



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:29 PM UTC

PDB ID : 2YPQ / pdb_00002ypq
Title : 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase with tryptophan and tyrosine bound
Authors : Blackmore, N.J.; Reichau, S.; Jiao, W.; Hutton, R.D.; Baker, E.N.; Jameson, G.B.; Parker, E.J.
Deposited on : 2012-10-31
Resolution : 2.76 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

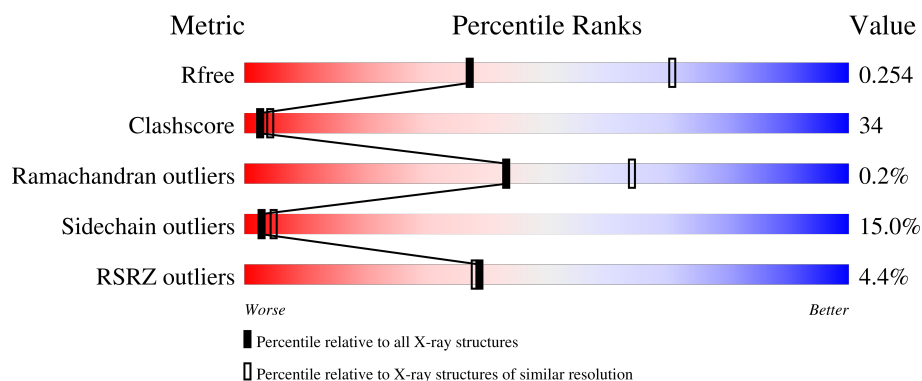
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	462	 5% 38% 48% 11% •
1	B	462	 4% 40% 46% 12% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	B	1468	-	-	X	-

2 Entry composition [i](#)

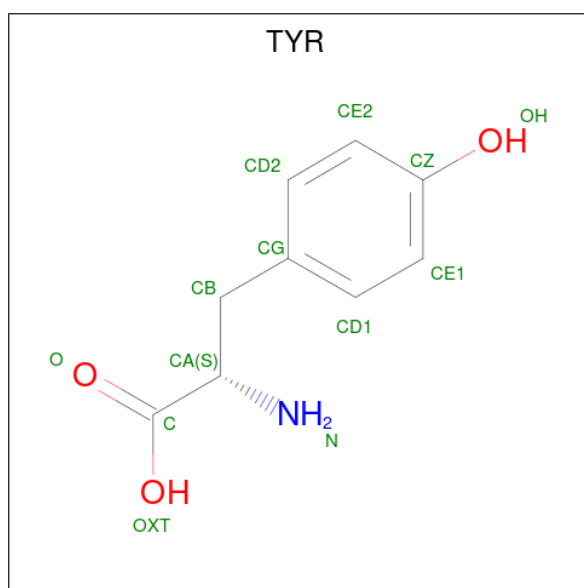
There are 9 unique types of molecules in this entry. The entry contains 7227 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE AROG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3514	2198	642	656	18			
1	B	457	Total	C	N	O	S	0	0	0
			3515	2194	640	663	18			

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).

