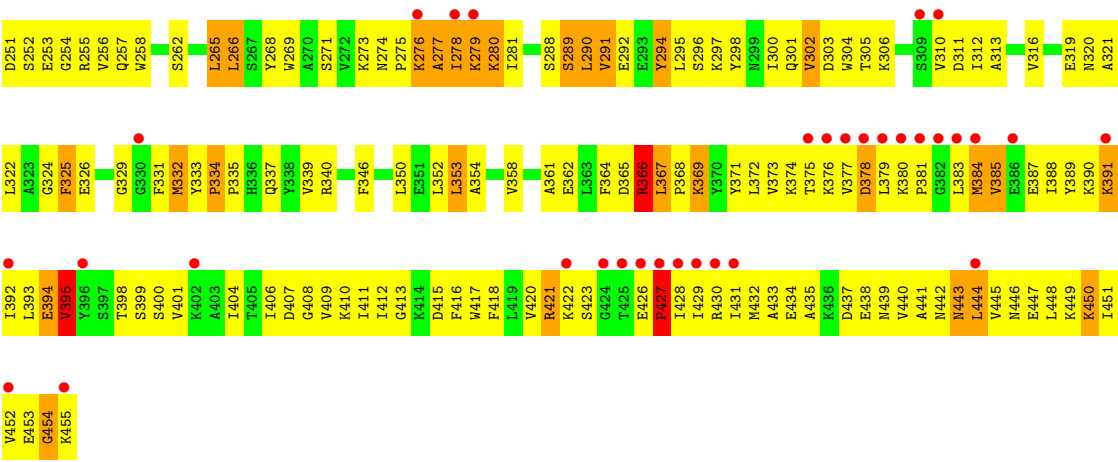
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 455aa long hypothetical phospho-sugar mutase



- Molecule 1: 455aa long hypothetical phospho-sugar mutase





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	161.90Å 161.90Å 170.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.80) 99.9 (50.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.280 0.228 , 0.279	Depositor DCC
R_{free} test set	1664 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.2	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	0.93	EDS
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: SO4

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	0.66	0/3592	1.14	24/4855 (0.5%)
1	B	0.62	0/3592	1.14	29/4855 (0.6%)
All	All	0.64	0/7184	1.14	53/9710 (0.5%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	N-CA-C	-9.43	99.08	111.24
1	A	68	VAL	N-CA-C	8.94	121.36	109.21
1	A	198	LYS	N-CA-C	-8.58	95.32	108.96
1	B	329	GLY	N-CA-C	-8.46	99.34	112.45
1	B	198	LYS	N-CA-C	-7.99	96.25	108.96
1	B	395	VAL	N-CA-C	7.72	118.47	110.36
1	A	151	VAL	N-CA-C	7.60	118.14	110.23
1	A	454	GLY	N-CA-C	-7.59	103.21	114.90
1	B	199	ILE	N-CA-C	7.53	118.72	107.80
1	A	329	GLY	N-CA-C	-7.38	101.00	112.45
1	B	366	ARG	N-CA-C	-7.34	104.42	113.15
1	A	182	SER	N-CA-C	7.27	119.50	109.18
1	A	2	GLY	N-CA-C	-7.13	96.28	113.18
1	B	367	LEU	CA-C-N	7.12	127.12	119.78
1	B	367	LEU	C-N-CA	7.12	127.12	119.78
1	B	326	GLU	N-CA-C	-6.88	100.62	110.59
1	B	294	TYR	N-CA-C	6.49	118.23	111.03
1	A	244	ALA	N-CA-C	6.37	120.20	111.54
1	B	165	ILE	N-CA-C	6.30	116.97	110.36
1	A	47	ARG	N-CA-C	6.25	124.12	110.80
1	A	242	GLY	N-CA-C	6.17	120.11	112.64
1	B	136	ILE	N-CA-C	6.09	117.94	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LYS	N-CA-C	-6.00	104.82	111.36
1	B	454	GLY	N-CA-C	-5.95	104.64	114.76
1	B	244	ALA	N-CA-C	5.90	119.56	111.54
1	A	199	ILE	N-CA-C	5.87	116.39	108.17
1	A	17	GLU	N-CA-C	-5.87	103.59	112.04
1	B	249	PHE	N-CA-C	5.84	118.06	110.53
1	B	212	ALA	N-CA-C	5.80	118.55	111.82
1	B	133	PHE	N-CA-C	5.78	118.96	109.76
1	B	151	VAL	N-CA-C	5.77	116.42	110.36
1	B	399	SER	N-CA-C	-5.70	106.16	113.23
1	B	68	VAL	N-CA-C	5.66	116.91	109.21
1	B	65	GLY	N-CA-C	5.64	123.59	114.90
1	A	202	ILE	N-CA-C	-5.63	100.28	108.17
1	A	212	ALA	N-CA-C	5.63	118.36	111.82
1	A	129	PHE	N-CA-C	5.61	117.47	111.36
1	A	334	PRO	N-CA-C	5.58	117.51	110.70
1	B	325	PHE	N-CA-C	5.56	116.97	108.52
1	B	48	ALA	N-CA-C	5.55	122.62	110.80
1	A	4	LEU	CA-C-N	5.51	128.93	121.05
1	A	4	LEU	C-N-CA	5.51	128.93	121.05
1	A	388	ILE	N-CA-C	-5.46	105.17	110.42
1	B	421	ARG	N-CA-C	5.41	117.91	109.52
1	B	378	ASP	N-CA-C	5.31	117.93	110.23
1	A	40	ILE	N-CA-C	5.25	115.46	108.11
1	B	444	LEU	N-CA-C	-5.22	105.59	111.28
1	A	175	VAL	N-CA-C	5.20	117.26	109.20
1	B	302	VAL	N-CA-C	5.16	114.17	106.85
1	B	145	VAL	N-CA-C	-5.10	102.28	109.21
1	B	334	PRO	N-CA-C	5.06	116.88	110.70
1	B	2	GLY	N-CA-C	-5.05	101.21	113.18
1	A	249	PHE	N-CA-C	5.04	117.99	110.52

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	3531	0	3616	209	1
1	B	3531	0	3616	297	1
2	A	5	0	0	0	0
3	A	34	0	0	1	0
3	B	12	0	0	0	0
All	All	7113	0	7232	498	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 35.

