



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:20 PM UTC

PDB ID : 2DUU / pdb_00002duu
Title : Crystal Structure of apo-form of NADP-Dependent Glyceraldehyde-3-Phosphate Dehydrogenase from *Synechococcus* Sp.
Authors : Kitatani, T.; Nakamura, Y.; Wada, K.; Kinoshita, T.; Tamoi, M.; Shigeoka, S.; Tada, T.
Deposited on : 2006-07-27
Resolution : 2.90 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

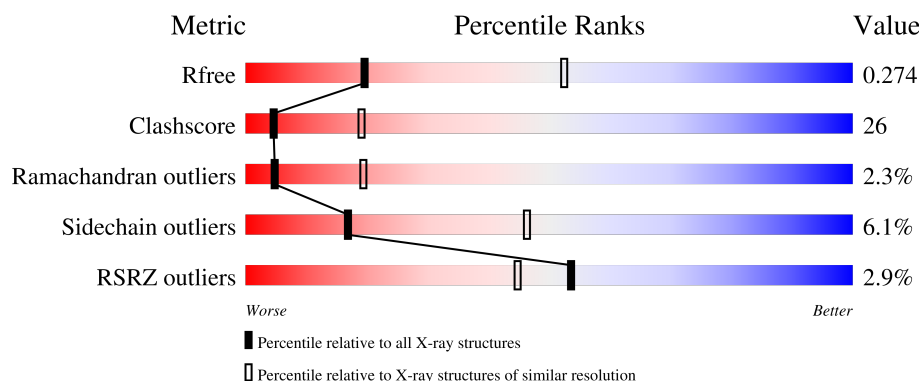
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	380	44% 34% 6% 15%
1	B	380	43% 35% 6% 15%
1	O	380	3% 46% 34% • • 15%
1	P	380	3% 44% 37% • 15%
1	Q	380	2% 44% 37% • 15%

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Mol	Chain	Length	Quality of chain
1	R	380	5% 43% 39% •• 15%

2 Entry composition [i](#)

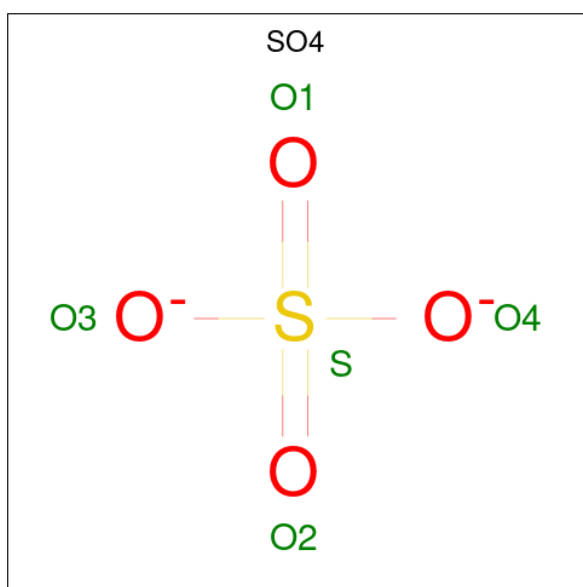
There are 3 unique types of molecules in this entry. The entry contains 15053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde 3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	B	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	O	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	P	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	Q	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			
1	R	322	Total	C	N	O	S	0	0	0
			2451	1544	423	475	9			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0

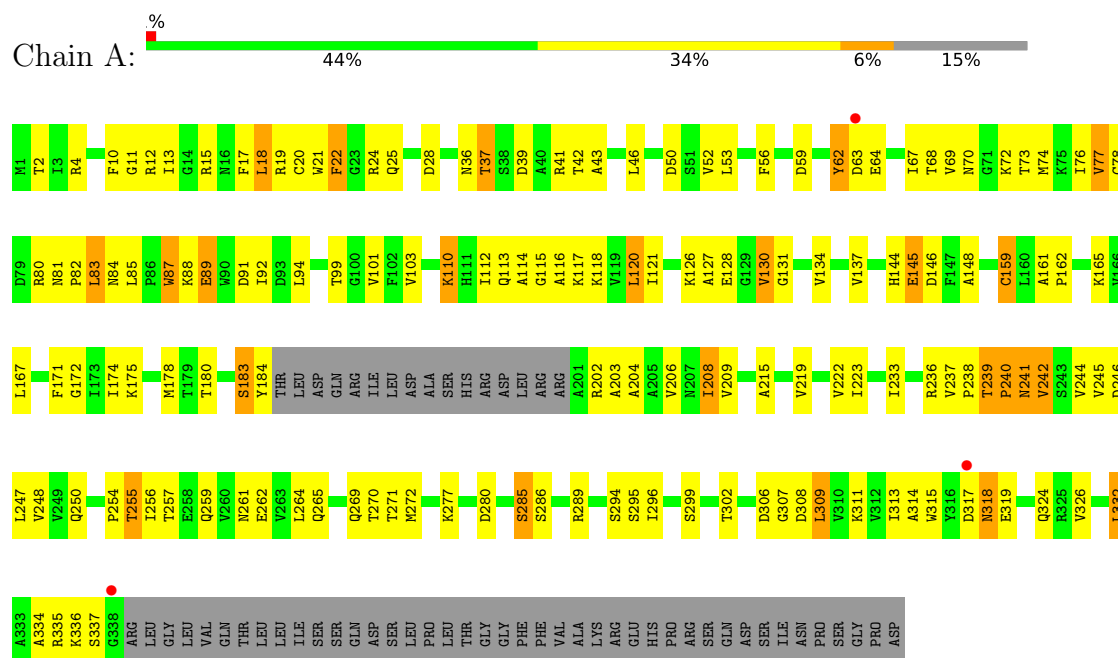
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	68	Total O 68 68	0	0
3	B	87	Total O 87 87	0	0
3	O	61	Total O 61 61	0	0
3	P	57	Total O 57 57	0	0
3	Q	19	Total O 19 19	0	0
3	R	25	Total O 25 25	0	0

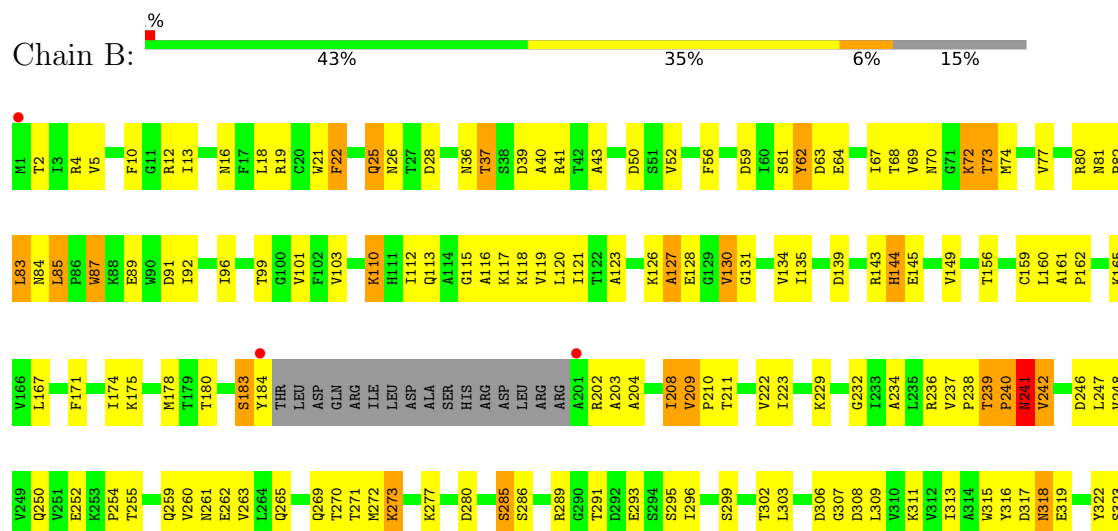
3 Residue-property plots

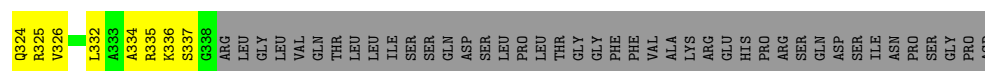
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

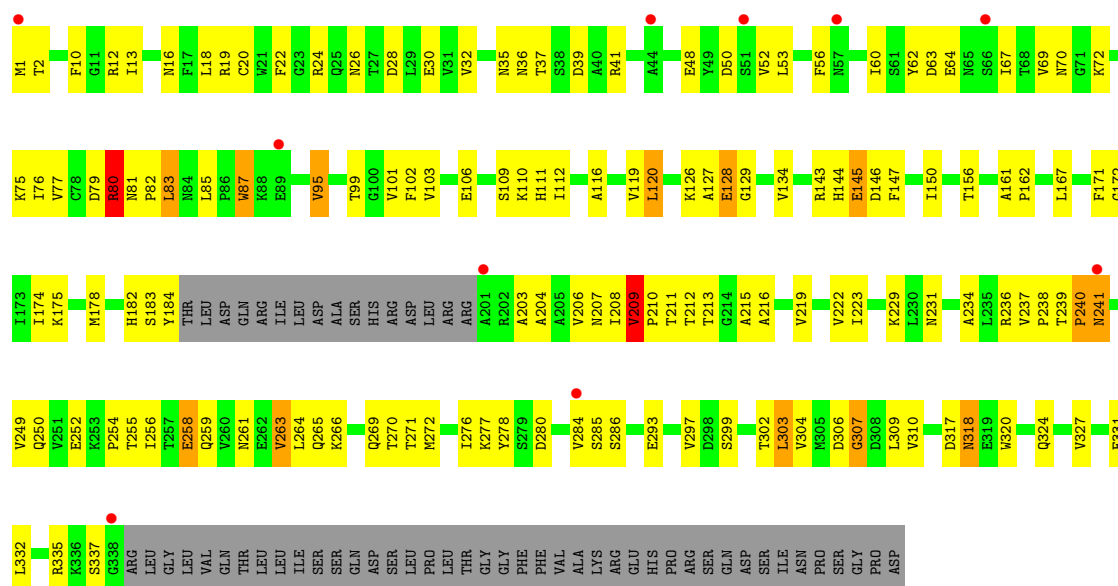


- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

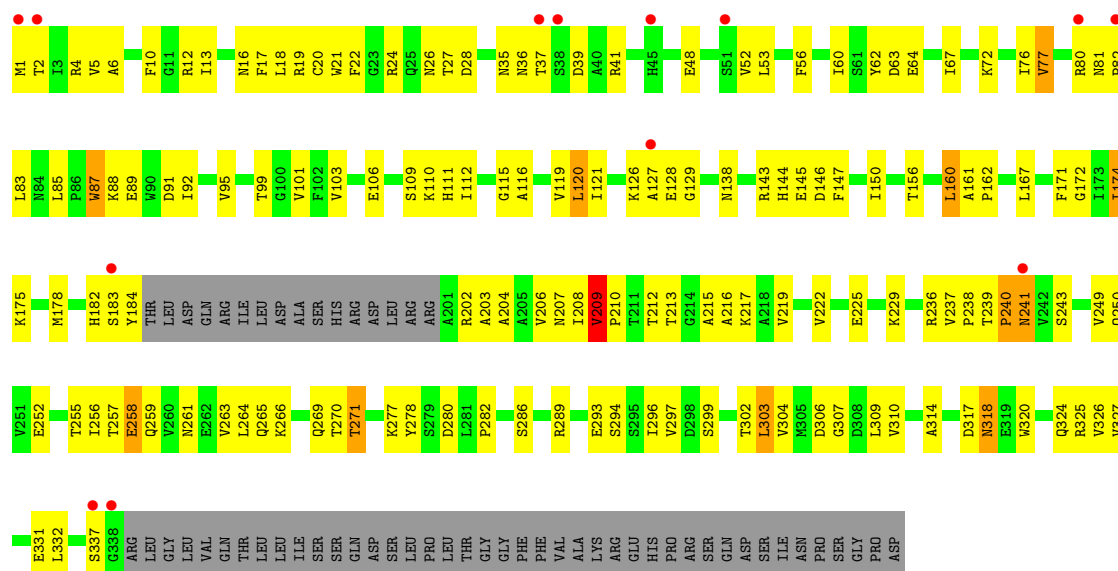
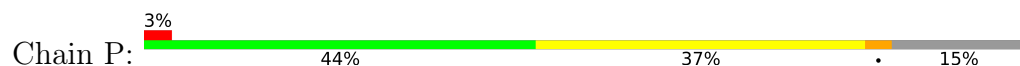




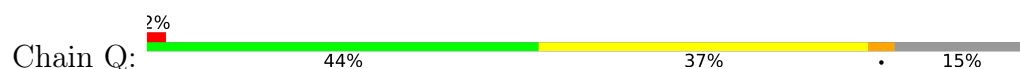
• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