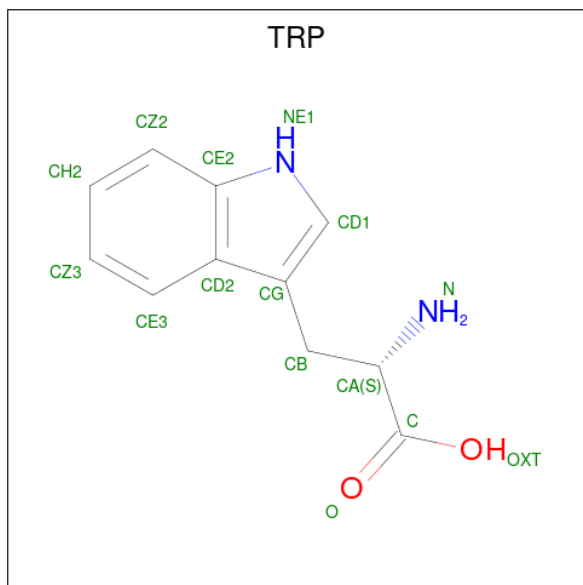


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

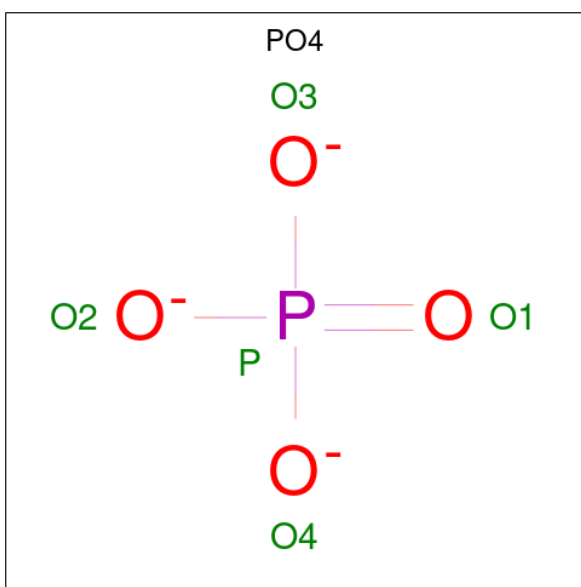
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



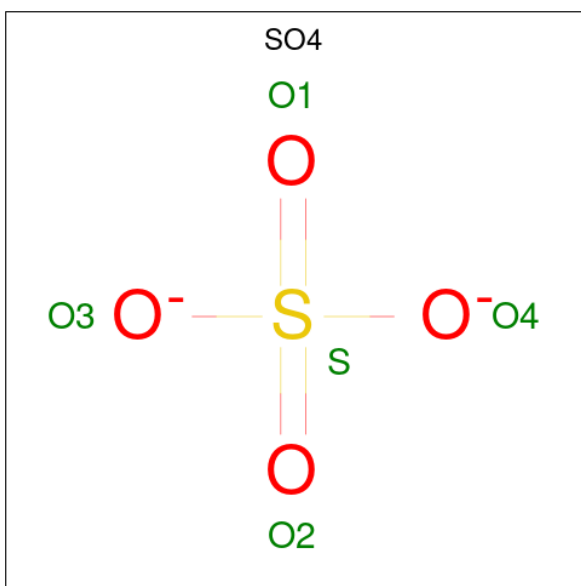
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).