All (498) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:CE1	1:B:10:VAL:HG23	1.74	1.22
1:A:1:MET:CE	1:A:6:GLY:HA3	1.74	1.18
1:B:5:PHE:CE1	1:B:10:VAL:CG2	2.31	1.14
1:B:3:LYS:HG3	1:B:4:LEU:H	0.92	1.08
1:A:1:MET:HE2	1:A:6:GLY:HA3	1.34	1.05
1:A:1:MET:HE3	1:A:7:THR:H	1.24	1.02
1:B:1:MET:HB2	1:B:11:ARG:HG2	1.39	1.01
1:B:3:LYS:CG	1:B:4:LEU:H	1.66	1.01
1:B:3:LYS:HG3	1:B:4:LEU:N	1.77	0.98
1:B:8:ASP:HB3	1:B:107:LYS:HE2	1.45	0.95
1:A:217:PRO:HB2	1:A:248:ILE:HD11	1.45	0.94
1:A:358:VAL:HG21	1:A:366:ARG:HH22	1.33	0.94
1:A:115:GLU:HG3	1:A:310:VAL:HG22	1.49	0.92
1:B:5:PHE:HE1	1:B:10:VAL:HG23	1.25	0.92
1:A:238:VAL:HG21	1:A:346:PHE:HD1	1.35	0.91
1:A:209:LEU:HD22	1:B:193:ARG:HD2	1.53	0.91
1:A:228:VAL:HA	1:A:231:THR:HG23	1.51	0.91
1:A:1:MET:HB3	1:A:6:GLY:CA	2.01	0.90
1:B:1:MET:HB2	1:B:11:ARG:CG	2.01	0.90
1:B:205:ASN:HD22	1:B:205:ASN:H	1.10	0.90
1:B:383:LEU:HD21	1:B:391:LYS:HZ2	1.37	0.89
1:A:425:THR:HG22	1:A:426:GLU:HG3	1.54	0.88
1:B:1:MET:HG3	1:B:11:ARG:CZ	2.03	0.88
1:B:288:SER:O	1:B:291:VAL:HG12	1.74	0.88
1:A:1:MET:HE3	1:A:7:THR:N	1.90	0.87
1:B:417:TRP:HH2	1:B:432:MET:HE2	1.39	0.86
1:B:375:THR:HG22	1:B:376:LYS:H	1.39	0.85
1:B:387:GLU:HG3	1:B:391:LYS:HE3	1.59	0.84
1:B:5:PHE:CD1	1:B:10:VAL:CG2	2.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:THR:HG22	1:B:401:VAL:HG22	1.60	0.84
1:B:1:MET:SD	1:B:6:GLY:HA3	2.17	0.84
1:A:398:THR:HG23	1:A:401:VAL:HG22	1.61	0.83
1:B:366:ARG:HB2	1:B:366:ARG:HH11	1.44	0.83
1:A:380:LYS:HD2	1:A:381:PRO:HD2	1.61	0.82
1:A:391:LYS:O	1:A:395:VAL:HG12	1.77	0.82
1:B:115:GLU:HB2	1:B:310:VAL:HG13	1.61	0.82
1:B:377:VAL:HG11	1:B:452:VAL:HG11	1.61	0.82
1:A:231:THR:HG21	1:B:231:THR:HG21	1.59	0.82
1:B:333:TYR:CE2	1:B:335:PRO:HG2	2.14	0.82
1:B:442:ASN:O	1:B:445:VAL:HG12	1.78	0.82
1:B:1:MET:CE	1:B:6:GLY:HA3	2.09	0.81
1:B:1:MET:HE1	1:B:6:GLY:CA	2.10	0.81
1:A:238:VAL:HG21	1:A:346:PHE:CD1	2.16	0.81
1:B:379:LEU:HD13	1:B:427:PRO:HB3	1.62	0.81
1:B:377:VAL:HG13	1:B:429:ILE:HB	1.63	0.81
1:A:1:MET:HE3	1:A:6:GLY:HA3	1.63	0.80
1:A:193:ARG:HD2	1:B:209:LEU:HD22	1.63	0.79
1:B:366:ARG:HH11	1:B:366:ARG:CG	1.96	0.79
1:B:417:TRP:CH2	1:B:432:MET:HE2	2.18	0.78
1:B:230:LYS:HE2	1:B:254:GLY:HA3	1.66	0.78
1:B:1:MET:HE1	1:B:6:GLY:C	2.09	0.77
1:B:5:PHE:CD1	1:B:10:VAL:HG22	2.19	0.76
1:B:1:MET:HG3	1:B:11:ARG:NE	2.00	0.76
1:B:26:LEU:O	1:B:30:ILE:HG13	1.86	0.75
1:B:443:ASN:HA	1:B:446:ASN:HD22	1.51	0.75
1:B:5:PHE:CD1	1:B:10:VAL:HG23	2.21	0.75
1:B:222:LEU:CD1	1:B:248:ILE:HD11	2.17	0.74
1:B:228:VAL:HA	1:B:231:THR:HG23	1.69	0.74
1:A:276:LYS:HD3	1:A:277:ALA:N	2.03	0.74
1:A:275:PRO:HA	1:A:279:LYS:NZ	2.03	0.73
1:B:379:LEU:HB3	1:B:427:PRO:HB3	1.69	0.73
1:B:178:ASP:OD2	1:B:225:THR:HG21	1.87	0.73
1:B:366:ARG:HH11	1:B:366:ARG:CB	2.00	0.73
1:B:188:THR:OG1	1:B:240:HIS:HE1	1.71	0.73
1:A:267:SER:OG	1:A:281:ILE:HG21	1.88	0.73
1:B:222:LEU:HD11	1:B:248:ILE:HD11	1.69	0.72
1:B:176:LEU:HD23	1:B:177:ILE:N	2.03	0.72
1:A:1:MET:HB3	1:A:6:GLY:HA2	1.70	0.72
1:A:333:TYR:CE2	1:A:335:PRO:HG2	2.25	0.72
1:B:176:LEU:HD23	1:B:176:LEU:C	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LYS:HD3	1:B:381:PRO:HD2	1.71	0.72
1:B:1:MET:CE	1:B:6:GLY:CA	2.67	0.72
1:A:178:ASP:OD2	1:A:225:THR:HG21	1.90	0.71
1:B:104:ASN:HD22	1:B:105:GLY:H	1.37	0.71
1:A:253:GLU:HG2	1:A:361:ALA:CB	2.19	0.71
1:B:443:ASN:HA	1:B:446:ASN:ND2	2.06	0.71
1:A:217:PRO:HB2	1:A:248:ILE:CD1	2.20	0.70
1:A:216:GLU:HG3	1:A:246:ARG:NH2	2.07	0.70
1:B:205:ASN:HD22	1:B:205:ASN:N	1.88	0.70
1:B:238:VAL:HG21	1:B:346:PHE:CD1	2.26	0.70
1:A:176:LEU:HD23	1:A:176:LEU:C	2.17	0.70
1:A:447:GLU:HA	1:A:450:LYS:HZ2	1.54	0.69
1:A:205:ASN:H	1:A:205:ASN:HD22	1.41	0.69
1:B:377:VAL:CG1	1:B:429:ILE:HB	2.23	0.69