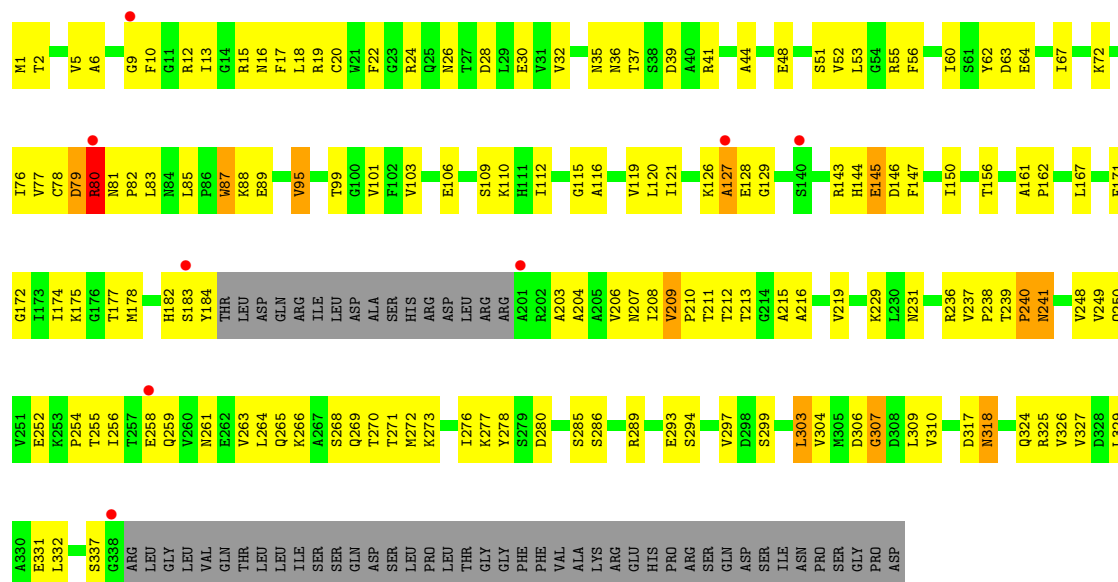


• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

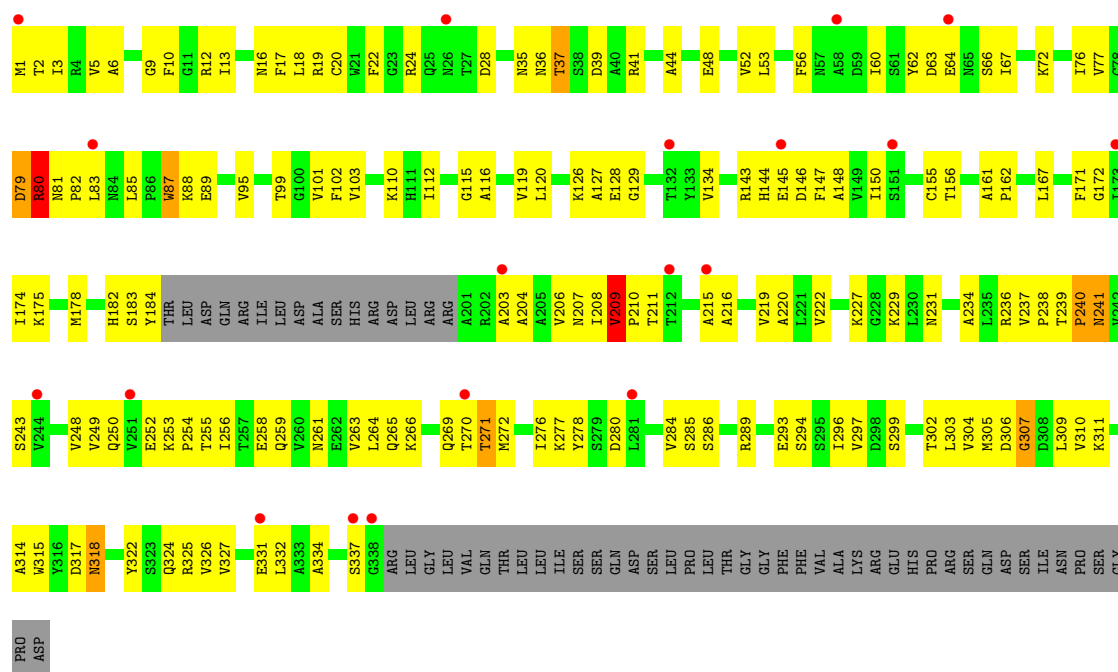
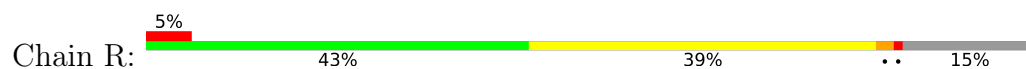


• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase





• Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.40Å 79.80Å 207.20Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 94.3 (50.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.275 0.218 , 0.274	Depositor DCC
R_{free} test set	5442 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15053	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.53	0/2490	1.08	15/3387 (0.4%)
1	B	0.54	0/2490	1.06	18/3387 (0.5%)
1	O	0.64	4/2490 (0.2%)	0.97	7/3387 (0.2%)
1	P	0.64	4/2490 (0.2%)	0.98	11/3387 (0.3%)
1	Q	0.89	12/2490 (0.5%)	1.18	16/3387 (0.5%)
1	R	0.69	7/2490 (0.3%)	0.99	8/3387 (0.2%)
All	All	0.66	27/14940 (0.2%)	1.05	75/20322 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	79	ASP	C-O	25.97	1.53	1.24
1	Q	80	ARG	N-CA	13.97	1.64	1.46
1	P	80	ARG	CZ-NH2	-12.84	1.16	1.33
1	Q	78	CYS	C-N	12.13	1.51	1.33
1	O	80	ARG	CZ-NH2	-11.73	1.18	1.33
1	Q	79	ASP	CA-C	11.25	1.67	1.53
1	P	80	ARG	CD-NE	-10.61	1.31	1.46
1	R	80	ARG	CB-CG	-9.71	1.23	1.52
1	R	80	ARG	CG-CD	-9.65	1.23	1.52
1	Q	80	ARG	CZ-NH2	-9.63	1.21	1.33
1	O	80	ARG	CZ-NH1	-9.30	1.19	1.32
1	R	80	ARG	CD-NE	-9.20	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	79	ASP	C-O	-9.04	1.13	1.24
1	R	80	ARG	CZ-NH2	-8.67	1.22	1.33
1	O	80	ARG	CD-NE	-8.18	1.34	1.46
1	Q	80	ARG	NE-CZ	-7.85	1.24	1.33
1	Q	80	ARG	CD-NE	-7.70	1.35	1.46
1	Q	80	ARG	CG-CD	-6.91	1.31	1.52
1	P	80	ARG	NE-CZ	-6.84	1.25	1.33
1	O	80	ARG	NE-CZ	-6.57	1.25	1.33
1	R	80	ARG	C-O	6.08	1.33	1.24
1	Q	80	ARG	CA-C	5.84	1.60	1.52
1	R	80	ARG	NE-CZ	-5.81	1.26	1.33
1	Q	80	ARG	C-O	5.28	1.30	1.24
1	Q	80	ARG	CZ-NH1	-5.09	1.25	1.32
1	P	80	ARG	CG-CD	-5.08	1.37	1.52
1	Q	80	ARG	C-N	5.07	1.39	1.33

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	79	ASP	CA-C-O	-22.48	92.25	120.57
1	Q	79	ASP	O-C-N	17.12	148.98	122.96
1	Q	78	CYS	CA-C-N	-14.43	101.35	123.13
1	Q	78	CYS	C-N-CA	-14.43	101.35	123.13
1	Q	80	ARG	N-CA-C	13.18	138.87	110.80
1	A	209	VAL	N-CA-C	12.15	119.58	107.55
1	Q	79	ASP	CA-C-N	-10.81	100.89	121.54
1	Q	79	ASP	C-N-CA	-10.81	100.89	121.54
1	B	22	PHE	N-CA-C	-10.24	97.02	110.43
1	A	22	PHE	N-CA-C	-9.01	98.10	110.35
1	B	209	VAL	N-CA-C	8.99	117.84	107.77
1	Q	79	ASP	N-CA-CB	8.85	125.30	110.69
1	A	208	ILE	N-CA-C	-8.52	93.73	107.28
1	A	20	CYS	N-CA-C	-8.41	102.19	111.36
1	P	80	ARG	CG-CD-NE	-8.33	93.67	112.00
1	Q	79	ASP	CA-CB-CG	8.12	120.72	112.60
1	R	80	ARG	CD-NE-CZ	-7.96	113.26	124.40
1	B	208	ILE	N-CA-C	-7.95	94.64	107.28
1	B	85	LEU	N-CA-C	7.65	119.35	109.64
1	A	174	ILE	N-CA-C	-7.24	106.04	111.90
1	P	80	ARG	NE-CZ-NH2	-7.13	112.79	119.20
1	Q	80	ARG	CG-CD-NE	-6.91	96.79	112.00
1	R	37	THR	N-CA-C	-6.90	103.98	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	80	ARG	O-C-N	6.89	131.75	122.59
1	B	174	ILE	N-CA-C	-6.86	105.16	111.67
1	P	241	ASN	N-CA-C	6.81	121.47	111.87
1	A	28	ASP	N-CA-C	-6.55	104.86	112.92
1	Q	241	ASN	N-CA-C	6.43	120.78	112.41
1	O	320	TRP	N-CA-C	6.20	117.70	111.07
1	B	28	ASP	N-CA-C	-6.16	104.94	112.88
1	P	174	ILE	N-CA-C	-6.15	106.92	111.90
1	R	209	VAL	N-CA-C	6.13	114.63	107.77
1	O	28	ASP	N-CA-C	-6.12	105.12	112.59
1	R	80	ARG	CA-CB-CG	6.07	126.24	114.10
1	B	13	ILE	N-CA-C	6.02	116.20	110.42
1	P	28	ASP	N-CA-C	-5.98	105.16	112.88
1	O	209	VAL	N-CA-C	5.96	115.08	108.05
1	P	209	VAL	N-CA-C	5.95	115.07	108.05
1	R	241	ASN	N-CA-C	5.93	120.12	112.41
1	B	209	VAL	CA-C-N	5.79	125.55	119.76
1	B	209	VAL	C-N-CA	5.79	125.55	119.76
1	R	28	ASP	N-CA-C	-5.76	105.56	112.59
1	A	13	ILE	N-CA-C	5.76	115.94	110.53
1	B	144	HIS	N-CA-C	5.75	119.11	111.75
1	P	320	TRP	N-CA-C	5.71	117.36	111.03
1	P	129	GLY	N-CA-C	-5.70	107.16	114.85
1	O	223	ILE	CA-C-N	5.61	125.72	119.32
1	O	223	ILE	C-N-CA	5.61	125.72	119.32
1	P	80	ARG	CD-NE-CZ	-5.58	116.59	124.40
1	A	223	ILE	CA-C-N	5.54	126.77	119.84
1	A	223	ILE	C-N-CA	5.54	126.77	119.84
1	A	110	LYS	N-CA-C	-5.52	105.42	111.82
1	R	129	GLY	N-CA-C	-5.51	106.92	114.64
1	A	146	ASP	N-CA-C	5.49	116.94	111.07
1	B	99	THR	N-CA-C	-5.47	106.61	113.72
1	B	110	LYS	N-CA-C	-5.45	105.50	111.82
1	A	148	ALA	N-CA-C	-5.42	105.03	111.69
1	P	80	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	O	129	GLY	N-CA-C	-5.41	107.07	114.64
1	B	223	ILE	CA-C-N	5.38	125.71	119.47
1	B	223	ILE	C-N-CA	5.38	125.71	119.47
1	Q	129	GLY	N-CA-C	-5.37	107.12	114.64
1	O	241	ASN	N-CA-C	5.33	119.55	112.30
1	Q	209	VAL	N-CA-C	5.32	114.33	108.05
1	A	255	THR	N-CA-C	5.28	115.25	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ASN	CB-CA-C	-5.19	108.97	116.54
1	R	148	ALA	N-CA-C	-5.13	106.86	113.23
1	A	37	THR	N-CA-C	-5.12	105.39	113.02
1	B	37	THR	N-CA-C	-5.12	105.39	113.02
1	Q	28	ASP	N-CA-C	-5.10	106.37	112.59
1	Q	80	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	B	85	LEU	CA-C-N	5.07	126.17	119.84
1	B	85	LEU	C-N-CA	5.07	126.17	119.84
1	P	160	LEU	N-CA-C	5.05	116.60	111.14
1	A	159	CYS	N-CA-C	-5.01	106.86	113.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Q	80	ARG	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2451	0	2474	127	0
1	B	2451	0	2474	129	0
1	O	2451	0	2474	138	0
1	P	2451	0	2474	133	0
1	Q	2451	0	2474	160	0
1	R	2451	0	2474	145	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
3	A	68	0	0	4	0
3	B	87	0	0	4	0
3	O	61	0	0	5	0
3	P	57	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	19	0	0	5	0
3	R	25	0	0	0	0
All	All	15053	0	14844	769	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 26.