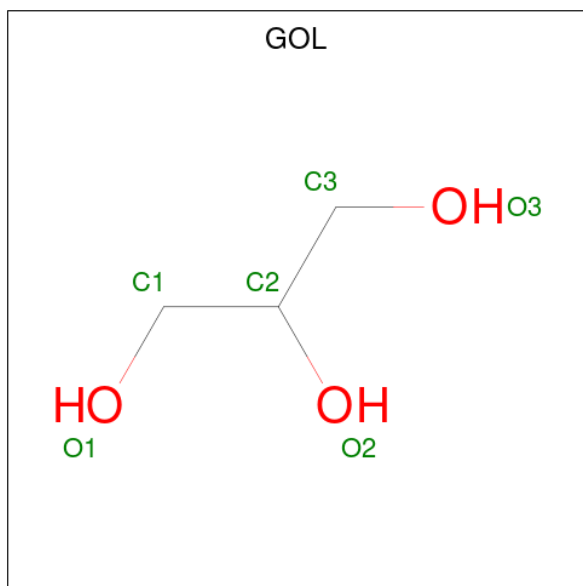


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

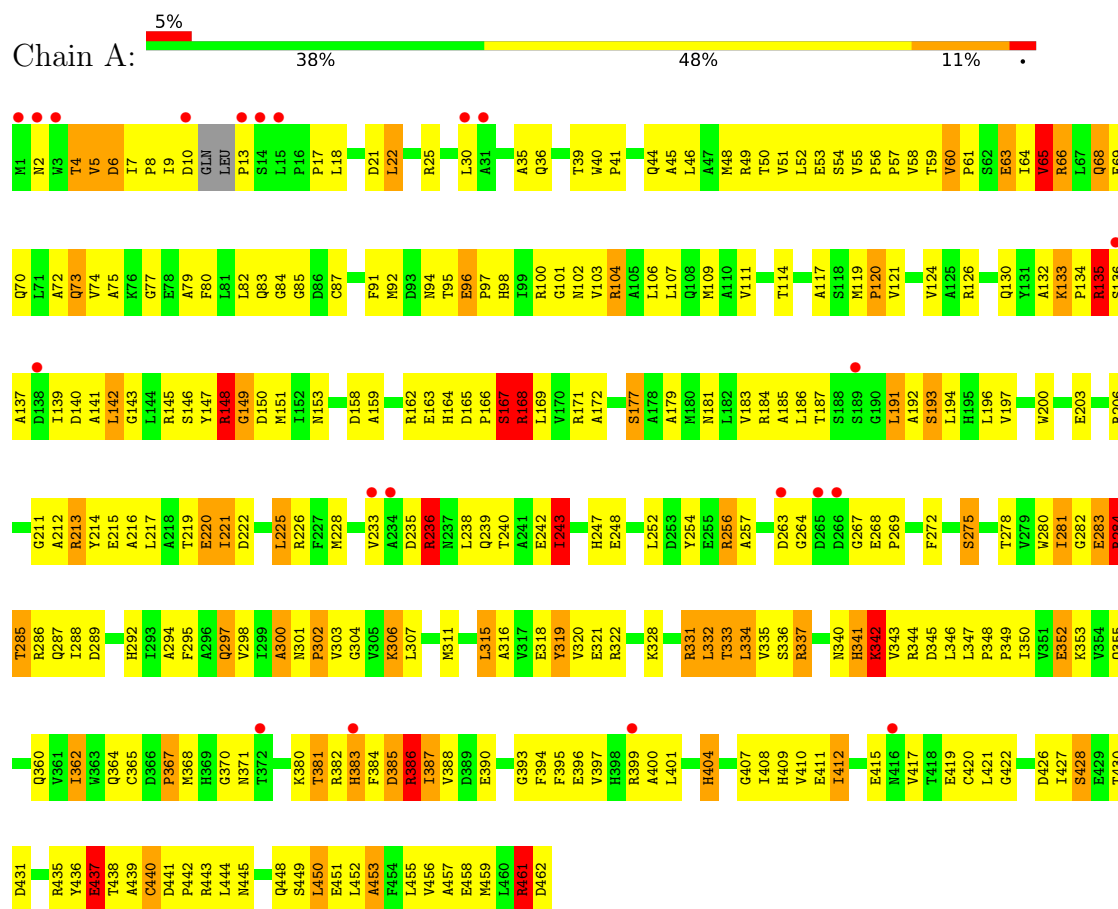
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	35	Total O 35 35	0	0
9	B	46	Total O 46 46	0	0