1:A:358:VAL:HG21	1:A:366:ARG:NH2	2.07	0.69
1:B:390:LYS:O	1:B:394:GLU:HG3	1.92	0.68
1:B:21:GLU:CD	1:B:21:GLU:H	2.00	0.68
1:B:379:LEU:CB	1:B:427:PRO:HB3	2.24	0.68
1:B:420:VAL:HG13	1:B:431:ILE:HG12	1.76	0.68
1:B:366:ARG:HH11	1:B:366:ARG:HG3	1.58	0.67
1:A:1:MET:CE	1:A:6:GLY:CA	2.65	0.67
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.10	0.67
1:B:277:ALA:O	1:B:279:LYS:HD2	1.94	0.67
1:B:371:TYR:O	1:B:434:GLU:HB2	1.94	0.67
1:B:83:VAL:HA	1:B:88:TYR:HB2	1.77	0.67
1:B:118:ARG:HH22	1:B:311:ASP:HB2	1.59	0.67
1:B:319:GLU:HG2	1:B:319:GLU:O	1.96	0.66
1:B:379:LEU:CD1	1:B:427:PRO:HB3	2.25	0.66
1:B:366:ARG:HB2	1:B:366:ARG:NH1	2.11	0.66
1:A:398:THR:CG2	1:A:401:VAL:HG22	2.25	0.66
1:B:305:THR:HA	1:B:406:ILE:HD13	1.77	0.66
1:B:373:VAL:HG21	1:B:442:ASN:HA	1.76	0.66
1:A:115:GLU:HG3	1:A:310:VAL:CG2	2.22	0.66
1:A:8:ASP:OD1	1:A:107:LYS:HE2	1.96	0.66
1:B:440:VAL:O	1:B:444:LEU:HB2	1.96	0.65
1:A:379:LEU:HG	1:A:429:ILE:HD11	1.77	0.65
1:B:251:ASP:OD2	1:B:255:ARG:HG3	1.97	0.65
1:B:278:ILE:HD12	1:B:280:LYS:NZ	2.10	0.65
1:B:136:ILE:HD11	1:B:141:LEU:HD13	1.79	0.64
1:A:275:PRO:HA	1:A:279:LYS:HZ3	1.60	0.64
1:A:280:LYS:HB2	1:A:280:LYS:HZ3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:O	1:A:241:ASP:HA	1.97	0.64
1:B:389:TYR:CE1	1:B:408:GLY:HA2	2.33	0.63
1:A:380:LYS:HD2	1:A:381:PRO:CD	2.27	0.63
1:A:33:PHE:HZ	1:A:120:LYS:HD3	1.64	0.63
1:A:188:THR:O	1:A:191:VAL:HG22	1.99	0.63
1:A:82:ALA:O	1:A:86:LEU:HB2	1.99	0.63
1:A:253:GLU:HG2	1:A:361:ALA:HB1	1.81	0.63
1:B:413:GLY:HA3	1:B:416:PHE:CE2	2.33	0.63
1:B:295:LEU:HD22	1:B:300:ILE:HD12	1.79	0.62
1:A:98:HIS:HB2	1:A:216:GLU:HB2	1.81	0.62
1:B:365:ASP:C	1:B:367:LEU:H	2.06	0.62
1:A:358:VAL:CG1	1:A:362:GLU:HB3	2.28	0.62
1:A:104:ASN:HD22	1:A:105:GLY:H	1.48	0.62
1:B:228:VAL:HA	1:B:231:THR:CG2	2.29	0.62
1:B:333:TYR:CD2	1:B:335:PRO:HG2	2.35	0.62
1:B:391:LYS:O	1:B:394:GLU:HB2	1.99	0.62
1:A:447:GLU:HA	1:A:450:LYS:NZ	2.15	0.61
1:A:1:MET:HE2	1:A:6:GLY:CA	2.21	0.61
1:B:119:GLU:H	1:B:119:GLU:CD	2.09	0.61
1:A:281:ILE:C	1:A:281:ILE:HD12	2.26	0.61
1:A:312:ILE:HG22	1:A:332:MET:HE2	1.83	0.61
1:B:429:ILE:HG22	1:B:431:ILE:HG13	1.81	0.61
1:A:253:GLU:HG2	1:A:361:ALA:HB2	1.82	0.61
1:B:401:VAL:HG12	1:B:413:GLY:HA2	1.83	0.60
1:B:33:PHE:CD2	1:B:124:ILE:HD11	2.36	0.60
1:B:120:LYS:HA	1:B:123:GLU:HG3	1.84	0.60
1:A:110:ASP:CG	1:A:111:LYS:H	2.09	0.60
1:B:133:PHE:C	1:B:135:THR:H	2.10	0.60
1:B:387:GLU:O	1:B:391:LYS:HG3	2.02	0.60
1:A:168:ILE:HD11	1:A:351:GLU:HG3	1.82	0.60
1:B:173:TYR:CZ	1:B:353:LEU:HD12	2.37	0.59
1:A:263:GLY:O	1:A:267:SER:HB2	2.03	0.59
1:A:437:ASP:HB3	1:A:440:VAL:HG13	1.83	0.59
1:B:21:GLU:OE1	1:B:21:GLU:N	2.34	0.59
1:B:332:MET:O	1:B:334:PRO:HD3	2.03	0.59
1:B:429:ILE:N	1:B:429:ILE:HD12	2.16	0.59
1:A:1:MET:HE3	1:A:6:GLY:CA	2.32	0.59
1:A:136:ILE:HD11	1:A:141:LEU:CD1	2.33	0.59
1:A:375:THR:HG22	1:A:376:LYS:N	2.18	0.59
1:B:58:GLU:HG2	1:B:68:VAL:HG11	1.84	0.59
1:A:392:ILE:HA	1:A:395:VAL:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:HG21	1:B:49:GLY:HA3	1.85	0.59
1:B:265:LEU:HD11	1:B:367:LEU:HD13	1.83	0.58
1:A:352:LEU:CD1	1:A:363:LEU:HD11	2.33	0.58
1:B:305:THR:HA	1:B:406:ILE:CD1	2.32	0.58
1:A:290:LEU:C	1:A:290:LEU:HD23	2.28	0.58
1:B:205:ASN:H	1:B:205:ASN:ND2	1.87	0.58
1:B:227:GLU:O	1:B:231:THR:HG22	2.04	0.58
1:B:290:LEU:HD23	1:B:290:LEU:C	2.28	0.58
1:B:449:LYS:HG2	1:B:453:GLU:OE2	2.03	0.58
1:B:398:THR:HG23	1:B:401:VAL:H	1.68	0.58
1:A:415:ASP:OD1	1:A:436:LYS:HD2	2.03	0.57
1:A:417:TRP:NE1	1:A:434:GLU:HG3	2.18	0.57
1:A:119:GLU:CD	1:A:119:GLU:H	2.12	0.57
1:B:411:ILE:HB	1:B:418:PHE:CE1	2.39	0.57
1:B:294:TYR:O	1:B:297:LYS:HG2	2.05	0.57
1:A:177:ILE:HD13	1:A:188:THR:HG22	1.87	0.57
1:B:276:LYS:O	1:B:276:LYS:HD3	2.05	0.56