All (769) 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:Q:261:ASN:ND2	1:Q:299:SER:HB2	1.75	1.01
1:P:12:ARG:H	1:P:12:ARG:HD3	1.24	1.00
1:R:12:ARG:H	1:R:12:ARG:HD3	1.30	0.97
1:Q:12:ARG:HD3	1:Q:12:ARG:H	1.31	0.94
1:Q:250:GLN:HE21	1:R:250:GLN:HE21	1.11	0.93
1:Q:36:ASN:ND2	1:Q:37:THR:H	1.65	0.92
1:P:36:ASN:ND2	1:P:37:THR:H	1.68	0.91
1:Q:207:ASN:ND2	1:R:286:SER:HB2	1.87	0.89
1:A:206:VAL:HA	3:A:6423:HOH:O	1.71	0.89
1:Q:175:LYS:HE2	1:R:306:ASP:HB3	1.55	0.89
1:Q:261:ASN:HD22	1:Q:299:SER:HB2	1.35	0.87
1:O:36:ASN:ND2	1:O:37:THR:H	1.73	0.86
1:R:80:ARG:N	1:R:80:ARG:HD2	1.88	0.85
1:A:184:TYR:HA	1:A:236:ARG:HH21	1.41	0.84
1:R:144:HIS:CD2	1:R:337:SER:HA	2.12	0.84
1:R:12:ARG:HD3	1:R:12:ARG:N	1.93	0.84
1:B:171:PHE:CE1	1:B:255:THR:HG21	2.13	0.84
1:O:12:ARG:H	1:O:12:ARG:HD3	1.43	0.84
1:R:36:ASN:ND2	1:R:37:THR:H	1.77	0.83
1:R:80:ARG:NE	1:R:80:ARG:H	1.77	0.82
1:P:12:ARG:HD3	1:P:12:ARG:N	1.94	0.82
1:R:171:PHE:CE1	1:R:255:THR:HG21	2.13	0.82
1:R:80:ARG:HD2	1:R:80:ARG:C	2.03	0.81
1:Q:171:PHE:CE1	1:Q:255:THR:HG21	2.14	0.81
1:B:252:GLU:HG3	1:O:143:ARG:HH12	1.44	0.81
1:P:63:ASP:CG	1:P:64:GLU:H	1.90	0.80
1:P:99:THR:OG1	1:P:101:VAL:HG12	1.81	0.80
1:Q:250:GLN:NE2	1:R:250:GLN:HE21	1.79	0.80
1:A:171:PHE:CE1	1:A:255:THR:HG21	2.16	0.79
1:O:12:ARG:HD3	1:O:12:ARG:N	1.98	0.79
1:B:19:ARG:NH2	1:B:50:ASP:HB2	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:207:ASN:HD21	1:R:286:SER:HB2	1.48	0.78
1:A:21:TRP:HH2	1:A:72:LYS:NZ	1.80	0.78
1:A:184:TYR:HA	1:A:236:ARG:NH2	1.99	0.78
1:Q:12:ARG:HD3	1:Q:12:ARG:N	1.99	0.78
1:O:174:ILE:O	1:O:229:LYS:HE2	1.84	0.77
1:A:82:PRO:HA	1:A:85:LEU:HD12	1.66	0.77
1:A:162:PRO:HB3	1:A:272:MET:HE2	1.67	0.77
1:B:59:ASP:H	1:B:70:ASN:HD21	1.30	0.77
1:O:1:MET:HG2	1:O:2:THR:HG22	1.66	0.77
1:O:250:GLN:HE21	1:P:250:GLN:HE21	1.34	0.76
1:Q:80:ARG:HE	1:Q:80:ARG:HA	1.50	0.76
1:B:204:ALA:HB2	3:B:6451:HOH:O	1.85	0.76
1:P:171:PHE:CE1	1:P:255:THR:HG21	2.21	0.76
1:B:184:TYR:HA	1:B:236:ARG:HH21	1.50	0.75
1:Q:261:ASN:ND2	1:Q:299:SER:CB	2.49	0.74
1:Q:80:ARG:HE	1:Q:80:ARG:CA	1.96	0.74
1:Q:15:ARG:HD2	3:Q:6466:HOH:O	1.87	0.74
1:A:43:ALA:HB3	1:A:67:ILE:HD11	1.68	0.74
1:O:182:HIS:HB2	1:O:236:ARG:HD3	1.70	0.73
1:O:204:ALA:O	1:O:238:PRO:HG3	1.88	0.73
1:R:85:LEU:HD13	1:R:87:TRP:CZ2	2.23	0.73
1:P:63:ASP:CG	1:P:64:GLU:N	2.45	0.73
1:R:174:ILE:O	1:R:229:LYS:HE2	1.89	0.73
1:B:43:ALA:HB3	1:B:67:ILE:HD11	1.70	0.73
1:A:59:ASP:H	1:A:70:ASN:HD21	1.34	0.72
1:P:225:GLU:HG3	3:P:6371:HOH:O	1.88	0.72
1:P:16:ASN:OD1	1:P:53:LEU:HD11	1.88	0.72
1:R:80:ARG:H	1:R:80:ARG:CD	2.02	0.72
1:Q:63:ASP:CG	1:Q:64:GLU:H	1.97	0.72
1:O:207:ASN:ND2	1:P:286:SER:HB2	2.05	0.71
1:A:285:SER:OG	1:B:208:ILE:HB	1.91	0.71
1:Q:277:LYS:HB2	1:Q:293:GLU:HG2	1.72	0.71
1:R:12:ARG:H	1:R:12:ARG:CD	2.03	0.71
1:B:184:TYR:HA	1:B:236:ARG:NH2	2.04	0.71
1:Q:306:ASP:HB3	1:R:175:LYS:HE2	1.71	0.71
1:R:80:ARG:N	1:R:80:ARG:CD	2.47	0.71
1:A:256:ILE:HB	1:O:106:GLU:OE1	1.89	0.71
1:O:171:PHE:CE1	1:O:255:THR:HG21	2.26	0.70
1:O:144:HIS:CD2	1:O:337:SER:HA	2.26	0.70
1:R:16:ASN:OD1	1:R:53:LEU:HD11	1.91	0.70
1:P:37:THR:HB	3:P:6382:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:63:ASP:CG	1:O:64:GLU:H	1.99	0.69
1:R:99:THR:OG1	1:R:101:VAL:HG12	1.92	0.69
1:R:277:LYS:HB2	1:R:293:GLU:HG2	1.75	0.69
1:P:144:HIS:CD2	1:P:337:SER:HA	2.28	0.69
1:P:182:HIS:HB2	1:P:236:ARG:HD3	1.75	0.69
1:Q:63:ASP:CG	1:Q:64:GLU:N	2.49	0.69
1:Q:182:HIS:HB2	1:Q:236:ARG:HD3	1.74	0.69
1:A:309:LEU:HB2	1:B:175:LYS:HE2	1.74	0.68
1:A:103:VAL:HA	1:A:121:ILE:HD13	1.76	0.68
1:Q:144:HIS:CD2	1:Q:337:SER:HA	2.29	0.68
1:O:81:ASN:HD21	1:O:83:LEU:CD2	2.07	0.68
1:O:258:GLU:HB2	3:O:6361:HOH:O	1.92	0.68
1:B:59:ASP:H	1:B:70:ASN:ND2	1.92	0.67
1:P:12:ARG:H	1:P:12:ARG:CD	2.03	0.67
1:Q:81:ASN:HD21	1:Q:83:LEU:HD23	1.59	0.67
1:Q:265:GLN:O	1:Q:269:GLN:HG3	1.95	0.67
1:O:63:ASP:CG	1:O:64:GLU:N	2.52	0.67
1:B:286:SER:HB3	1:B:289:ARG:HH11	1.59	0.67
1:A:19:ARG:NH2	1:A:50:ASP:HB2	2.10	0.67
1:R:174:ILE:HD11	1:R:252:GLU:HB3	1.77	0.67
1:A:134:VAL:HG23	1:A:222:VAL:HG11	1.77	0.66
1:B:36:ASN:ND2	1:B:37:THR:H	1.93	0.66
1:R:161:ALA:HB3	1:R:162:PRO:HD3	1.77	0.66
1:O:145:GLU:CD	1:O:145:GLU:H	2.03	0.66
1:Q:174:ILE:O	1:Q:229:LYS:HE2	1.95	0.66
1:A:36:ASN:ND2	1:A:37:THR:H	1.91	0.66
1:Q:286:SER:HB2	1:R:207:ASN:HD21	1.61	0.66
1:B:59:ASP:N	1:B:70:ASN:HD21	1.94	0.66
1:B:162:PRO:HB3	1:B:272:MET:HE2	1.78	0.66
1:O:207:ASN:HD21	1:P:286:SER:HB2	1.60	0.66
1:O:85:LEU:HD13	1:O:87:TRP:CZ2	2.30	0.66
1:Q:12:ARG:H	1:Q:12:ARG:CD	2.09	0.66
1:A:204:ALA:HB2	3:A:6561:HOH:O	1.95	0.66
1:O:128:GLU:HA	3:O:6601:HOH:O	1.94	0.66
1:Q:204:ALA:O	1:Q:238:PRO:HG3	1.96	0.66
1:R:204:ALA:O	1:R:238:PRO:HG3	1.96	0.65
1:Q:174:ILE:HD11	1:Q:252:GLU:HB3	1.76	0.65
1:R:81:ASN:HD21	1:R:83:LEU:HD23	1.62	0.65
1:O:99:THR:OG1	1:O:101:VAL:HG12	1.96	0.65
1:P:174:ILE:O	1:P:229:LYS:HE2	1.97	0.65
1:R:63:ASP:CG	1:R:64:GLU:H	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:HG23	1:B:240:PRO:HD2	1.77	0.64
1:P:174:ILE:HD11	1:P:252:GLU:HB3	1.80	0.64
1:Q:16:ASN:OD1	1:Q:53:LEU:HD11	1.97	0.64
1:O:95:VAL:CG1	1:O:119:VAL:HG22	2.28	0.64
1:B:21:TRP:CH2	1:B:72:LYS:NZ	2.66	0.64
1:Q:145:GLU:CD	1:Q:145:GLU:H	2.04	0.64
1:Q:250:GLN:HE21	1:R:250:GLN:NE2	1.89	0.64
1:P:95:VAL:CG1	1:P:119:VAL:HG22	2.28	0.64
1:B:103:VAL:HA	1:B:121:ILE:HD13	1.79	0.64
1:B:252:GLU:HG3	1:O:143:ARG:NH1	2.13	0.64
1:A:59:ASP:N	1:A:70:ASN:HD21	1.96	0.64
1:A:162:PRO:HB3	1:A:272:MET:CE	2.27	0.64
1:B:52:VAL:HG13	1:B:241:ASN:ND2	2.13	0.64
1:O:264:LEU:HD13	1:O:297:VAL:HG11	1.80	0.64
1:O:12:ARG:H	1:O:12:ARG:CD	2.12	0.63
1:O:16:ASN:OD1	1:O:53:LEU:HD11	1.99	0.63
1:P:36:ASN:ND2	1:P:37:THR:N	2.44	0.63
1:Q:95:VAL:CG1	1:Q:119:VAL:HG22	2.29	0.63
1:A:250:GLN:NE2	1:B:250:GLN:NE2	2.46	0.63
1:A:261:ASN:HD21	1:A:302:THR:CB	2.11	0.63
1:R:237:VAL:HG23	1:R:239:THR:HG23	1.79	0.63
1:O:75:LYS:HG3	3:O:6628:HOH:O	1.97	0.63
1:R:63:ASP:CG	1:R:64:GLU:N	2.57	0.63
1:Q:286:SER:HB2	1:R:207:ASN:ND2	2.14	0.63
1:R:264:LEU:HD13	1:R:297:VAL:HG11	1.81	0.63
1:Q:22:PHE:HE1	1:Q:72:LYS:HD2	1.64	0.63
1:P:143:ARG:HB2	1:P:146:ASP:OD1	1.98	0.63
1:Q:81:ASN:HD21	1:Q:83:LEU:CD2	2.10	0.63
1:Q:231:ASN:HB3	1:R:303:LEU:HD11	1.79	0.63
1:O:239:THR:HB	1:O:240:PRO:HD2	1.81	0.63
1:B:171:PHE:CD1	1:B:255:THR:HG21	2.34	0.62
1:R:265:GLN:O	1:R:269:GLN:HG3	1.99	0.62
1:B:144:HIS:CD2	1:B:337:SER:HA	2.34	0.62
1:R:144:HIS:HD2	1:R:337:SER:HA	1.61	0.62
1:O:215:ALA:O	1:O:219:VAL:HG23	1.98	0.62
1:B:2:THR:HG23	1:B:2:THR:O	2.00	0.62
1:B:81:ASN:HB3	1:B:84:ASN:HD22	1.65	0.62
1:O:182:HIS:HB2	1:O:236:ARG:CD	2.29	0.62
1:Q:99:THR:OG1	1:Q:101:VAL:HG12	1.99	0.62
1:B:126:LYS:O	1:B:127:ALA:HB3	1.99	0.61
1:O:272:MET:HG3	1:O:276:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:239:THR:HB	1:R:240:PRO:HD2	1.81	0.61
1:O:81:ASN:HD21	1:O:83:LEU:HD22	1.64	0.61
1:Q:80:ARG:CA	1:Q:80:ARG:NE	2.54	0.61
1:P:215:ALA:O	1:P:219:VAL:HG23	1.99	0.61
3:A:6433:HOH:O	1:O:106:GLU:HG3	2.00	0.61
1:O:250:GLN:NE2	1:P:250:GLN:HE21	1.98	0.61
1:R:182:HIS:HB2	1:R:236:ARG:HD3	1.82	0.61
1:A:59:ASP:H	1:A:70:ASN:ND2	1.98	0.61
1:O:39:ASP:OD1	1:O:41:ARG:HG2	2.01	0.61
1:Q:215:ALA:O	1:Q:219:VAL:HG23	2.01	0.61
1:A:144:HIS:CD2	1:A:337:SER:HA	2.36	0.61
1:O:306:ASP:HB3	1:P:175:LYS:HE2	1.83	0.61
1:R:215:ALA:O	1:R:219:VAL:HG23	2.00	0.61
1:R:80:ARG:HD2	1:R:81:ASN:N	2.15	0.61
1:Q:36:ASN:ND2	1:Q:37:THR:N	2.43	0.60
1:A:19:ARG:CZ	1:A:56:PHE:HB2	2.31	0.60
1:O:36:ASN:ND2	1:O:37:THR:N	2.48	0.60
1:A:81:ASN:HB3	1:A:84:ASN:ND2	2.15	0.60
1:A:239:THR:HG23	1:A:240:PRO:HD2	1.81	0.60
1:Q:85:LEU:HD13	1:Q:87:TRP:CZ2	2.36	0.60
1:B:270:THR:O	1:B:273:LYS:HB2	2.01	0.60
1:R:81:ASN:HD21	1:R:83:LEU:CD2	2.14	0.60
1:R:95:VAL:CG1	1:R:119:VAL:HG22	2.32	0.60
1:O:22:PHE:HE1	1:O:72:LYS:HD2	1.65	0.60
1:R:145:GLU:H	1:R:145:GLU:CD	2.09	0.60
1:R:183:SER:O	1:R:184:TYR:C	2.45	0.60
1:O:19:ARG:NH2	1:O:56:PHE:HB2	2.17	0.60
1:O:286:SER:HB2	1:P:207:ASN:ND2	2.17	0.59
1:Q:52:VAL:HG13	1:Q:241:ASN:ND2	2.16	0.59
1:R:35:ASN:HA	1:R:77:VAL:O	2.02	0.59
1:Q:210:PRO:HG3	1:R:315:TRP:HZ2	1.67	0.59
1:O:80:ARG:HH11	1:O:80:ARG:HG3	1.67	0.59
1:P:81:ASN:HD21	1:P:83:LEU:HD23	1.66	0.59
1:A:68:THR:HG23	1:A:73:THR:HG22	1.83	0.59
1:A:81:ASN:HB3	1:A:84:ASN:HD22	1.68	0.59
1:P:282:PRO:HA	3:P:6587:HOH:O	2.01	0.59
1:Q:182:HIS:HB2	1:Q:236:ARG:CD	2.32	0.59
1:O:12:ARG:HG2	1:O:13:ILE:H	1.68	0.59
1:P:241:ASN:HA	1:P:318:ASN:ND2	2.18	0.59
1:Q:80:ARG:HA	1:Q:80:ARG:NE	2.18	0.59
1:R:19:ARG:NH2	1:R:56:PHE:HB2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:41:ARG:HB3	1:Q:62:TYR:CE1	2.38	0.59
1:Q:35:ASN:HA	1:Q:77:VAL:O	2.02	0.59
1:B:183:SER:OG	1:B:239:THR:HG22	2.03	0.59
1:P:204:ALA:O	1:P:238:PRO:HG3	2.02	0.59
1:Q:264:LEU:HD13	1:Q:297:VAL:HG11	1.84	0.59
1:Q:210:PRO:HG3	1:R:315:TRP:CZ2	2.38	0.58
1:A:18:LEU:HD22	1:A:22:PHE:CE2	2.38	0.58
1:Q:161:ALA:HB3	1:Q:162:PRO:HD3	1.84	0.58
1:P:85:LEU:HD13	1:P:87:TRP:CZ2	2.38	0.58
1:A:12:ARG:HH22	1:A:50:ASP:CG	2.11	0.58
1:Q:261:ASN:HD22	1:Q:299:SER:CB	2.13	0.58
1:A:145:GLU:H	1:A:145:GLU:CD	2.11	0.58
1:O:81:ASN:C	1:O:81:ASN:HD22	2.11	0.58
1:Q:67:ILE:HG23	1:Q:76:ILE:CD1	2.34	0.58
1:P:182:HIS:HB2	1:P:236:ARG:CD	2.34	0.58
1:P:120:LEU:C	1:P:120:LEU:HD12	2.28	0.58
1:P:81:ASN:HD21	1:P:83:LEU:CD2	2.17	0.57
1:B:145:GLU:CD	1:B:145:GLU:H	2.11	0.57
1:A:255:THR:HG22	1:A:259:GLN:OE1	2.03	0.57
1:O:12:ARG:HG2	1:O:13:ILE:N	2.20	0.57
1:O:183:SER:O	1:O:184:TYR:C	2.47	0.57
1:O:250:GLN:HE21	1:P:250:GLN:NE2	2.01	0.57
1:R:266:LYS:NZ	1:R:270:THR:HG21	2.19	0.57
1:A:120:LEU:C	1:A:120:LEU:HD12	2.29	0.57
1:Q:209:VAL:HG13	1:R:284:VAL:CG1	2.35	0.57
1:O:41:ARG:HB3	1:O:62:TYR:CE1	2.40	0.57
1:P:22:PHE:HE1	1:P:72:LYS:HD2	1.69	0.57
1:Q:208:ILE:HB	1:R:285:SER:HB3	1.87	0.57
1:R:48:GLU:HB2	1:R:60:ILE:HD12	1.86	0.57
1:A:21:TRP:CH2	1:A:72:LYS:NZ	2.64	0.57
1:P:62:TYR:HA	1:P:67:ILE:HA	1.86	0.57
1:Q:183:SER:O	1:Q:184:TYR:C	2.48	0.57
1:Q:239:THR:HB	1:Q:240:PRO:HD2	1.84	0.57
1:A:126:LYS:O	1:A:127:ALA:HB3	2.04	0.57
1:O:67:ILE:HG23	1:O:76:ILE:CD1	2.34	0.57
1:P:255:THR:HG22	1:P:259:GLN:NE2	2.20	0.57
1:Q:229:LYS:O	1:R:305:MET:HE2	2.05	0.56
1:R:241:ASN:HA	1:R:318:ASN:ND2	2.20	0.56
1:B:89:GLU:OE1	1:B:89:GLU:N	2.36	0.56
1:P:183:SER:O	1:P:184:TYR:C	2.48	0.56
1:Q:175:LYS:CE	1:R:306:ASP:HB3	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:MET:HE1	1:A:180:THR:HB	1.87	0.56
1:O:206:VAL:C	1:O:207:ASN:HD22	2.13	0.56
1:Q:280:ASP:HA	1:Q:299:SER:OG	2.05	0.56
1:O:265:GLN:O	1:O:269:GLN:HG3	2.06	0.56
1:A:246:ASP:HA	1:A:313:ILE:HD13	1.87	0.56
1:R:143:ARG:HB2	1:R:146:ASP:OD1	2.06	0.56
1:P:81:ASN:HD22	1:P:82:PRO:CD	2.19	0.56
1:B:18:LEU:HD22	1:B:22:PHE:CE2	2.41	0.56
1:O:146:ASP:HB3	1:O:147:PHE:CE1	2.40	0.56
1:O:161:ALA:HB3	1:O:162:PRO:HD3	1.88	0.56
1:P:81:ASN:HD22	1:P:82:PRO:N	2.03	0.56
1:A:87:TRP:HA	1:A:87:TRP:HE3	1.71	0.56
1:Q:120:LEU:HD13	1:Q:150:ILE:HG13	1.88	0.56
1:A:87:TRP:HA	1:A:87:TRP:CE3	2.41	0.55
1:P:239:THR:HB	1:P:240:PRO:HD2	1.88	0.55
1:R:62:TYR:HA	1:R:67:ILE:HA	1.88	0.55
1:A:2:THR:O	1:A:2:THR:HG23	2.05	0.55
1:B:239:THR:HG23	1:B:240:PRO:CD	2.35	0.55
1:P:35:ASN:HA	1:P:77:VAL:O	2.06	0.55
1:A:159:CYS:HA	1:A:295:SER:HB2	1.89	0.55
1:P:303:LEU:C	1:P:303:LEU:HD23	2.32	0.55
1:A:4:ARG:HD3	1:A:91:ASP:O	2.05	0.55
1:A:256:ILE:HB	1:O:106:GLU:CD	2.32	0.55