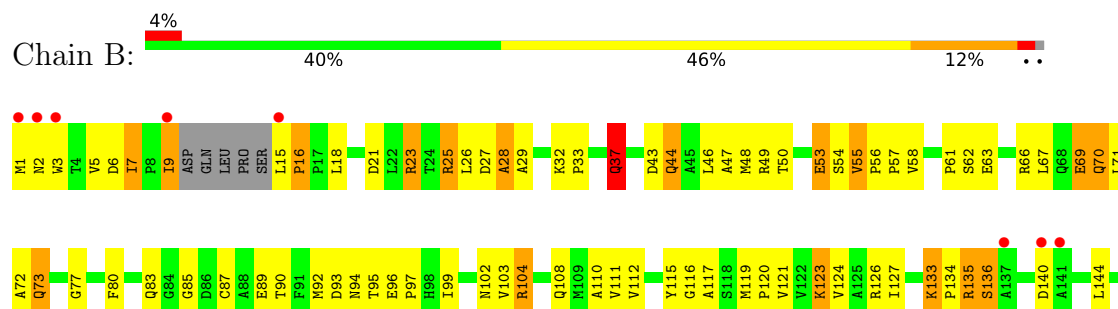
3 Residue-property plots

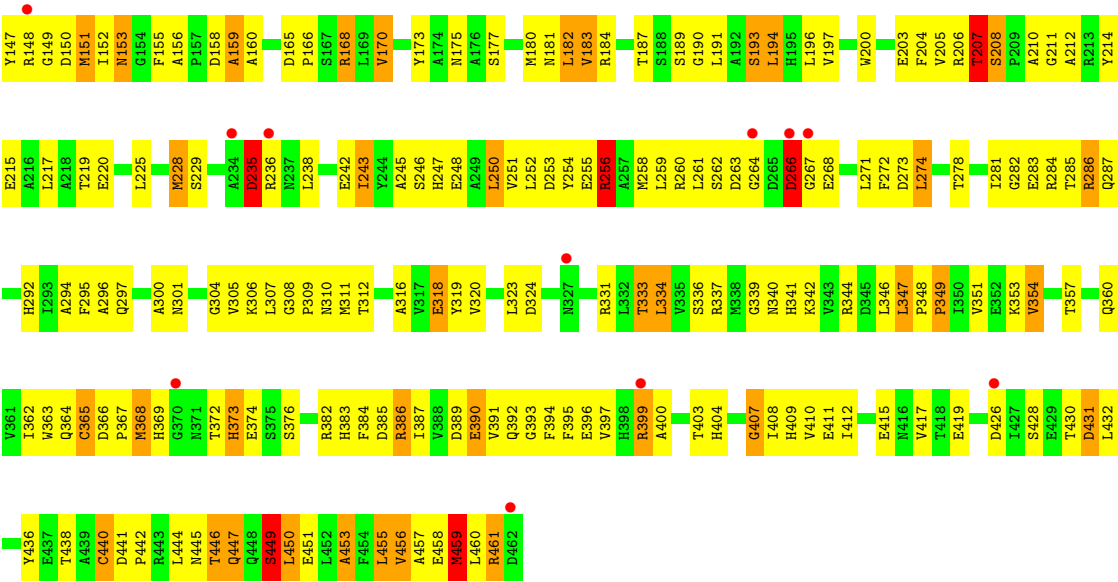
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE AROG



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE AROG





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	202.78Å 202.78Å 66.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	175.67 – 2.76 175.61 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.1 (175.67-2.76) 98.1 (175.61-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	27.88 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.249 0.199 , 0.254	Depositor DCC
R_{free} test set	2716 reflections (6.67%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7227	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: PO4, CL, GOL, SO4, MN

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	1.01	2/3587 (0.1%)	1.71	83/4881 (1.7%)
1	B	1.03	6/3587 (0.2%)	1.73	76/4879 (1.6%)
All	All	1.02	8/7174 (0.1%)	1.72	159/9760 (1.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	ASP	C-O	-6.58	1.17	1.23
1	A	57	PRO	N-CA	-5.56	1.41	1.46
1	B	207	THR	CA-C	5.22	1.60	1.52
1	B	334	LEU	C-O	-5.18	1.18	1.24
1	B	57	PRO	N-CA	-5.18	1.41	1.46
1	B	70	GLN	C-O	5.10	1.30	1.24
1	B	324	ASP	CA-C	-5.08	1.47	1.53
1	A	225	LEU	C-O	-5.07	1.18	1.24