1:A:288:SER:OG	1:A:290:LEU:HB3	2.05	0.56
1:A:372:LEU:HA	1:A:434:GLU:HB3	1.86	0.56
1:A:384:MET:SD	1:A:385:VAL:HG12	2.46	0.56
1:B:251:ASP:OD2	1:B:255:ARG:NH1	2.38	0.56
1:A:340:ARG:HG3	3:A:461:HOH:O	2.05	0.56
1:B:302:VAL:HG23	1:B:302:VAL:O	2.04	0.56
1:A:253:GLU:HA	1:A:253:GLU:OE1	2.06	0.56
1:B:115:GLU:HB2	1:B:310:VAL:CG1	2.34	0.56
1:B:383:LEU:CD1	1:B:387:GLU:HG2	2.35	0.56
1:B:268:TYR:O	1:B:271:SER:HB3	2.06	0.56
1:B:289:SER:HB3	1:B:417:TRP:CD1	2.41	0.56
1:B:156:VAL:HG13	1:B:191:VAL:HG12	1.88	0.56
1:B:248:ILE:O	1:B:248:ILE:HG13	2.06	0.56
1:B:437:ASP:OD2	1:B:439:ASN:HB2	2.05	0.56
1:A:83:VAL:HG11	1:A:109:VAL:HG21	1.88	0.56
1:A:379:LEU:HG	1:A:429:ILE:CD1	2.35	0.56
1:B:104:ASN:ND2	1:B:105:GLY:H	2.02	0.56
1:B:379:LEU:HD13	1:B:427:PRO:CB	2.34	0.56
1:A:14:VAL:HG21	1:A:49:GLY:HA3	1.88	0.55
1:A:278:ILE:N	1:A:278:ILE:HD13	2.21	0.55
1:A:280:LYS:NZ	1:A:280:LYS:CB	2.68	0.55
1:A:288:SER:HA	1:A:417:TRP:CZ2	2.40	0.55
1:A:220:ASP:O	1:A:223:LYS:HB2	2.06	0.55
1:B:104:ASN:HD22	1:B:105:GLY:N	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:SER:OG	1:A:183:VAL:N	2.40	0.55
1:A:289:SER:HG	1:A:417:TRP:CD1	2.25	0.55
1:A:198:LYS:HA	1:B:211:SER:OG	2.06	0.55
1:B:366:ARG:HG3	1:B:366:ARG:NH1	2.22	0.55
1:A:228:VAL:CA	1:A:231:THR:HG23	2.31	0.54
1:B:121:GLU:O	1:B:125:GLU:HG3	2.07	0.54
1:B:290:LEU:HD23	1:B:291:VAL:N	2.22	0.54
1:A:375:THR:CG2	1:A:376:LYS:N	2.71	0.54
1:A:115:GLU:HG3	1:A:310:VAL:HG13	1.89	0.54
1:A:369:LYS:HE2	1:A:371:TYR:HE1	1.71	0.54
1:B:238:VAL:HG21	1:B:346:PHE:HD1	1.72	0.54
1:A:378:ASP:HA	1:A:428:ILE:HG13	1.90	0.54
1:B:126:ASP:O	1:B:130:THR:HG23	2.08	0.54
1:B:379:LEU:C	1:B:379:LEU:HD23	2.32	0.54
1:B:383:LEU:HD21	1:B:391:LYS:NZ	2.16	0.54
1:B:278:ILE:HD12	1:B:280:LYS:HZ3	1.72	0.54
1:B:288:SER:HA	1:B:417:TRP:CZ2	2.43	0.54
1:A:352:LEU:O	1:A:356:GLU:HG2	2.07	0.54
1:A:136:ILE:HD11	1:A:141:LEU:HD13	1.90	0.53
1:A:449:LYS:HG2	1:A:453:GLU:OE2	2.08	0.53
1:A:397:SER:C	1:A:398:THR:HG22	2.33	0.53
1:B:17:GLU:O	1:B:19:THR:HG23	2.09	0.53
1:B:133:PHE:O	1:B:135:THR:N	2.39	0.53
1:A:265:LEU:HD13	1:A:367:LEU:HD11	1.90	0.53
1:B:385:VAL:HG23	1:B:389:TYR:CE2	2.43	0.53
1:B:1:MET:HG3	1:B:11:ARG:CD	2.38	0.53
1:A:1:MET:CB	1:A:6:GLY:CA	2.82	0.53
1:B:10:VAL:HG21	1:B:26:LEU:HD11	1.90	0.53
1:B:383:LEU:HD23	1:B:388:ILE:HD11	1.90	0.53
1:B:1:MET:C	1:B:3:LYS:N	2.65	0.53
1:B:1:MET:HE3	1:B:9:GLY:O	2.09	0.53
1:B:108:VAL:HG23	1:B:116:ILE:HG12	1.89	0.53
1:B:273:LYS:HE3	1:B:333:TYR:OH	2.09	0.53
1:B:1:MET:HE1	1:B:7:THR:N	2.23	0.53
1:B:418:PHE:HB3	1:B:433:ALA:HB2	1.91	0.53
1:A:76:THR:N	1:A:77:PRO:CD	2.72	0.52
1:A:78:ALA:HA	1:A:155:TYR:CD1	2.44	0.52
1:B:443:ASN:N	1:B:443:ASN:HD22	2.06	0.52
1:B:4:LEU:HD12	1:B:5:PHE:H	1.74	0.52
1:A:96:ALA:HB2	1:A:104:ASN:HA	1.91	0.52
1:B:383:LEU:HD11	1:B:391:LYS:HZ1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASN:H	1:A:205:ASN:ND2	2.07	0.52
1:A:96:ALA:HB2	1:A:104:ASN:CA	2.40	0.52
1:A:177:ILE:HG22	1:A:179:PRO:HD3	1.91	0.52
1:A:371:TYR:O	1:A:434:GLU:HB2	2.10	0.52
1:B:296:SER:C	1:B:298:TYR:H	2.17	0.52
1:A:316:VAL:HG13	1:A:321:ALA:HB3	1.90	0.52
1:B:75:PRO:HA	1:B:183:VAL:HG11	1.92	0.52
1:B:171:LYS:HG2	1:B:173:TYR:CZ	2.44	0.52
1:B:281:ILE:HG13	1:B:281:ILE:O	2.08	0.52
1:A:21:GLU:CD	1:A:21:GLU:H	2.17	0.52
1:A:252:SER:N	1:A:360:SER:OG	2.38	0.52
1:B:36:LYS:O	1:B:37:ASN:HB2	2.09	0.52
1:A:371:TYR:O	1:A:434:GLU:CB	2.58	0.51
1:A:117:ARG:HB3	1:A:119:GLU:OE1	2.10	0.51
1:A:115:GLU:CG	1:A:310:VAL:HG13	2.40	0.51
1:B:173:TYR:OH	1:B:353:LEU:HD12	2.10	0.51
1:B:440:VAL:CG2	1:B:441:ALA:N	2.74	0.51
1:B:313:ALA:HA	1:B:332:MET:HE2	1.93	0.51
1:B:372:LEU:HD12	1:B:433:ALA:O	2.09	0.51
1:B:411:ILE:HD13	1:B:418:PHE:CZ	2.46	0.51