1:Q:261:ASN:HD21	1:Q:299:SER:CA	2.19	0.55
1:A:171:PHE:CD1	1:A:255:THR:HG21	2.42	0.55
1:P:161:ALA:HB3	1:P:162:PRO:HD3	1.89	0.55
1:B:18:LEU:HD22	1:B:22:PHE:HE2	1.71	0.55
1:B:19:ARG:CZ	1:B:56:PHE:HB2	2.37	0.55
1:O:82:PRO:HB2	1:O:110:LYS:HB3	1.89	0.55
1:R:278:TYR:CE1	1:R:299:SER:HB3	2.41	0.55
1:B:246:ASP:HA	1:B:313:ILE:HD13	1.88	0.55
1:A:324:GLN:OE1	1:A:324:GLN:HA	2.07	0.55
1:P:156:THR:OG1	1:P:182:HIS:HE1	1.90	0.55
1:A:99:THR:OG1	1:A:101:VAL:HG22	2.06	0.54
1:B:81:ASN:HB3	1:B:84:ASN:ND2	2.22	0.54
1:B:237:VAL:HG23	1:B:239:THR:HB	1.89	0.54
1:Q:87:TRP:HA	1:Q:87:TRP:CE3	2.42	0.54
1:Q:143:ARG:HB2	1:Q:146:ASP:OD1	2.07	0.54
1:B:87:TRP:HA	1:B:87:TRP:CE3	2.42	0.54
1:Q:87:TRP:HA	1:Q:87:TRP:HE3	1.73	0.54
1:Q:241:ASN:HA	1:Q:318:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:19:ARG:NH2	1:Q:56:PHE:HB2	2.22	0.54
1:A:265:GLN:O	1:A:269:GLN:HG3	2.07	0.54
1:B:202:ARG:O	1:B:204:ALA:N	2.40	0.54
1:A:183:SER:OG	1:A:239:THR:HG22	2.08	0.54
1:B:87:TRP:HA	1:B:87:TRP:HE3	1.73	0.54
1:O:81:ASN:HD22	1:O:82:PRO:N	2.05	0.54
1:P:87:TRP:HE3	1:P:87:TRP:HA	1.73	0.54
1:R:82:PRO:HB2	1:R:110:LYS:HB3	1.90	0.54
1:A:63:ASP:OD1	1:A:64:GLU:N	2.40	0.54
1:P:10:PHE:CZ	1:P:18:LEU:HD12	2.43	0.54
1:P:216:ALA:HB3	3:P:6367:HOH:O	2.07	0.54
1:Q:9:GLY:HA3	1:Q:99:THR:HG22	1.90	0.54
1:R:324:GLN:OE1	1:R:324:GLN:HA	2.07	0.54
1:P:289:ARG:HH12	1:R:289:ARG:HH22	1.55	0.54
1:A:87:TRP:CE3	1:A:92:ILE:HG13	2.43	0.54
1:Q:277:LYS:HB2	1:Q:293:GLU:CG	2.38	0.53
1:B:59:ASP:N	1:B:70:ASN:ND2	2.55	0.53
1:O:95:VAL:HG13	1:O:119:VAL:HG22	1.91	0.53
1:O:286:SER:HB2	1:P:207:ASN:HD21	1.72	0.53
1:P:87:TRP:HA	1:P:87:TRP:CE3	2.43	0.53
1:Q:62:TYR:HA	1:Q:67:ILE:HA	1.89	0.53
1:B:156:THR:HB	2:B:2339:SO4:O3	2.07	0.53
1:R:270:THR:OG1	1:R:271:THR:N	2.42	0.53
1:B:87:TRP:CE3	1:B:92:ILE:HG13	2.43	0.53
1:A:239:THR:HG23	1:A:240:PRO:CD	2.38	0.53
1:B:261:ASN:HD21	1:B:302:THR:CB	2.21	0.53
1:A:237:VAL:HG23	1:A:239:THR:HB	1.91	0.53
1:B:254:PRO:HA	1:B:307:GLY:O	2.08	0.53
1:P:112:ILE:HA	1:P:116:ALA:O	2.08	0.53
1:Q:272:MET:HG3	1:Q:276:ILE:HD12	1.90	0.53
1:R:1:MET:HG2	1:R:2:THR:HG22	1.91	0.53
1:R:249:VAL:O	1:R:309:LEU:HD12	2.08	0.53
1:A:21:TRP:HH2	1:A:72:LYS:HZ2	1.39	0.53
1:P:81:ASN:HD22	1:P:81:ASN:C	2.17	0.53
1:P:264:LEU:HD13	1:P:297:VAL:HG11	1.91	0.53
1:B:64:GLU:OE2	1:B:64:GLU:HA	2.09	0.53
1:O:209:VAL:HG21	3:O:6496:HOH:O	2.08	0.53
1:P:237:VAL:HG23	1:P:239:THR:HG23	1.91	0.53
1:O:80:ARG:HH11	1:O:80:ARG:CG	2.20	0.53
1:A:67:ILE:HD12	1:A:76:ILE:HD11	1.91	0.52
1:B:4:ARG:HD3	1:B:91:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:277:LYS:HB2	1:O:293:GLU:HG2	1.91	0.52
1:P:88:LYS:HB3	1:P:115:GLY:HA3	1.91	0.52
1:Q:206:VAL:C	1:Q:207:ASN:HD22	2.16	0.52
1:B:19:ARG:HH22	1:B:50:ASP:HB2	1.73	0.52
1:Q:81:ASN:C	1:Q:81:ASN:HD22	2.17	0.52
1:Q:112:ILE:HA	1:Q:116:ALA:O	2.10	0.52
1:R:22:PHE:HE1	1:R:72:LYS:HD2	1.74	0.52
1:B:178:MET:HE1	1:B:180:THR:HB	1.91	0.52
1:O:303:LEU:C	1:O:303:LEU:HD23	2.35	0.52
1:P:19:ARG:NH2	1:P:56:PHE:HB2	2.23	0.52
1:Q:39:ASP:OD1	1:Q:41:ARG:HG2	2.09	0.52
1:R:303:LEU:C	1:R:303:LEU:HD23	2.34	0.52
1:O:241:ASN:HA	1:O:318:ASN:ND2	2.25	0.52
1:P:138:ASN:CG	1:P:222:VAL:HG12	2.35	0.52
1:B:160:LEU:HD22	1:B:178:MET:HE3	1.91	0.52
1:Q:208:ILE:CG1	1:R:239:THR:HG21	2.39	0.52
1:O:79:ASP:HB2	1:O:85:LEU:CD2	2.40	0.52
1:R:41:ARG:HB3	1:R:62:TYR:CE1	2.45	0.52
1:O:35:ASN:HA	1:O:77:VAL:O	2.09	0.52
1:O:48:GLU:HB2	1:O:60:ILE:HD12	1.91	0.52
1:A:94:LEU:HA	1:A:118:LYS:O	2.10	0.51
1:B:82:PRO:HA	1:B:85:LEU:HD12	1.92	0.51
1:P:103:VAL:HA	1:P:121:ILE:HD13	1.92	0.51
1:R:182:HIS:HB2	1:R:236:ARG:CD	2.39	0.51
1:R:289:ARG:HA	1:R:317:ASP:OD2	2.10	0.51
1:A:52:VAL:HG13	1:A:241:ASN:ND2	2.25	0.51
1:A:255:THR:CG2	1:A:259:GLN:OE1	2.58	0.51
1:B:211:THR:HG23	1:B:234:ALA:HB3	1.91	0.51
1:P:213:THR:HA	2:P:4339:SO4:O2	2.10	0.51
1:P:261:ASN:ND2	1:P:302:THR:OG1	2.36	0.51
1:R:266:LYS:HZ2	1:R:270:THR:HG21	1.74	0.51
1:O:24:ARG:HH11	1:O:24:ARG:HG3	1.76	0.51
1:Q:41:ARG:HB3	1:Q:62:TYR:CZ	2.45	0.51
1:Q:303:LEU:C	1:Q:303:LEU:HD23	2.34	0.51
1:A:202:ARG:O	1:A:204:ALA:N	2.43	0.51
1:P:81:ASN:HD22	1:P:82:PRO:HD2	1.76	0.51
1:A:11:GLY:HA2	1:A:15:ARG:HH21	1.74	0.51
1:A:59:ASP:N	1:A:70:ASN:ND2	2.57	0.51
1:O:254:PRO:HA	1:O:307:GLY:O	2.11	0.51
1:Q:12:ARG:HG2	1:Q:13:ILE:N	2.26	0.51
1:Q:81:ASN:HD22	1:Q:82:PRO:N	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:CE	1:B:306:ASP:HB3	2.40	0.51
1:B:134:VAL:HG23	1:B:222:VAL:HG11	1.91	0.51
1:P:39:ASP:OD1	1:P:41:ARG:HG2	2.10	0.51
1:P:41:ARG:HB3	1:P:62:TYR:CE1	2.46	0.51
1:R:112:ILE:HA	1:R:116:ALA:O	2.11	0.51
1:R:184:TYR:C	1:R:184:TYR:CD1	2.89	0.51
1:A:89:GLU:OE1	1:A:89:GLU:N	2.40	0.51
1:B:12:ARG:HH22	1:B:50:ASP:CG	2.19	0.51
1:P:182:HIS:HA	1:P:243:SER:OG	2.10	0.51
1:Q:248:VAL:HG11	1:R:248:VAL:HG11	1.93	0.51
1:Q:324:GLN:HA	1:Q:324:GLN:OE1	2.10	0.51
1:P:106:GLU:O	1:P:109:SER:HB2	2.11	0.50
1:Q:67:ILE:HG23	1:Q:76:ILE:HD11	1.93	0.50
1:Q:88:LYS:HB3	1:Q:115:GLY:HA3	1.93	0.50
1:A:39:ASP:OD1	1:A:41:ARG:HB3	2.10	0.50
1:Q:1:MET:HG2	1:Q:2:THR:HG22	1.94	0.50
1:Q:212:THR:HG22	1:Q:213:THR:N	2.25	0.50
1:R:67:ILE:HG23	1:R:76:ILE:CD1	2.41	0.50
1:O:182:HIS:HD2	1:O:236:ARG:HE	1.60	0.50
1:Q:10:PHE:CZ	1:Q:18:LEU:HD12	2.46	0.50
1:B:270:THR:OG1	1:B:271:THR:N	2.45	0.50
1:A:18:LEU:HD22	1:A:22:PHE:HE2	1.77	0.50
1:B:41:ARG:HA	1:B:62:TYR:HD1	1.76	0.50
1:P:62:TYR:HB2	1:P:67:ILE:HG22	1.93	0.50
1:P:277:LYS:HB2	1:P:293:GLU:HG2	1.94	0.50
1:R:12:ARG:HG2	1:R:13:ILE:N	2.27	0.50
1:A:117:LYS:NZ	3:A:6346:HOH:O	2.44	0.50
1:O:80:ARG:CG	1:O:80:ARG:NH1	2.65	0.50
1:Q:249:VAL:O	1:Q:309:LEU:HD12	2.12	0.50
1:P:278:TYR:CE1	1:P:299:SER:HB3	2.47	0.50
1:B:286:SER:HA	1:B:289:ARG:HD3	1.93	0.49
1:O:87:TRP:HE3	1:O:87:TRP:HA	1.77	0.49
1:O:237:VAL:HG23	1:O:239:THR:HG23	1.94	0.49
1:Q:48:GLU:HB2	1:Q:60:ILE:HD12	1.93	0.49
1:R:120:LEU:HD13	1:R:150:ILE:HG13	1.94	0.49
1:Q:261:ASN:HD21	1:Q:299:SER:HB2	1.70	0.49
1:R:39:ASP:OD1	1:R:41:ARG:HG2	2.11	0.49
1:R:134:VAL:HG23	1:R:222:VAL:HG11	1.93	0.49
1:A:175:LYS:NZ	1:A:250:GLN:OE1	2.45	0.49
1:O:52:VAL:HG13	1:O:241:ASN:ND2	2.26	0.49
1:P:24:ARG:HG3	1:P:24:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:184:TYR:C	1:P:184:TYR:CD1	2.89	0.49
1:A:41:ARG:HA	1:A:62:TYR:HD1	1.78	0.49
1:A:59:ASP:O	1:A:69:VAL:HA	2.12	0.49
1:A:120:LEU:HD12	1:A:121:ILE:N	2.28	0.49
1:B:59:ASP:O	1:B:69:VAL:HA	2.12	0.49
1:B:162:PRO:HB3	1:B:272:MET:CE	2.41	0.49
1:O:41:ARG:HB3	1:O:62:TYR:CZ	2.48	0.49
1:O:87:TRP:HA	1:O:87:TRP:CE3	2.47	0.49
1:Q:317:ASP:O	1:Q:318:ASN:C	2.55	0.49
1:A:317:ASP:O	1:A:318:ASN:C	2.56	0.49
1:B:277:LYS:HB3	1:B:296:ILE:HG23	1.93	0.49
1:O:62:TYR:HA	1:O:67:ILE:HA	1.95	0.49
1:O:146:ASP:HB3	1:O:147:PHE:CD1	2.48	0.49
1:P:294:SER:HG	1:P:325:ARG:HH11	1.59	0.49
1:R:171:PHE:CD1	1:R:255:THR:HG21	2.47	0.49
1:R:317:ASP:O	1:R:318:ASN:C	2.56	0.49
1:A:68:THR:CG2	1:A:73:THR:HG22	2.43	0.49
1:O:249:VAL:O	1:O:309:LEU:HD12	2.12	0.49
1:B:334:ALA:C	1:B:336:LYS:H	2.21	0.49
1:P:1:MET:HG2	1:P:2:THR:HG22	1.93	0.49
1:Q:266:LYS:HZ2	1:Q:270:THR:HG21	1.78	0.49
1:R:277:LYS:HB2	1:R:293:GLU:CG	2.42	0.49
1:O:67:ILE:HG23	1:O:76:ILE:HD11	1.93	0.49
1:O:335:ARG:NH2	3:O:6627:HOH:O	2.45	0.49
1:Q:81:ASN:HD22	1:Q:82:PRO:CD	2.26	0.49
1:R:10:PHE:CZ	1:R:18:LEU:HD12	2.48	0.49
1:P:265:GLN:O	1:P:269:GLN:HG3	2.12	0.48
1:R:41:ARG:HB3	1:R:62:TYR:CZ	2.48	0.48
1:B:255:THR:HG22	1:B:259:GLN:OE1	2.13	0.48
1:P:1:MET:HE2	1:P:2:THR:HG22	1.95	0.48
1:Q:24:ARG:HD3	3:Q:6401:HOH:O	2.12	0.48
1:R:52:VAL:HG13	1:R:241:ASN:ND2	2.28	0.48
1:A:280:ASP:HA	1:A:299:SER:OG	2.14	0.48
1:P:145:GLU:H	1:P:145:GLU:CD	2.20	0.48
1:Q:250:GLN:NE2	1:R:250:GLN:NE2	2.55	0.48
1:R:82:PRO:HB2	1:R:110:LYS:CB	2.42	0.48
1:A:248:VAL:HG11	1:B:248:VAL:HG11	1.96	0.48
1:O:261:ASN:ND2	1:O:302:THR:OG1	2.44	0.48
1:A:308:ASP:OD2	1:B:175:LYS:HE3	2.13	0.48
1:P:48:GLU:HB2	1:P:60:ILE:HD12	1.95	0.48
1:R:62:TYR:HB2	1:R:67:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:317:ASP:O	1:O:318:ASN:C	2.55	0.48
1:P:1:MET:HE2	1:P:2:THR:CG2	2.44	0.48
1:P:12:ARG:HG2	1:P:13:ILE:N	2.28	0.48
1:R:216:ALA:HB1	1:R:231:ASN:HA	1.95	0.48
1:A:42:THR:O	1:A:46:LEU:HG	2.13	0.48
1:B:317:ASP:O	1:B:318:ASN:C	2.56	0.48
1:O:82:PRO:HB2	1:O:110:LYS:CB	2.44	0.48
1:O:10:PHE:CZ	1:O:18:LEU:HD12	2.49	0.48
1:Q:77:VAL:HG23	3:Q:6376:HOH:O	2.13	0.48
1:Q:36:ASN:HD22	1:Q:37:THR:H	1.54	0.48
1:Q:266:LYS:NZ	1:Q:270:THR:HG21	2.29	0.48
1:R:272:MET:HG3	1:R:276:ILE:HD12	1.94	0.48
1:A:315:TRP:HZ2	1:B:210:PRO:CG	2.27	0.48
1:A:250:GLN:HE21	1:B:250:GLN:HE22	1.61	0.47
1:A:334:ALA:C	1:A:336:LYS:H	2.21	0.47
1:O:255:THR:O	1:O:307:GLY:HA2	2.14	0.47
1:P:120:LEU:HD13	1:P:150:ILE:HG13	1.96	0.47
1:P:317:ASP:O	1:P:318:ASN:C	2.57	0.47
1:R:12:ARG:HG2	1:R:13:ILE:H	1.78	0.47
1:R:24:ARG:HG3	1:R:24:ARG:HH11	1.80	0.47
1:O:184:TYR:C	1:O:184:TYR:CD1	2.92	0.47
1:Q:184:TYR:C	1:Q:184:TYR:CD1	2.93	0.47
1:R:81:ASN:HD22	1:R:82:PRO:N	2.12	0.47
1:B:247:LEU:O	1:B:311:LYS:HA	2.14	0.47
1:O:278:TYR:CE1	1:O:299:SER:HB3	2.49	0.47
1:Q:56:PHE:HD2	1:Q:60:ILE:HD11	1.79	0.47
1:A:10:PHE:CZ	1:A:18:LEU:HD12	2.50	0.47
1:A:83:LEU:HD13	1:A:110:LYS:HB3	1.97	0.47
1:B:117:LYS:NZ	3:B:6553:HOH:O	2.46	0.47
1:B:240:PRO:HG2	1:B:241:ASN:H	1.79	0.47
1:P:10:PHE:CE1	1:P:18:LEU:HD12	2.49	0.47
1:P:12:ARG:HG2	1:P:13:ILE:H	1.80	0.47
1:P:206:VAL:C	1:P:207:ASN:HD22	2.23	0.47
1:Q:1:MET:HE2	1:Q:2:THR:HG22	1.97	0.47
1:Q:44:ALA:HB2	1:Q:62:TYR:HB3	1.96	0.47
1:Q:55:ARG:HB3	3:Q:6444:HOH:O	2.15	0.47
1:R:17:PHE:CE2	1:R:326:VAL:HG12	2.50	0.47
1:R:88:LYS:HB3	1:R:115:GLY:HA3	1.96	0.47
1:B:130:VAL:HG23	1:B:131:GLY:N	2.29	0.47
1:B:296:ILE:HD12	1:B:315:TRP:O	2.15	0.47
1:O:81:ASN:HD21	1:O:83:LEU:HD23	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:327:VAL:O	1:P:331:GLU:HB2	2.15	0.47
1:Q:209:VAL:HG13	1:R:284:VAL:HG12	1.94	0.47
1:A:315:TRP:HZ2	1:B:210:PRO:HG3	1.79	0.47
1:B:145:GLU:N	1:B:145:GLU:OE2	2.47	0.47
1:Q:67:ILE:HG23	1:Q:76:ILE:HD12	1.97	0.47
1:R:20:CYS:HB3	1:R:324:GLN:OE1	2.15	0.47
1:A:254:PRO:HA	1:A:307:GLY:O	2.15	0.46
1:O:212:THR:HG22	1:O:213:THR:N	2.30	0.46
1:R:56:PHE:HD2	1:R:60:ILE:HD11	1.80	0.46
1:B:322:TYR:O	1:B:326:VAL:HG23	2.14	0.46
1:O:19:ARG:CZ	1:O:56:PHE:HB2	2.45	0.46
1:P:289:ARG:HA	1:P:317:ASP:OD2	2.15	0.46
1:Q:82:PRO:HB2	1:Q:110:LYS:HB3	1.97	0.46
1:P:138:ASN:ND2	1:P:222:VAL:HG12	2.31	0.46
1:Q:82:PRO:HB2	1:Q:110:LYS:CB	2.45	0.46
1:R:3:ILE:HD13	1:R:334:ALA:HA	1.97	0.46
1:R:36:ASN:ND2	1:R:37:THR:N	2.55	0.46
1:A:89:GLU:H	1:A:89:GLU:CD	2.22	0.46
1:A:334:ALA:C	1:A:336:LYS:N	2.73	0.46
1:Q:62:TYR:HB2	1:Q:67:ILE:HG22	1.98	0.46
1:R:67:ILE:HG23	1:R:76:ILE:HD11	1.98	0.46
1:B:85:LEU:HD13	1:B:87:TRP:CZ2	2.50	0.46
1:Q:103:VAL:HG23	1:Q:126:LYS:HB2	1.97	0.46
1:R:261:ASN:ND2	1:R:302:THR:OG1	2.40	0.46
1:A:208:ILE:HB	1:B:285:SER:OG	2.15	0.46
1:B:119:VAL:CG1	1:B:149:VAL:HG22	2.46	0.46
1:P:160:LEU:HD12	1:P:160:LEU:O	2.16	0.46
1:A:296:ILE:HD12	1:A:315:TRP:O	2.15	0.46
1:P:21:TRP:HE1	1:P:27:THR:HG21	1.81	0.46
1:R:206:VAL:C	1:R:207:ASN:HD22	2.24	0.46
1:B:334:ALA:C	1:B:336:LYS:N	2.72	0.46
1:O:112:ILE:HA	1:O:116:ALA:O	2.16	0.46
1:O:209:VAL:HA	1:O:210:PRO:HD3	1.76	0.46
1:P:5:VAL:HG12	1:P:6:ALA:N	2.30	0.46
1:Q:177:THR:OG1	1:R:311:LYS:HD2	2.16	0.46
1:R:81:ASN:HD22	1:R:82:PRO:CD	2.29	0.46
1:R:255:THR:O	1:R:307:GLY:HA2	2.16	0.46