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ALA	N-CA-C	-10.06	100.27	111.14
1	A	283	GLU	N-CA-C	-9.75	98.89	112.45
1	B	47	ALA	N-CA-C	-9.44	99.07	111.24
1	B	44	GLN	N-CA-C	-9.13	101.70	113.12
1	B	400	ALA	N-CA-C	-9.12	101.58	112.89
1	A	117	ALA	N-CA-C	-8.86	102.47	113.28
1	A	451	GLU	N-CA-C	-8.83	101.66	111.28
1	B	67	LEU	N-CA-C	-8.70	100.99	111.69
1	B	37	GLN	N-CA-C	-8.60	99.24	110.07
1	B	89	GLU	N-CA-C	-8.51	99.30	110.53
1	A	142	LEU	N-CA-C	-8.19	103.19	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	VAL	CB-CA-C	-8.17	101.33	112.04
1	B	295	PHE	N-CA-C	-8.06	102.44	111.14
1	B	456	VAL	N-CA-C	7.98	118.78	110.72
1	B	449	SER	CA-C-N	-7.86	109.95	120.63
1	B	449	SER	C-N-CA	-7.86	109.95	120.63
1	B	190	GLY	N-CA-C	7.75	123.00	114.40
1	B	58	VAL	CB-CA-C	-7.74	101.54	112.22
1	A	220	GLU	CA-C-N	-7.72	110.67	120.56
1	A	220	GLU	C-N-CA	-7.72	110.67	120.56
1	B	170	VAL	CB-CA-C	-7.72	100.77	111.65
1	B	349	PRO	N-CA-C	-7.71	103.24	113.65
1	B	449	SER	N-CA-C	-7.61	102.99	111.28
1	B	159	ALA	CA-C-O	7.59	129.42	120.92
1	A	300	ALA	N-CA-C	7.56	121.76	112.54
1	B	69	GLU	N-CA-C	-7.52	103.16	111.36
1	B	219	THR	N-CA-C	-7.46	103.22	111.36
1	A	167	SER	N-CA-C	-7.40	103.51	112.54
1	B	365	CYS	N-CA-C	7.28	120.87	107.99
1	B	208	SER	CA-C-N	7.25	126.87	119.19
1	B	208	SER	C-N-CA	7.25	126.87	119.19
1	B	431	ASP	CA-C-N	7.23	132.17	120.60
1	B	431	ASP	C-N-CA	7.23	132.17	120.60
1	A	60	VAL	N-CA-C	7.10	117.04	109.01
1	A	278	THR	N-CA-C	-7.10	98.28	109.50
1	A	135	ARG	N-CA-C	6.97	121.03	109.95
1	A	295	PHE	N-CA-C	-6.92	102.96	111.40
1	B	28	ALA	N-CA-C	-6.86	103.73	111.07
1	B	368	MET	N-CA-C	6.84	118.39	111.07
1	A	380	LYS	N-CA-C	-6.83	100.87	110.50
1	B	182	LEU	N-CA-C	-6.81	103.97	112.90
1	B	235	ASP	CB-CA-C	-6.81	102.40	113.37
1	B	455	LEU	CA-C-N	-6.78	110.80	120.42
1	B	455	LEU	C-N-CA	-6.78	110.80	120.42
1	B	318	GLU	N-CA-C	-6.70	104.06	111.36
1	A	206	ARG	N-CA-C	-6.66	103.27	111.33
1	A	272	PHE	N-CA-C	6.65	120.35	109.85
1	A	85	GLY	N-CA-C	-6.50	101.80	110.58
1	B	55	VAL	CA-C-N	6.47	127.04	120.38
1	B	55	VAL	C-N-CA	6.47	127.04	120.38
1	A	73	GLN	N-CA-C	-6.46	104.32	111.36
1	B	54	SER	N-CA-C	6.45	122.22	113.97