1:A:417:TRP:NE1	1:A:434:GLU:CG	2.74	0.51
1:B:262:SER:O	1:B:266:LEU:HB2	2.11	0.51
1:B:372:LEU:HD12	1:B:373:VAL:H	1.75	0.51
1:B:380:LYS:HD3	1:B:381:PRO:CD	2.40	0.51
1:B:444:LEU:O	1:B:444:LEU:HD23	2.11	0.50
1:B:265:LEU:CD1	1:B:367:LEU:HD13	2.41	0.50
1:B:364:PHE:O	1:B:367:LEU:HB2	2.11	0.50
1:B:383:LEU:CD2	1:B:388:ILE:HD11	2.41	0.50
1:A:295:LEU:HB3	1:A:300:ILE:HB	1.93	0.50
1:B:136:ILE:HD11	1:B:141:LEU:CD1	2.41	0.50
1:B:230:LYS:HG3	1:B:254:GLY:HA3	1.93	0.50
1:A:174:LYS:O	1:A:234:VAL:HG13	2.11	0.50
1:A:388:ILE:O	1:A:392:ILE:HG12	2.11	0.50
1:A:4:LEU:HB2	1:A:125:GLU:OE2	2.11	0.50
1:A:279:LYS:O	1:A:280:LYS:HB2	2.10	0.50
1:A:219:PHE:O	1:A:223:LYS:HD3	2.12	0.50
1:A:389:TYR:O	1:A:393:LEU:HB2	2.11	0.50
1:B:1:MET:O	1:B:3:LYS:N	2.44	0.50
1:B:118:ARG:O	1:B:121:GLU:HB2	2.12	0.50
1:B:411:ILE:O	1:B:417:TRP:HA	2.11	0.50
1:A:110:ASP:CG	1:A:111:LYS:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:VAL:HG23	1:B:441:ALA:N	2.27	0.50
1:A:401:VAL:HB	1:A:412:ILE:O	2.11	0.50
1:B:389:TYR:O	1:B:393:LEU:HB2	2.11	0.50
1:A:275:PRO:HA	1:A:279:LYS:HZ1	1.77	0.49
1:B:388:ILE:O	1:B:389:TYR:C	2.55	0.49
1:B:398:THR:CG2	1:B:401:VAL:H	2.24	0.49
1:A:1:MET:HB3	1:A:6:GLY:HA3	1.89	0.49
1:B:435:ALA:N	1:B:441:ALA:HB2	2.27	0.49
1:B:137:GLU:O	1:B:138:TRP:C	2.55	0.49
1:B:428:ILE:C	1:B:429:ILE:HD12	2.37	0.49
1:B:4:LEU:CD1	1:B:5:PHE:H	2.26	0.49
1:B:294:TYR:CD1	1:B:367:LEU:HD12	2.46	0.49
1:B:375:THR:HG22	1:B:376:LYS:N	2.18	0.49
1:B:384:MET:O	1:B:387:GLU:HB3	2.12	0.49
1:B:404:ILE:HG22	1:B:406:ILE:HG22	1.94	0.49
1:B:447:GLU:O	1:B:450:LYS:HB2	2.13	0.49
1:A:94:ILE:HD12	1:A:94:ILE:N	2.28	0.49
1:A:211:SER:OG	1:B:198:LYS:HA	2.12	0.49
1:B:1:MET:HB2	1:B:11:ARG:CD	2.42	0.49
1:B:8:ASP:O	1:B:107:LYS:HG2	2.13	0.49
1:B:23:VAL:HG21	1:B:53:LEU:HD22	1.93	0.49
1:A:333:TYR:CD2	1:A:335:PRO:HG2	2.48	0.49
1:B:118:ARG:NH2	1:B:311:ASP:HB2	2.27	0.49
1:B:177:ILE:HD13	1:B:188:THR:HG22	1.94	0.49
1:B:292:GLU:HG3	1:B:302:VAL:HG22	1.93	0.49
1:B:372:LEU:HA	1:B:434:GLU:HB3	1.93	0.49
1:B:246:ARG:HD2	1:B:340:ARG:NH1	2.27	0.49
1:A:265:LEU:O	1:A:268:TYR:HB3	2.13	0.49
1:B:443:ASN:HD22	1:B:444:LEU:N	2.11	0.49
1:A:447:GLU:CD	1:A:450:LYS:HZ1	2.19	0.48
1:A:222:LEU:O	1:A:223:LYS:C	2.56	0.48
1:B:431:ILE:HD11	1:B:452:VAL:HG21	1.95	0.48
1:A:8:ASP:CG	1:A:107:LYS:HE2	2.39	0.48
1:A:174:LYS:HE2	1:A:200:TYR:CE1	2.48	0.48
1:B:24:LEU:O	1:B:27:SER:HB2	2.14	0.48
1:B:251:ASP:HB2	1:B:361:ALA:HA	1.96	0.48
1:A:293:GLU:OE2	1:A:436:LYS:NZ	2.32	0.48
1:A:294:TYR:CD1	1:A:367:LEU:HD12	2.48	0.48
1:B:358:VAL:HG13	1:B:362:GLU:OE2	2.13	0.48
1:A:386:GLU:O	1:A:386:GLU:HG2	2.14	0.48
1:A:405:THR:HG22	1:A:409:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PRO:HG2	1:B:187:SER:OG	2.14	0.48
1:B:257:GLN:OE1	1:B:364:PHE:CD2	2.67	0.48
1:B:392:ILE:HG13	1:B:393:LEU:N	2.28	0.48
1:A:47:ARG:CZ	1:A:96:ALA:HB3	2.44	0.48
1:A:110:ASP:HB2	1:A:116:ILE:HG22	1.96	0.48
1:A:288:SER:O	1:A:291:VAL:HG12	2.14	0.48
1:B:173:TYR:OH	1:B:354:ALA:HA	2.14	0.48
1:B:306:LYS:HB3	1:B:407:ASP:OD2	2.14	0.48
1:B:398:THR:HG23	1:B:400:SER:H	1.79	0.48
1:A:44:ARG:O	1:A:73:MET:HA	2.14	0.47
1:A:228:VAL:HA	1:A:231:THR:CG2	2.34	0.47
1:A:238:VAL:HG22	1:A:249:PHE:CD2	2.48	0.47
1:A:258:TRP:HA	1:A:258:TRP:CE3	2.48	0.47
1:B:295:LEU:HD22	1:B:300:ILE:CD1	2.44	0.47
1:A:1:MET:CB	1:A:6:GLY:HA3	2.45	0.47
1:B:215:PRO:O	1:B:241:ASP:HA	2.13	0.47
1:A:371:TYR:CD1	1:A:371:TYR:N	2.80	0.47
1:A:396:TYR:O	1:A:398:THR:HG22	2.15	0.47
1:B:75:PRO:HA	1:B:183:VAL:CG1	2.45	0.47
1:B:423:SER:HB2	1:B:430:ARG:NE	2.30	0.47
1:A:255:ARG:HH22	1:A:365:ASP:CG	2.23	0.47
1:A:278:ILE:HD13	1:A:278:ILE:H	1.79	0.47
1:A:319:GLU:O	1:A:320:ASN:C	2.57	0.47
1:B:452:VAL:C	1:B:454:GLY:H	2.21	0.47