1:B:159:CYS:SG	1:B:316:TYR:HB3	2.56	0.46
1:A:332:LEU:HD22	1:A:336:LYS:HG3	1.97	0.45
1:B:139:ASP:OD1	1:B:139:ASP:N	2.49	0.45
1:O:156:THR:OG1	1:O:182:HIS:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:212:THR:HG22	1:P:213:THR:N	2.31	0.45
1:O:303:LEU:HD23	1:O:304:VAL:N	2.31	0.45
1:B:280:ASP:HA	1:B:299:SER:OG	2.16	0.45
1:O:56:PHE:HD2	1:O:60:ILE:HD11	1.81	0.45
1:P:95:VAL:HG13	1:P:119:VAL:HG22	1.98	0.45
1:P:249:VAL:O	1:P:309:LEU:HD12	2.15	0.45
1:Q:327:VAL:O	1:Q:331:GLU:HB2	2.17	0.45
1:A:17:PHE:CE2	1:A:326:VAL:HG12	2.51	0.45
1:P:255:THR:O	1:P:307:GLY:HA2	2.16	0.45
1:P:257:THR:HA	1:P:304:VAL:HG23	1.98	0.45
1:P:256:ILE:HG13	1:P:259:GLN:H	1.81	0.45
1:Q:126:LYS:O	1:Q:127:ALA:HB3	2.16	0.45
1:B:255:THR:HB	1:B:259:GLN:OE1	2.16	0.45
1:R:254:PRO:HA	1:R:307:GLY:O	2.16	0.45
1:B:39:ASP:OD1	1:B:41:ARG:HB3	2.16	0.45
1:B:159:CYS:HA	1:B:295:SER:HB2	1.99	0.45
1:B:161:ALA:O	1:B:165:LYS:HB2	2.17	0.45
1:Q:156:THR:OG1	1:Q:182:HIS:HE1	1.99	0.45
1:R:87:TRP:HA	1:R:87:TRP:HE3	1.82	0.45
1:R:280:ASP:HA	1:R:299:SER:OG	2.17	0.45
1:O:20:CYS:HB3	1:O:324:GLN:OE1	2.17	0.45
1:O:67:ILE:HG23	1:O:76:ILE:HD12	1.98	0.45
1:O:208:ILE:CG1	1:P:239:THR:HG21	2.47	0.45
1:Q:20:CYS:HB3	1:Q:324:GLN:OE1	2.16	0.45
1:Q:171:PHE:CD1	1:Q:255:THR:HG21	2.52	0.45
1:R:146:ASP:HB3	1:R:147:PHE:CD1	2.52	0.45
1:R:44:ALA:HB2	1:R:62:TYR:HB3	1.98	0.45
1:R:63:ASP:HB3	1:R:66:SER:O	2.17	0.45
1:B:324:GLN:HA	1:B:324:GLN:OE1	2.17	0.45
1:O:280:ASP:HA	1:O:299:SER:OG	2.17	0.45
1:R:303:LEU:HD23	1:R:304:VAL:N	2.31	0.45
1:A:88:LYS:HB3	1:A:89:GLU:OE1	2.18	0.44
1:O:106:GLU:O	1:O:109:SER:HB2	2.16	0.44
1:O:250:GLN:NE2	1:P:250:GLN:NE2	2.64	0.44
1:O:324:GLN:OE1	1:O:324:GLN:HA	2.16	0.44
1:P:20:CYS:HB3	1:P:324:GLN:OE1	2.17	0.44
1:P:265:GLN:HG3	1:P:278:TYR:CD2	2.52	0.44
1:Q:81:ASN:HD22	1:Q:82:PRO:HD2	1.82	0.44
1:Q:212:THR:CG2	1:Q:213:THR:N	2.80	0.44
1:R:81:ASN:HD22	1:R:82:PRO:HD2	1.82	0.44
1:A:77:VAL:CG2	1:A:78:CYS:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:O	1:A:242:VAL:C	2.60	0.44
1:B:255:THR:CG2	1:B:259:GLN:OE1	2.65	0.44
1:Q:41:ARG:HD3	3:Q:6624:HOH:O	2.15	0.44
1:Q:256:ILE:HG13	1:Q:259:GLN:H	1.83	0.44
1:A:286:SER:HB3	1:A:289:ARG:HH11	1.82	0.44
1:R:9:GLY:HA3	1:R:99:THR:HG22	1.98	0.44
1:A:24:ARG:NH1	1:A:324:GLN:OE1	2.50	0.44
1:O:79:ASP:HB2	1:O:85:LEU:HD21	2.00	0.44
1:O:182:HIS:CD2	1:O:236:ARG:HE	2.36	0.44
1:O:256:ILE:HG13	1:O:259:GLN:H	1.82	0.44
1:P:52:VAL:HG13	1:P:241:ASN:ND2	2.33	0.44
1:R:79:ASP:HB2	1:R:85:LEU:HD23	2.00	0.44
1:A:59:ASP:HB2	1:A:70:ASN:HD22	1.82	0.44
1:A:175:LYS:HE2	1:B:306:ASP:HB3	1.99	0.44
1:B:10:PHE:CZ	1:B:18:LEU:HD12	2.53	0.44
1:B:211:THR:CG2	1:B:234:ALA:HB3	2.48	0.44
1:B:265:GLN:O	1:B:269:GLN:HG3	2.18	0.44
1:P:324:GLN:OE1	1:P:324:GLN:HA	2.17	0.44
1:A:87:TRP:HB2	1:A:114:ALA:O	2.17	0.44
1:A:315:TRP:CZ2	1:B:210:PRO:HG3	2.53	0.44
1:B:334:ALA:O	1:B:336:LYS:N	2.51	0.44
1:P:4:ARG:HD3	1:P:91:ASP:O	2.18	0.44
1:P:17:PHE:CE2	1:P:326:VAL:HG12	2.52	0.44
1:Q:145:GLU:CD	1:Q:145:GLU:N	2.72	0.44
1:Q:261:ASN:HB3	1:Q:278:TYR:OH	2.18	0.44
1:Q:120:LEU:HD12	1:Q:120:LEU:C	2.43	0.44
1:A:277:LYS:HB3	1:A:296:ILE:HG23	1.99	0.43
1:B:21:TRP:HH2	1:B:72:LYS:NZ	2.13	0.43
1:O:175:LYS:HE2	1:P:306:ASP:HB3	1.99	0.43
1:Q:12:ARG:HG2	1:Q:13:ILE:H	1.81	0.43
1:R:87:TRP:HA	1:R:87:TRP:CE3	2.52	0.43
1:O:62:TYR:HB2	1:O:67:ILE:HG22	1.99	0.43
1:O:284:VAL:O	1:O:285:SER:C	2.61	0.43
1:O:134:VAL:HG23	1:O:222:VAL:HG11	2.01	0.43
1:P:56:PHE:HD2	1:P:60:ILE:HD11	1.83	0.43
1:P:182:HIS:HD2	1:P:236:ARG:HE	1.65	0.43
1:Q:37:THR:O	1:Q:37:THR:HG22	2.18	0.43
1:R:120:LEU:C	1:R:120:LEU:HD12	2.43	0.43
1:R:296:ILE:O	1:R:314:ALA:HA	2.17	0.43
1:A:50:ASP:OD1	1:A:53:LEU:HB2	2.17	0.43
1:B:68:THR:HG23	1:B:73:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ILE:HB	1:B:325:ARG:HD3	1.99	0.43
1:P:103:VAL:HG23	1:P:126:LYS:HB2	1.99	0.43
1:P:146:ASP:HB3	1:P:147:PHE:CD1	2.54	0.43
1:P:217:LYS:HE3	3:P:6492:HOH:O	2.16	0.43
1:Q:255:THR:O	1:Q:307:GLY:HA2	2.17	0.43
1:R:1:MET:HE2	1:R:2:THR:HG22	2.00	0.43
1:A:43:ALA:CB	1:A:67:ILE:HD11	2.43	0.43
1:A:204:ALA:O	1:A:238:PRO:HG3	2.18	0.43
1:Q:106:GLU:O	1:Q:109:SER:HB2	2.19	0.43
1:R:327:VAL:O	1:R:331:GLU:HB2	2.19	0.43
1:P:202:ARG:NH2	1:Q:51:SER:OG	2.52	0.43
1:P:270:THR:OG1	1:P:271:THR:N	2.49	0.43
1:P:296:ILE:O	1:P:314:ALA:HA	2.18	0.43
1:Q:254:PRO:HA	1:Q:307:GLY:O	2.18	0.43
1:R:209:VAL:HA	1:R:210:PRO:HD3	1.73	0.43
1:A:250:GLN:NE2	1:B:250:GLN:HE22	2.14	0.43
1:A:306:ASP:HB3	1:B:175:LYS:HE3	2.00	0.43
1:A:308:ASP:OD2	1:B:175:LYS:CE	2.67	0.43
1:Q:22:PHE:CE1	1:Q:72:LYS:HD2	2.49	0.43
1:Q:146:ASP:HB3	1:Q:147:PHE:CD1	2.54	0.43
1:R:211:THR:HG21	1:R:236:ARG:NE	2.33	0.43
1:B:291:THR:HG22	1:B:293:GLU:H	1.83	0.43
1:O:22:PHE:CE1	1:O:72:LYS:HD2	2.51	0.43
1:Q:294:SER:HG	1:Q:325:ARG:HH11	1.66	0.43
1:R:101:VAL:HG13	1:R:102:PHE:CD1	2.53	0.43
1:A:233:ILE:HD11	1:B:303:LEU:HD13	2.01	0.43
1:B:260:VAL:O	1:B:263:VAL:HG22	2.19	0.43
1:Q:207:ASN:CG	1:R:286:SER:HB2	2.43	0.43
1:O:22:PHE:CZ	1:O:69:VAL:HB	2.54	0.42
1:O:145:GLU:CD	1:O:145:GLU:N	2.75	0.42
1:A:112:ILE:HA	1:A:116:ALA:O	2.18	0.42
1:A:256:ILE:O	1:A:257:THR:C	2.62	0.42
1:A:334:ALA:O	1:A:336:LYS:N	2.52	0.42
1:B:118:LYS:HG3	1:B:119:VAL:N	2.34	0.42
1:O:259:GLN:O	1:O:263:VAL:HG13	2.19	0.42
1:P:212:THR:CG2	1:P:213:THR:N	2.82	0.42
1:R:10:PHE:CE1	1:R:18:LEU:HD12	2.54	0.42
1:B:113:GLN:C	1:B:115:GLY:H	2.26	0.42
1:Q:36:ASN:CG	1:Q:37:THR:H	2.23	0.42
1:Q:48:GLU:O	1:Q:55:ARG:HA	2.20	0.42
1:Q:209:VAL:HG13	1:R:284:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:79:ASP:HB2	1:R:85:LEU:CD2	2.49	0.42
1:B:121:ILE:HG22	1:B:123:ALA:H	1.83	0.42
1:O:69:VAL:O	1:O:70:ASN:C	2.60	0.42
1:O:79:ASP:HB2	1:O:85:LEU:HD23	2.02	0.42
1:O:211:THR:HG23	1:O:234:ALA:HB3	2.02	0.42
1:P:67:ILE:HG23	1:P:76:ILE:CD1	2.49	0.42
1:Q:24:ARG:HG3	1:Q:24:ARG:HH11	1.84	0.42
1:Q:268:SER:O	1:Q:273:LYS:HA	2.18	0.42
1:R:156:THR:OG1	1:R:182:HIS:HE1	2.02	0.42
1:Q:120:LEU:HD11	1:Q:329:LEU:HD23	2.01	0.42
1:Q:211:THR:HG21	1:Q:236:ARG:NE	2.35	0.42
1:Q:303:LEU:HD23	1:Q:304:VAL:N	2.34	0.42
1:A:137:VAL:HG13	1:A:165:LYS:HG3	2.01	0.42
1:A:175:LYS:HE2	1:B:308:ASP:OD2	2.20	0.42
1:B:204:ALA:O	1:B:238:PRO:HG3	2.20	0.42
1:B:209:VAL:HA	1:B:210:PRO:HD3	1.78	0.42
1:O:182:HIS:O	1:O:237:VAL:HG22	2.19	0.42
1:O:265:GLN:HG3	1:O:278:TYR:CD2	2.55	0.42
1:R:220:ALA:CB	1:R:227:LYS:HA	2.50	0.42
1:A:50:ASP:OD1	1:A:53:LEU:HD12	2.19	0.42
1:B:63:ASP:OD1	1:B:64:GLU:N	2.53	0.42
1:O:81:ASN:C	1:O:81:ASN:ND2	2.78	0.42
1:O:327:VAL:O	1:O:331:GLU:HB2	2.20	0.42
1:Q:10:PHE:CE1	1:Q:18:LEU:HD12	2.54	0.42
1:P:5:VAL:CG1	1:P:6:ALA:N	2.83	0.42
1:P:144:HIS:HD2	3:P:6357:HOH:O	2.03	0.42
1:Q:30:GLU:O	1:Q:32:VAL:HG13	2.19	0.42
1:Q:289:ARG:HA	1:Q:317:ASP:OD2	2.19	0.42
1:B:5:VAL:HG11	1:B:96:ILE:HD13	2.02	0.42
1:B:61:SER:OG	1:B:68:THR:HB	2.20	0.42
1:B:121:ILE:HG22	1:B:123:ALA:N	2.35	0.42
1:Q:18:LEU:HD23	1:Q:18:LEU:HA	1.90	0.42
1:Q:261:ASN:HD21	1:Q:299:SER:HA	1.85	0.42
1:R:37:THR:O	1:R:37:THR:HG22	2.19	0.42
1:A:130:VAL:HG23	1:A:131:GLY:N	2.35	0.41
1:B:178:MET:O	1:B:232:GLY:HA2	2.20	0.41
1:O:317:ASP:OD1	1:O:317:ASP:C	2.63	0.41
1:P:171:PHE:CD1	1:P:255:THR:HG21	2.55	0.41
1:P:280:ASP:HA	1:P:299:SER:OG	2.19	0.41
1:R:103:VAL:HG23	1:R:126:LYS:HB2	2.01	0.41
1:B:161:ALA:HB3	1:B:162:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASN:O	1:B:242:VAL:C	2.63	0.41
1:O:143:ARG:HB2	1:O:146:ASP:OD1	2.21	0.41
1:P:241:ASN:HA	1:P:318:ASN:HD22	1.85	0.41
1:Q:17:PHE:CE2	1:Q:326:VAL:HG12	2.55	0.41
1:Q:208:ILE:HD11	1:R:239:THR:HG21	2.00	0.41
1:R:211:THR:HG23	1:R:234:ALA:HB3	2.02	0.41
1:R:294:SER:HG	1:R:325:ARG:HH11	1.64	0.41
1:A:184:TYR:CA	1:A:236:ARG:NH2	2.77	0.41
1:A:241:ASN:HB2	1:A:242:VAL:H	1.52	0.41
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.88	0.41
3:B:6634:HOH:O	1:P:258:GLU:HB2	2.19	0.41
1:O:101:VAL:HG13	1:O:102:PHE:CD1	2.55	0.41
1:O:266:LYS:HZ2	1:O:270:THR:HG21	1.86	0.41
1:P:209:VAL:HA	1:P:210:PRO:HD3	1.69	0.41
1:Q:241:ASN:HA	1:Q:318:ASN:HD22	1.83	0.41
1:R:182:HIS:HA	1:R:243:SER:OG	2.19	0.41
1:O:266:LYS:NZ	1:O:270:THR:HG21	2.35	0.41
1:B:126:LYS:O	1:B:127:ALA:CB	2.63	0.41
1:B:143:ARG:NH2	1:O:252:GLU:OE1	2.53	0.41
1:O:95:VAL:HG11	1:O:111:HIS:HB3	2.01	0.41
1:O:103:VAL:HG23	1:O:126:LYS:HB2	2.02	0.41
1:P:22:PHE:CE1	1:P:72:LYS:HD2	2.53	0.41
1:R:81:ASN:HD22	1:R:81:ASN:C	2.29	0.41
1:B:40:ALA:HB3	1:B:63:ASP:O	2.20	0.41
1:P:36:ASN:HD22	1:P:37:THR:H	1.60	0.41
1:R:19:ARG:CZ	1:R:56:PHE:HB2	2.50	0.41
1:A:161:ALA:O	1:A:165:LYS:HB2	2.21	0.41
1:B:5:VAL:CG1	1:B:96:ILE:HD13	2.50	0.41
1:B:83:LEU:HD13	1:B:110:LYS:HG2	2.01	0.41
1:B:229:LYS:NZ	1:O:143:ARG:HH21	2.19	0.41
1:P:182:HIS:CD2	1:P:236:ARG:HE	2.39	0.41
1:Q:83:LEU:H	1:Q:83:LEU:HD22	1.86	0.41
1:R:5:VAL:HG12	1:R:6:ALA:N	2.35	0.41
1:R:256:ILE:HG13	1:R:259:GLN:H	1.85	0.41
1:A:247:LEU:O	1:A:311:LYS:HA	2.21	0.41
1:O:36:ASN:CG	1:O:37:THR:N	2.78	0.41
1:Q:182:HIS:O	1:Q:237:VAL:HG22	2.20	0.41
1:Q:182:HIS:HD2	1:Q:236:ARG:HE	1.68	0.41
1:Q:241:ASN:C	1:Q:318:ASN:ND2	2.79	0.41
1:Q:261:ASN:HD21	1:Q:299:SER:CB	2.26	0.41
1:A:82:PRO:HA	1:A:85:LEU:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:HB	1:A:259:GLN:OE1	2.20	0.41
1:A:270:THR:OG1	1:A:271:THR:N	2.54	0.41
1:B:16:ASN:HB3	1:B:323:SER:OG	2.20	0.41
1:B:25:GLN:NE2	1:B:26:ASN:H	2.18	0.41
1:O:10:PHE:CE1	1:O:18:LEU:HD12	2.56	0.41
1:O:30:GLU:O	1:O:32:VAL:HG13	2.21	0.41
1:O:239:THR:HG21	1:P:208:ILE:CG1	2.51	0.41
1:P:303:LEU:C	1:P:303:LEU:CD2	2.93	0.41
1:Q:95:VAL:HG13	1:Q:119:VAL:HG22	2.02	0.41
1:Q:175:LYS:HE2	1:R:306:ASP:CB	2.39	0.41
1:A:36:ASN:ND2	1:A:37:THR:N	2.65	0.41
1:O:36:ASN:CG	1:O:37:THR:H	2.28	0.41
1:P:82:PRO:HB2	1:P:110:LYS:CB	2.51	0.41
1:Q:36:ASN:CG	1:Q:37:THR:N	2.79	0.41
1:Q:103:VAL:HA	1:Q:121:ILE:HD13	2.02	0.41
1:A:241:ASN:HA	1:A:318:ASN:ND2	2.36	0.40
1:O:120:LEU:HD13	1:O:150:ILE:HG13	2.02	0.40
1:R:171:PHE:HE1	1:R:255:THR:HG21	1.78	0.40
1:R:325:ARG:NE	1:R:325:ARG:HA	2.36	0.40
1:B:112:ILE:HA	1:B:116:ALA:O	2.21	0.40
1:P:95:VAL:HG11	1:P:111:HIS:HB3	2.04	0.40
1:Q:52:VAL:HG13	1:Q:241:ASN:CG	2.45	0.40
1:R:155:CYS:HB3	1:R:322:TYR:HB2	2.03	0.40
1:B:25:GLN:HG3	3:B:6584:HOH:O	2.21	0.40
1:B:63:ASP:CG	1:B:64:GLU:N	2.79	0.40
1:O:50:ASP:C	1:O:52:VAL:H	2.28	0.40
1:P:92:ILE:O	1:P:116:ALA:HA	2.21	0.40
1:P:266:LYS:NZ	1:P:270:THR:HG21	2.37	0.40
1:Q:285:SER:HB3	1:R:208:ILE:HB	2.03	0.40
1:A:4:ARG:CD	1:A:91:ASP:O	2.69	0.40
1:A:113:GLN:C	1:A:115:GLY:H	2.30	0.40
1:A:244:VAL:HG23	1:A:314:ALA:O	2.21	0.40
1:B:277:LYS:HB2	1:B:293:GLU:CG	2.51	0.40
1:O:18:LEU:HA	1:O:18:LEU:HD23	1.91	0.40
1:O:216:ALA:HB1	1:O:231:ASN:HA	2.04	0.40
1:P:19:ARG:CZ	1:P:56:PHE:HB2	2.51	0.40
1:P:41:ARG:NH2	3:P:6476:HOH:O	2.53	0.40
1:Q:5:VAL:HG12	1:Q:6:ALA:N	2.35	0.40
1:Q:216:ALA:HB1	1:Q:231:ASN:HA	2.02	0.40
1:A:215:ALA:O	1:A:219:VAL:HG23	2.22	0.40
1:A:236:ARG:HE	1:A:236:ARG:HB3	1.63	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	318/380 (84%)	282 (89%)	28 (9%)	8 (2%)	4	17
1	B	318/380 (84%)	282 (89%)	28 (9%)	8 (2%)	4	17
1	O	318/380 (84%)	286 (90%)	25 (8%)	7 (2%)	5	20
1	P	318/380 (84%)	291 (92%)	21 (7%)	6 (2%)	6	23
1	Q	318/380 (84%)	284 (89%)	26 (8%)	8 (2%)	4	17
1	R	318/380 (84%)	287 (90%)	24 (8%)	7 (2%)	5	20
All	All	1908/2280 (84%)	1712 (90%)	152 (8%)	44 (2%)	5	19