1	A	168	ARG	N-CA-C	-6.41	105.32	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	VAL	N-CA-C	-6.40	103.33	112.35
1	B	56	PRO	CB-CA-C	-6.39	103.12	110.92
1	B	120	PRO	CB-CA-C	-6.39	103.22	111.46
1	A	387	ILE	CB-CA-C	-6.35	103.56	111.94
1	B	266	ASP	N-CA-C	-6.32	104.67	112.38
1	B	134	PRO	CA-C-N	-6.30	112.79	122.62
1	B	134	PRO	C-N-CA	-6.30	112.79	122.62
1	B	312	THR	CB-CA-C	-6.27	99.47	108.88
1	A	333	THR	CA-C-O	-6.26	114.08	121.16
1	B	53	GLU	N-CA-C	-6.25	105.51	113.01
1	A	437	GLU	CB-CA-C	-6.23	101.41	111.06
1	A	94	ASN	N-CA-C	-6.22	100.28	109.62
1	A	162	ARG	CA-C-N	-6.21	112.05	120.87
1	A	162	ARG	C-N-CA	-6.21	112.05	120.87
1	B	450	LEU	N-CA-C	-6.21	104.13	111.03
1	B	183	VAL	CB-CA-C	-6.21	103.92	112.24
1	B	196	LEU	N-CA-C	-6.21	104.05	111.69
1	B	261	LEU	N-CA-C	-6.20	99.08	109.07
1	B	447	GLN	CA-CB-CG	-6.20	101.70	114.10
1	B	256	ARG	CA-C-N	6.16	128.44	120.44
1	B	256	ARG	C-N-CA	6.16	128.44	120.44
1	A	453	ALA	N-CA-C	-6.12	104.88	112.90
1	B	57	PRO	N-CA-C	-6.10	101.59	111.77
1	B	112	VAL	N-CA-C	-6.07	103.50	111.09
1	A	134	PRO	N-CA-C	-6.04	101.68	111.77
1	A	179	ALA	N-CA-C	-6.03	104.04	111.40
1	A	243	ILE	CB-CA-C	-6.02	103.17	110.99
1	A	236	ARG	N-CA-C	-5.98	104.84	111.71
1	B	407	GLY	CA-C-O	-5.97	115.66	121.75
1	B	459	MET	N-CA-C	-5.96	104.78	111.28
1	A	184	ARG	N-CA-C	5.94	118.27	111.02
1	B	153	ASN	N-CA-C	5.93	116.25	107.88
1	A	263	ASP	CB-CA-C	-5.90	100.65	110.68
1	A	455	LEU	N-CA-C	-5.90	104.98	111.82
1	B	50	THR	CA-CB-OG1	-5.87	100.80	109.60
1	A	390	GLU	N-CA-C	-5.85	104.98	111.36
1	A	461	ARG	CB-CA-C	-5.83	103.44	112.07
1	A	58	VAL	N-CA-C	-5.81	104.16	112.35
1	A	386	ARG	N-CA-C	-5.79	105.10	111.82
1	A	57	PRO	N-CA-C	-5.78	102.12	111.77
1	A	177	SER	CA-CB-OG	-5.77	99.56	111.10
1	A	320	VAL	CA-C-O	-5.77	115.05	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ASP	N-CA-C	-5.76	103.75	112.04
1	A	371	ASN	N-CA-C	5.72	119.58	112.59
1	A	101	GLY	CA-C-N	-5.71	112.63	120.28
1	A	101	GLY	C-N-CA	-5.71	112.63	120.28
1	B	46	LEU	CA-C-O	5.69	126.58	120.20
1	A	370	GLY	N-CA-C	5.68	120.71	114.40
1	A	225	LEU	CB-CA-C	-5.67	101.94	110.90
1	A	319	TYR	O-C-N	5.67	128.15	122.08
1	B	304	GLY	O-C-N	-5.67	118.15	123.25
1	B	324	ASP	CB-CA-C	-5.59	103.95	111.11