1:B:278:ILE:HD11	1:B:320:ASN:O	2.14	0.47
1:A:133:PHE:O	1:A:135:THR:N	2.40	0.47
1:A:45:ASP:OD1	1:A:45:ASP:C	2.57	0.47
1:B:133:PHE:C	1:B:135:THR:N	2.73	0.47
1:B:305:THR:HG23	1:B:306:LYS:O	2.15	0.47
1:B:415:ASP:O	1:B:435:ALA:HB1	2.15	0.47
1:A:288:SER:HA	1:A:417:TRP:CE2	2.50	0.47
1:B:366:ARG:CG	1:B:366:ARG:NH1	2.65	0.47
1:B:383:LEU:HD12	1:B:387:GLU:HG2	1.95	0.47
1:A:308:GLY:O	1:A:312:ILE:HG13	2.15	0.46
1:B:388:ILE:O	1:B:391:LYS:HB2	2.15	0.46
1:B:398:THR:HG23	1:B:400:SER:N	2.30	0.46
1:A:176:LEU:HA	1:A:200:TYR:O	2.15	0.46
1:A:219:PHE:CD2	1:A:256:VAL:HG22	2.50	0.46
1:B:346:PHE:CZ	1:B:350:LEU:HD11	2.50	0.46
1:A:3:LYS:HA	1:A:3:LYS:HD3	1.59	0.46
1:A:406:ILE:HG13	1:A:406:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD12	1:B:248:ILE:HD11	1.93	0.46
1:B:365:ASP:C	1:B:367:LEU:N	2.71	0.46
1:B:369:LYS:HE2	1:B:371:TYR:HE1	1.80	0.46
1:B:383:LEU:HD11	1:B:387:GLU:HG2	1.97	0.46
1:A:392:ILE:HG23	1:A:451:ILE:HG21	1.96	0.46
1:A:230:LYS:HE3	1:A:253:GLU:O	2.16	0.46
1:B:49:GLY:O	1:B:53:LEU:HG	2.15	0.46
1:B:429:ILE:N	1:B:429:ILE:CD1	2.79	0.46
1:A:171:LYS:O	1:A:172:ASN:C	2.57	0.46
1:A:371:TYR:O	1:A:434:GLU:HA	2.16	0.46
1:A:374:LYS:CB	1:A:374:LYS:NZ	2.79	0.46
1:B:418:PHE:CD2	1:B:448:LEU:HD11	2.51	0.45
1:B:435:ALA:HB3	1:B:441:ALA:HB2	1.96	0.45
1:B:266:LEU:HB3	1:B:331:PHE:CE1	2.51	0.45
1:A:136:ILE:HD11	1:A:141:LEU:HD12	1.98	0.45
1:B:22:LEU:HD23	1:B:22:LEU:O	2.17	0.45
1:B:101:ALA:N	1:B:102:PRO:HD2	2.31	0.45
1:B:388:ILE:HG21	1:B:452:VAL:HG22	1.98	0.45
1:B:316:VAL:HG13	1:B:321:ALA:HB3	1.97	0.45
1:B:417:TRP:NE1	1:B:434:GLU:CG	2.80	0.45
1:B:281:ILE:HD12	1:B:325:PHE:CE1	2.51	0.45
1:B:176:LEU:HB2	1:B:234:VAL:HG21	1.97	0.45
1:B:269:TRP:CE3	1:B:352:LEU:HD23	2.52	0.45
1:A:219:PHE:CE2	1:A:256:VAL:HG22	2.52	0.45
1:B:440:VAL:HA	1:B:443:ASN:HD21	1.81	0.45
1:B:371:TYR:CG	1:B:438:GLU:HB3	2.52	0.45
1:B:378:ASP:OD2	1:B:428:ILE:HG12	2.17	0.45
1:B:411:ILE:HD13	1:B:418:PHE:CE2	2.52	0.45
1:B:443:ASN:N	1:B:443:ASN:ND2	2.65	0.45
1:A:222:LEU:HD11	1:A:248:ILE:HD11	1.99	0.45
1:A:234:VAL:CG1	1:A:236:LEU:O	2.65	0.45
1:B:4:LEU:HD12	1:B:125:GLU:OE2	2.16	0.45
1:B:138:TRP:CG	1:B:139:SER:N	2.84	0.45
1:B:371:TYR:O	1:B:434:GLU:CB	2.63	0.45
1:B:450:LYS:O	1:B:451:ILE:C	2.60	0.45
1:A:94:ILE:N	1:A:94:ILE:CD1	2.80	0.44
1:A:374:LYS:HB3	1:A:374:LYS:HZ3	1.82	0.44
1:B:1:MET:HG3	1:B:11:ARG:NH1	2.31	0.44
1:A:225:THR:HA	1:A:228:VAL:HG22	1.98	0.44
1:A:309:SER:OG	1:A:340:ARG:HD3	2.17	0.44
1:A:324:GLY:C	1:A:332:MET:HG2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TYR:HB3	1:A:411:ILE:HD12	1.99	0.44
1:B:182:SER:O	1:B:184:GLY:N	2.50	0.44
1:B:418:PHE:HB3	1:B:433:ALA:CB	2.48	0.44
1:A:104:ASN:HD22	1:A:105:GLY:N	2.15	0.44
1:B:404:ILE:CG2	1:B:406:ILE:HG22	2.48	0.44
1:B:440:VAL:O	1:B:443:ASN:ND2	2.51	0.44
1:B:218:THR:O	1:B:219:PHE:C	2.60	0.44
1:A:216:GLU:HG3	1:A:246:ARG:HH21	1.83	0.44
1:B:225:THR:O	1:B:228:VAL:HG22	2.18	0.44
1:B:333:TYR:CE2	1:B:335:PRO:CG	2.94	0.44
1:B:409:VAL:HG12	1:B:411:ILE:CD1	2.48	0.44
1:B:445:VAL:CG1	1:B:446:ASN:N	2.81	0.44
1:B:114:ILE:HG22	1:B:115:GLU:N	2.33	0.43
1:B:253:GLU:CG	1:B:361:ALA:HB1	2.48	0.43
1:B:276:LYS:HB2	1:B:276:LYS:HE2	1.78	0.43
1:B:296:SER:C	1:B:298:TYR:N	2.77	0.43
1:A:83:VAL:HG11	1:A:109:VAL:CG2	2.49	0.43
1:A:173:TYR:OH	1:A:354:ALA:HA	2.18	0.43
1:A:269:TRP:HH2	1:A:355:ASN:OD1	2.01	0.43
1:B:337:GLN:HG3	1:B:339:VAL:HG22	2.00	0.43
1:B:271:SER:HA	1:B:322:LEU:HD11	2.00	0.43
1:A:180:ALA:HB2	1:A:213:ARG:NH2	2.33	0.43
1:A:222:LEU:HD11	1:A:248:ILE:CD1	2.48	0.43
1:A:298:TYR:O	1:A:299:ASN:HB2	2.19	0.43
1:A:398:THR:C	1:A:400:SER:H	2.27	0.43
1:A:413:GLY:HA3	1:A:416:PHE:CE2	2.54	0.43
1:B:108:VAL:HG21	1:B:116:ILE:HD11	2.00	0.43
1:A:159:ILE:HG23	1:A:344:MET:CE	2.48	0.43