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA
1	A	318	ASN
1	B	203	ALA
1	B	242	VAL
1	B	318	ASN
1	O	128	GLU
1	O	240	PRO
1	O	318	ASN
1	P	128	GLU
1	P	240	PRO
1	P	318	ASN
1	Q	80	ARG
1	Q	240	PRO
1	Q	318	ASN
1	R	240	PRO
1	R	318	ASN
1	A	183	SER

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Mol	Chain	Res	Type
1	A	242	VAL
1	B	183	SER
1	B	285	SER
1	O	203	ALA
1	O	307	GLY
1	P	203	ALA
1	Q	128	GLU
1	Q	203	ALA
1	R	128	GLU
1	R	203	ALA
1	A	240	PRO
1	A	285	SER
1	B	127	ALA
1	B	240	PRO
1	R	127	ALA
1	A	335	ARG
1	O	127	ALA
1	P	127	ALA
1	Q	127	ALA
1	Q	172	GLY
1	B	335	ARG
1	P	172	GLY
1	Q	307	GLY
1	R	172	GLY
1	O	172	GLY
1	R	307	GLY
1	A	172	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	269/321 (84%)	247 (92%)	22 (8%)	10	32
1	B	269/321 (84%)	248 (92%)	21 (8%)	11	35
1	O	269/321 (84%)	253 (94%)	16 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	269/321 (84%)	255 (95%)	14 (5%)	21	52
1	Q	269/321 (84%)	255 (95%)	14 (5%)	21	52
1	R	269/321 (84%)	257 (96%)	12 (4%)	24	58
All	All	1614/1926 (84%)	1515 (94%)	99 (6%)	17	46