1	B	354	VAL	O-C-N	5.58	127.38	121.91
1	A	149	GLY	CA-C-O	-5.58	116.97	121.77
1	B	177	SER	CB-CA-C	-5.55	101.57	110.79
1	A	163	GLU	CB-CA-C	5.51	119.08	109.65
1	A	278	THR	CA-CB-OG1	5.49	117.83	109.60
1	B	347	LEU	CA-C-N	-5.49	114.73	120.38
1	B	347	LEU	C-N-CA	-5.49	114.73	120.38
1	A	114	THR	N-CA-C	5.48	116.93	111.07
1	B	151	MET	N-CA-C	-5.46	106.46	113.01
1	A	242	GLU	N-CA-C	-5.43	100.32	109.07
1	B	399	ARG	N-CA-C	-5.42	105.37	111.28
1	B	447	GLN	N-CA-C	5.41	118.67	111.75
1	A	148	ARG	N-CA-C	5.40	119.56	112.92
1	B	73	GLN	N-CA-C	-5.40	105.40	111.28
1	A	400	ALA	CA-C-N	-5.37	112.66	122.38
1	A	400	ALA	C-N-CA	-5.37	112.66	122.38
1	A	342	LYS	N-CA-C	5.37	119.52	112.92
1	B	69	GLU	CA-C-O	5.36	126.10	120.42
1	B	16	PRO	CB-CA-C	-5.35	104.39	110.92
1	A	63	GLU	N-CA-C	-5.34	105.62	111.82
1	B	324	ASP	CA-C-O	-5.32	115.96	121.07
1	A	65	VAL	N-CA-C	-5.30	104.47	111.09
1	A	50	THR	O-C-N	-5.29	116.52	122.12
1	A	298	VAL	N-CA-C	5.28	116.06	110.72
1	B	304	GLY	N-CA-C	5.25	120.38	111.19
1	B	253	ASP	N-CA-CB	5.23	117.90	110.16
1	A	66	ARG	N-CA-CB	-5.22	102.27	110.30
1	B	339	GLY	N-CA-C	-5.21	106.11	112.68
1	A	302	PRO	CB-CA-C	-5.21	105.02	111.64
1	A	263	ASP	N-CA-C	-5.20	105.03	111.33
1	A	106	LEU	N-CA-C	-5.20	105.53	111.14
1	B	453	ALA	CA-C-N	-5.17	113.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	ALA	C-N-CA	-5.17	113.56	120.54
1	A	56	PRO	CB-CA-C	-5.16	104.62	110.92
1	A	284	ARG	N-CA-C	5.16	119.44	113.20
1	A	221	ILE	N-CA-C	-5.16	105.68	110.53
1	A	191	LEU	CA-C-N	-5.14	115.00	122.86
1	A	191	LEU	C-N-CA	-5.14	115.00	122.86
1	A	272	PHE	CB-CA-C	-5.14	99.69	109.66
1	B	274	LEU	N-CA-C	-5.12	105.29	112.25
1	A	404	HIS	N-CA-C	5.11	116.11	109.72
1	A	102	ASN	N-CA-C	5.11	116.84	111.28
1	B	384	PHE	N-CA-C	-5.09	105.73	111.28
1	B	333	THR	N-CA-C	-5.08	101.99	110.17
1	A	59	THR	CB-CA-C	-5.07	100.47	111.11
1	A	121	VAL	CB-CA-C	-5.07	103.84	110.98
1	A	284	ARG	CA-C-N	-5.06	113.70	122.14
1	A	284	ARG	C-N-CA	-5.06	113.70	122.14
1	A	321	GLU	N-CA-CB	5.05	118.08	110.30
1	A	53	GLU	CB-CA-C	-5.05	100.51	110.11
1	A	135	ARG	CA-CB-CG	-5.04	104.02	114.10
1	A	318	GLU	N-CA-C	-5.03	105.80	111.28
1	A	120	PRO	CB-CA-C	-5.02	105.18	111.56
1	A	213	ARG	N-CA-C	-5.02	105.82	112.34