1:B:138:TRP:CD2	1:B:139:SER:N	2.87	0.43
1:B:176:LEU:C	1:B:176:LEU:CD2	2.87	0.43
1:B:392:ILE:O	1:B:395:VAL:HG13	2.19	0.43
1:B:393:LEU:O	1:B:394:GLU:C	2.61	0.43
1:A:416:PHE:CD1	1:A:416:PHE:C	2.95	0.42
1:B:277:ALA:O	1:B:278:ILE:C	2.62	0.42
1:A:392:ILE:HG12	1:A:392:ILE:H	1.73	0.42
1:B:303:ASP:OD2	1:B:319:GLU:OE1	2.36	0.42
1:B:377:VAL:HG13	1:B:377:VAL:O	2.19	0.42
1:B:422:LYS:O	1:B:423:SER:C	2.62	0.42
1:A:1:MET:CG	1:A:6:GLY:HA3	2.48	0.42
1:A:188:THR:O	1:A:191:VAL:CG2	2.66	0.42
1:A:297:LYS:HZ3	1:A:298:TYR:HE2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LYS:O	1:B:369:LYS:HG2	2.18	0.42
1:B:383:LEU:HD11	1:B:391:LYS:NZ	2.34	0.42
1:B:421:ARG:O	1:B:429:ILE:HA	2.18	0.42
1:A:251:ASP:HB2	1:A:360:SER:OG	2.20	0.42
1:A:373:VAL:HG12	1:A:445:VAL:HG21	2.02	0.42
1:A:333:TYR:CZ	1:A:335:PRO:CG	3.03	0.42
1:B:411:ILE:O	1:B:417:TRP:HB2	2.19	0.42
1:B:55:LYS:HA	1:B:55:LYS:HD3	1.66	0.42
1:A:373:VAL:CG1	1:A:445:VAL:HG21	2.49	0.42
1:B:302:VAL:HG23	1:B:304:TRP:NE1	2.34	0.42
1:A:159:ILE:HG23	1:A:344:MET:HE3	2.02	0.42
1:B:3:LYS:CG	1:B:4:LEU:N	2.44	0.42
1:B:279:LYS:HD2	1:B:279:LYS:N	2.34	0.42
1:A:118:ARG:NH2	1:A:310:VAL:HB	2.35	0.42
1:A:1:MET:HE3	1:A:6:GLY:C	2.44	0.41
1:A:211:SER:HG	1:B:198:LYS:HA	1.84	0.41
1:A:284:ALA:C	1:A:286:SER:H	2.28	0.41
1:B:82:ALA:O	1:B:86:LEU:HB2	2.19	0.41
1:B:416:PHE:CD1	1:B:444:LEU:HD11	2.55	0.41
1:A:225:THR:O	1:A:228:VAL:HG22	2.20	0.41
1:A:398:THR:C	1:A:400:SER:N	2.76	0.41
1:B:188:THR:OG1	1:B:240:HIS:CE1	2.62	0.41
1:B:234:VAL:CG1	1:B:236:LEU:H	2.33	0.41
1:B:334:PRO:N	1:B:335:PRO:HD2	2.35	0.41
1:A:51:ASP:O	1:A:52:MET:C	2.62	0.41
1:A:230:LYS:HB2	1:A:230:LYS:NZ	2.36	0.41
1:A:452:VAL:C	1:A:454:GLY:H	2.28	0.41
1:B:251:ASP:OD1	1:B:253:GLU:HB2	2.20	0.41
1:A:393:LEU:HD21	1:A:405:THR:HG21	2.01	0.41
1:B:324:GLY:O	1:B:332:MET:HG2	2.21	0.41
1:B:450:LYS:NZ	1:B:450:LYS:CB	2.83	0.41
1:A:193:ARG:CD	1:B:209:LEU:HD22	2.41	0.41
1:A:297:LYS:HG3	1:A:298:TYR:CE2	2.55	0.41
1:B:41:LEU:HD23	1:B:42:VAL:N	2.35	0.41
1:B:410:LYS:HE3	1:B:412:ILE:HD11	2.03	0.41
1:A:333:TYR:CZ	1:A:335:PRO:HG2	2.55	0.41
1:B:1:MET:C	1:B:3:LYS:H	2.27	0.41
1:B:31:GLY:HA3	1:B:64:VAL:HG21	2.02	0.41
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.95	0.41
1:B:253:GLU:HG2	1:B:361:ALA:CB	2.51	0.41
1:B:258:TRP:HA	1:B:258:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HG3	1:A:310:VAL:CG1	2.50	0.41
1:A:201:THR:O	1:B:202:ILE:HD12	2.21	0.41
1:A:398:THR:HG23	1:A:401:VAL:H	1.84	0.41
1:A:440:VAL:O	1:A:444:LEU:HG	2.21	0.41
1:B:22:LEU:HD23	1:B:22:LEU:C	2.46	0.41
1:B:105:GLY:O	1:B:106:ILE:HD13	2.20	0.41
1:A:217:PRO:CB	1:A:248:ILE:HD11	2.33	0.41
1:A:324:GLY:CA	1:A:332:MET:HG2	2.51	0.41
1:B:76:THR:N	1:B:77:PRO:CD	2.83	0.41
1:B:265:LEU:O	1:B:268:TYR:HB3	2.20	0.41
1:A:291:VAL:HG13	1:A:292:GLU:N	2.36	0.40
1:A:297:LYS:NZ	1:A:298:TYR:HE2	2.19	0.40
1:B:369:LYS:NZ	1:B:369:LYS:HB3	2.36	0.40
1:B:178:ASP:OD1	1:B:178:ASP:C	2.64	0.40
1:B:251:ASP:CG	1:B:255:ARG:HG3	2.45	0.40
1:B:367:LEU:HA	1:B:368:PRO:HD3	1.92	0.40
1:B:437:ASP:O	1:B:440:VAL:HG22	2.21	0.40
1:B:450:LYS:C	1:B:455:LYS:HA	2.47	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:48:ALA:O	1:A:141:LEU:O[7_554]	2.10	0.10
1:B:2:GLY:O	1:B:126:ASP:OD1[10_444]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	453/455 (100%)	408 (90%)	40 (9%)	5 (1%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	453/455 (100%)	384 (85%)	59 (13%)	10 (2%)	5	19
All	All	906/910 (100%)	792 (87%)	99 (11%)	15 (2%)	7	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	SER
1	B	183	VAL
1	B	278	ILE
1	A	183	VAL
1	A	278	ILE
1	B	134	ASN
1	B	427	PRO
1	A	280	LYS
1	B	47	ARG
1	B	277	ALA
1	B	394	GLU
1	B	275	PRO
1	B	391	LYS