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	GLN
1	A	62	TYR
1	A	74	MET
1	A	77	VAL
1	A	80	ARG
1	A	83	LEU
1	A	87	TRP
1	A	89	GLU
1	A	120	LEU
1	A	128	GLU
1	A	130	VAL
1	A	145	GLU
1	A	167	LEU
1	A	239	THR
1	A	241	ASN
1	A	245	VAL
1	A	262	GLU
1	A	294	SER
1	A	309	LEU
1	A	319	GLU
1	A	332	LEU
1	B	25	GLN
1	B	62	TYR
1	B	72	LYS
1	B	73	THR
1	B	74	MET
1	B	77	VAL
1	B	80	ARG
1	B	83	LEU
1	B	87	TRP
1	B	101	VAL
1	B	120	LEU

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Mol	Chain	Res	Type
1	B	128	GLU
1	B	130	VAL
1	B	167	LEU
1	B	239	THR
1	B	241	ASN
1	B	262	GLU
1	B	273	LYS
1	B	309	LEU
1	B	319	GLU
1	B	332	LEU
1	O	26	ASN
1	O	80	ARG
1	O	83	LEU
1	O	87	TRP
1	O	95	VAL
1	O	120	LEU
1	O	145	GLU
1	O	167	LEU
1	O	178	MET
1	O	209	VAL
1	O	258	GLU
1	O	263	VAL
1	O	271	THR
1	O	303	LEU
1	O	310	VAL
1	O	332	LEU
1	P	26	ASN
1	P	77	VAL
1	P	87	TRP
1	P	89	GLU
1	P	120	LEU
1	P	167	LEU
1	P	178	MET
1	P	209	VAL
1	P	258	GLU
1	P	263	VAL
1	P	271	THR
1	P	303	LEU
1	P	310	VAL
1	P	332	LEU
1	Q	26	ASN
1	Q	79	ASP