1	A	398	THR
1	A	330	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/386 (100%)	328 (85%)	58 (15%)	3	10
1	B	386/386 (100%)	337 (87%)	49 (13%)	4	15
All	All	772/772 (100%)	665 (86%)	107 (14%)	3	12

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	14	VAL
1	A	16	LYS
1	A	26	LEU
1	A	28	LYS
1	A	41	LEU
1	A	51	ASP
1	A	52	MET
1	A	79	LEU
1	A	83	VAL
1	A	86	LEU
1	A	92	VAL
1	A	94	ILE
1	A	108	VAL
1	A	109	VAL
1	A	115	GLU
1	A	125	GLU
1	A	145	VAL
1	A	151	VAL
1	A	183	VAL
1	A	190	LEU
1	A	205	ASN
1	A	209	LEU
1	A	223	LYS
1	A	230	LYS
1	A	231	THR
1	A	234	VAL
1	A	246	ARG
1	A	252	SER
1	A	256	VAL
1	A	265	LEU
1	A	266	LEU
1	A	276	LYS
1	A	278	ILE
1	A	280	LYS
1	A	290	LEU
1	A	302	VAL
1	A	332	MET
1	A	352	LEU
1	A	353	LEU
1	A	363	LEU
1	A	367	LEU
1	A	369	LYS

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Mol	Chain	Res	Type
1	A	374	LYS
1	A	377	VAL
1	A	379	LEU
1	A	384	MET
1	A	391	LYS
1	A	392	ILE
1	A	393	LEU
1	A	395	VAL
1	A	398	THR
1	A	411	ILE
1	A	425	THR
1	A	428	ILE
1	A	429	ILE
1	A	440	VAL
1	A	450	LYS
1	B	1	MET
1	B	4	LEU
1	B	26	LEU
1	B	39	LYS
1	B	41	LEU
1	B	52	MET
1	B	79	LEU
1	B	83	VAL
1	B	86	LEU
1	B	92	VAL
1	B	109	VAL
1	B	145	VAL
1	B	151	VAL
1	B	175	VAL
1	B	183	VAL
1	B	190	LEU
1	B	191	VAL
1	B	205	ASN
1	B	225	THR
1	B	227	GLU
1	B	231	THR
1	B	234	VAL
1	B	238	VAL
1	B	246	ARG
1	B	252	SER
1	B	256	VAL
1	B	265	LEU

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Mol	Chain	Res	Type
1	B	266	LEU
1	B	274	ASN
1	B	276	LYS
1	B	279	LYS
1	B	280	LYS
1	B	289	SER
1	B	290	LEU
1	B	291	VAL
1	B	301	GLN
1	B	312	ILE
1	B	332	MET
1	B	353	LEU
1	B	366	ARG
1	B	369	LYS
1	B	374	LYS
1	B	384	MET
1	B	385	VAL
1	B	395	VAL
1	B	426	GLU
1	B	427	PRO
1	B	443	ASN
1	B	450	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	122	ASN
1	A	203	ASN
1	A	205	ASN
1	A	214	GLN
1	A	274	ASN
1	A	299	ASN
1	A	355	ASN
1	A	357	ASN
1	B	37	ASN
1	B	98	HIS
1	B	104	ASN
1	B	122	ASN
1	B	157	ASN
1	B	162	HIS
1	B	205	ASN

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Mol	Chain	Res	Type
1	B	214	GLN
1	B	240	HIS
1	B	274	ASN
1	B	299	ASN
1	B	301	GLN
1	B	314	HIS
1	B	328	ASN
1	B	336	HIS
1	B	355	ASN
1	B	357	ASN
1	B	443	ASN
1	B	446	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](#)

1 ligand is 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	SO4	A	460	-	4,4,4	1.17	0	6,6,6	1.34	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	460	SO4	O4-S-O3	2.89	124.47	108.54

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 [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	455/455 (100%)	-0.11	6 (1%) 75 66	19, 37, 59, 79	0
1	B	455/455 (100%)	0.40	41 (9%) 15 11	24, 48, 99, 100	0
All	All	910/910 (100%)	0.15	47 (5%) 33 25	19, 41, 89, 100	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	GLY	6.5
1	A	2	GLY	5.2
1	A	1	MET	4.7
1	B	4	LEU	4.4
1	B	377	VAL	3.8
1	B	379	LEU	3.6
1	B	425	THR	3.4
1	B	427	PRO	3.3
1	B	431	ILE	3.2
1	B	386	GLU	3.2
1	B	5	PHE	3.2
1	B	2	GLY	3.1
1	B	391	LYS	3.1
1	B	428	ILE	3.0
1	B	384	MET	3.0
1	B	430	ARG	2.9
1	B	381	PRO	2.8
1	B	424	GLY	2.7
1	B	8	ASP	2.7
1	B	3	LYS	2.6
1	B	422	LYS	2.6
1	B	455	LYS	2.5
1	A	3	LYS	2.5
1	B	309	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	279	LYS	2.4
1	B	392	ILE	2.4
1	B	9	GLY	2.3
1	B	375	THR	2.3
1	B	383	LEU	2.3
1	B	429	ILE	2.3
1	A	375	THR	2.3
1	B	276	LYS	2.2
1	B	396	TYR	2.2
1	B	330	GLY	2.2
1	B	444	LEU	2.2
1	B	380	LYS	2.2
1	A	384	MET	2.2
1	B	376	LYS	2.2
1	B	426	GLU	2.2
1	B	378	ASP	2.1
1	B	49	GLY	2.1
1	B	137	GLU	2.1
1	A	455	LYS	2.1
1	B	452	VAL	2.1
1	B	310	VAL	2.1
1	B	278	ILE	2.0
1	B	402	LYS	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	460	5/5	0.91	0.09	68,68,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.