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Mol	Chain	Res	Type
1	Q	87	TRP
1	Q	89	GLU
1	Q	95	VAL
1	Q	145	GLU
1	Q	167	LEU
1	Q	178	MET
1	Q	258	GLU
1	Q	263	VAL
1	Q	271	THR
1	Q	303	LEU
1	Q	310	VAL
1	Q	332	LEU
1	R	80	ARG
1	R	87	TRP
1	R	89	GLU
1	R	167	LEU
1	R	178	MET
1	R	209	VAL
1	R	253	LYS
1	R	258	GLU
1	R	263	VAL
1	R	271	THR
1	R	310	VAL
1	R	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	36	ASN
1	A	65	ASN
1	A	70	ASN
1	A	84	ASN
1	A	144	HIS
1	A	158	ASN
1	A	182	HIS
1	A	261	ASN
1	A	265	GLN
1	B	25	GLN
1	B	36	ASN
1	B	65	ASN
1	B	70	ASN

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	144	HIS
1	B	158	ASN
1	B	241	ASN
1	B	261	ASN
1	B	265	GLN
1	O	36	ASN
1	O	81	ASN
1	O	84	ASN
1	O	144	HIS
1	O	152	ASN
1	O	158	ASN
1	O	182	HIS
1	O	207	ASN
1	O	259	GLN
1	O	261	ASN
1	O	265	GLN
1	P	36	ASN
1	P	81	ASN
1	P	84	ASN
1	P	144	HIS
1	P	158	ASN
1	P	182	HIS
1	P	207	ASN
1	P	250	GLN
1	P	259	GLN
1	P	261	ASN
1	P	265	GLN
1	Q	36	ASN
1	Q	45	HIS
1	Q	70	ASN
1	Q	81	ASN
1	Q	84	ASN
1	Q	144	HIS
1	Q	152	ASN
1	Q	158	ASN
1	Q	182	HIS
1	Q	207	ASN
1	Q	250	GLN
1	Q	259	GLN
1	Q	261	ASN
1	Q	265	GLN

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Mol	Chain	Res	Type
1	Q	318	ASN
1	R	36	ASN
1	R	81	ASN
1	R	152	ASN
1	R	158	ASN
1	R	182	HIS
1	R	207	ASN
1	R	259	GLN
1	R	261	ASN
1	R	265	GLN
1	R	269	GLN
1	R	318	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	2339	-	4,4,4	0.38	0	6,6,6	0.19	0
2	SO4	A	1339	-	4,4,4	0.37	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	O	3339	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	Q	5339	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	P	4339	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	R	6339	-	4,4,4	0.23	0	6,6,6	0.10	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2339	SO4	1	0
2	P	4339	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/380 (84%)	-0.07	3 (0%) 81 75	20, 43, 80, 92	0
1	B	322/380 (84%)	-0.16	3 (0%) 81 75	17, 40, 73, 91	0
1	O	322/380 (84%)	0.07	10 (3%) 51 42	19, 48, 80, 92	0
1	P	322/380 (84%)	0.19	13 (4%) 42 34	22, 52, 89, 92	0
1	Q	322/380 (84%)	0.64	8 (2%) 58 48	56, 85, 92, 92	0
1	R	322/380 (84%)	0.81	19 (5%) 28 22	43, 85, 92, 92	0
All	All	1932/2280 (84%)	0.25	56 (2%) 53 45	17, 61, 91, 92	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	45	HIS	5.2
1	A	338	GLY	4.7
1	R	173	ILE	3.3
1	O	338	GLY	3.3
1	P	183	SER	3.2
1	B	201	ALA	3.2
1	P	338	GLY	3.1
1	Q	80	ARG	3.1
1	O	201	ALA	3.1
1	P	337	SER	3.0
1	R	215	ALA	3.0
1	R	203	ALA	3.0
1	R	151	SER	2.9
1	O	89	GLU	2.8
1	R	337	SER	2.7
1	Q	140	SER	2.7
1	B	1	MET	2.7
1	P	51	SER	2.6
1	R	338	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	1	MET	2.6
1	Q	183	SER	2.5
1	Q	127	ALA	2.5
1	O	1	MET	2.5
1	R	251	VAL	2.4
1	R	64	GLU	2.4
1	P	37	THR	2.4
1	P	2	THR	2.4
1	O	44	ALA	2.4
1	P	38	SER	2.4
1	R	331	GLU	2.3
1	O	51	SER	2.3
1	O	57	ASN	2.3
1	B	184	TYR	2.3
1	P	127	ALA	2.3
1	P	80	ARG	2.3
1	O	241	ASN	2.2
1	Q	258	GLU	2.2
1	R	83	LEU	2.2
1	Q	201	ALA	2.2
1	O	66	SER	2.2
1	P	82	PRO	2.2
1	A	317	ASP	2.1
1	R	212	THR	2.1
1	R	145	GLU	2.1
1	Q	338	GLY	2.1
1	R	270	THR	2.1
1	R	58	ALA	2.1
1	P	1	MET	2.1
1	A	63	ASP	2.1
1	O	284	VAL	2.0
1	R	244	VAL	2.0
1	Q	9	GLY	2.0
1	R	132	THR	2.0
1	R	281	LEU	2.0
1	P	241	ASN	2.0
1	R	26	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	SO4	Q	5339	5/5	0.90	0.11	87,88,88,89	5
2	SO4	R	6339	5/5	0.90	0.10	64,67,68,68	5
2	SO4	O	3339	5/5	0.95	0.07	30,30,32,32	5
2	SO4	P	4339	5/5	0.96	0.09	45,46,48,49	5
2	SO4	B	2339	5/5	0.96	0.10	41,42,43,44	5
2	SO4	A	1339	5/5	0.96	0.09	29,30,33,34	5

6.5 Other polymers [i](#)

There are no such residues in this entry.