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	3514	0	3466	250	0
1	B	3515	0	3464	241	0
2	A	13	0	8	0	0
2	B	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	9	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	5	0	0	1	0
6	B	5	0	0	2	0
7	A	2	0	0	1	0
8	A	6	0	8	1	0
8	B	18	0	24	3	0
9	A	35	0	0	2	0
9	B	46	0	0	6	0
All	All	7227	0	7004	483	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 34.

All (483) 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:133:LYS:HE3	1:B:440:CYS:SG	1.67	1.33
1:B:21:ASP:O	1:B:25:ARG:HG3	1.39	1.22
1:B:150:ASP:O	1:B:168:ARG:HG2	1.37	1.20
1:B:228:MET:HE3	1:B:238:LEU:HD11	1.22	1.15
1:A:48:MET:CE	1:A:167:SER:HA	1.79	1.12
1:B:391:VAL:CG1	1:B:459:MET:HE1	1.82	1.09
1:B:391:VAL:HG12	1:B:459:MET:CE	1.84	1.07
1:A:332:LEU:HD21	1:A:334:LEU:HD21	1.36	1.07
1:A:30:LEU:HD12	1:A:256:ARG:NH2	1.67	1.06
1:A:148:ARG:HB3	1:A:148:ARG:NH1	1.69	1.04
1:B:151:MET:HE1	1:B:254:TYR:CD2	1.93	1.03
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.22	1.00
1:B:307:LEU:HD11	1:B:334:LEU:HD22	1.41	0.99
1:B:391:VAL:HG12	1:B:459:MET:HE1	1.42	0.98
1:B:228:MET:CE	1:B:238:LEU:HD11	1.94	0.97
1:A:133:LYS:NZ	1:A:440:CYS:SG	2.38	0.97
1:B:393:GLY:O	1:B:397:VAL:HG23	1.65	0.96
1:B:26:LEU:O	1:B:29:ALA:HB3	1.65	0.96
1:B:133:LYS:CE	1:B:440:CYS:SG	2.54	0.96
1:B:365:CYS:O	1:B:367:PRO:HD3	1.65	0.96
1:B:340:ASN:HB2	1:B:389:ASP:OD2	1.68	0.93
1:A:48:MET:HE2	1:A:167:SER:HA	1.48	0.92
1:B:250:LEU:HD12	1:B:250:LEU:O	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLY:HA2	1:A:404:HIS:CD2	2.04	0.92
1:B:194:LEU:HD12	1:B:238:LEU:HD22	1.52	0.90
1:B:99:ILE:O	1:B:103:VAL:HG23	1.71	0.90
1:B:382:ARG:HD2	1:B:442:PRO:HG2	1.51	0.90
1:A:226:ARG:NH2	7:A:1468:CL:CL	2.43	0.89
1:B:252:LEU:O	1:B:256:ARG:HB3	1.72	0.89
1:B:48:MET:HG3	1:B:166:PRO:O	1.72	0.89
1:B:150:ASP:O	1:B:168:ARG:CG	2.22	0.88
1:A:194:LEU:HD23	1:A:225:LEU:HD21	1.56	0.87
1:A:48:MET:HE3	1:A:167:SER:HA	1.56	0.85
1:B:135:ARG:HG3	6:B:1468:SO4:O2	1.77	0.84
1:A:228:MET:HE1	1:A:238:LEU:HD11	1.58	0.84
1:B:85:GLY:HA3	1:B:126:ARG:HB2	1.58	0.83
1:A:382:ARG:HD2	1:A:442:PRO:HG2	1.59	0.82
1:A:286:ARG:NH1	1:A:311:MET:HE1	1.94	0.82
1:A:148:ARG:HB3	1:A:148:ARG:HH11	1.44	0.81
1:A:303:VAL:HG22	1:A:331:ARG:HH11	1.44	0.81
1:A:303:VAL:HG22	1:A:331:ARG:NH1	1.95	0.81
1:A:30:LEU:CD1	1:A:256:ARG:NH2	2.44	0.80
1:B:242:GLU:OE1	8:B:1470:GOL:H31	1.80	0.80
1:B:7:ILE:O	1:B:9:ILE:HD12	1.82	0.80
1:B:21:ASP:O	1:B:25:ARG:CG	2.25	0.80
1:A:306:LYS:O	1:A:307:LEU:HD23	1.83	0.79
1:A:48:MET:HG3	1:A:166:PRO:O	1.82	0.79
1:A:168:ARG:HG2	1:A:168:ARG:NH1	1.97	0.78
1:A:252:LEU:O	1:A:256:ARG:HB3	1.82	0.78
1:B:395:PHE:O	1:B:399:ARG:HG2	1.83	0.78
1:B:391:VAL:HG12	1:B:459:MET:HE3	1.63	0.78
1:A:80:PHE:CE1	1:A:407:GLY:HA2	2.18	0.78
1:A:5:VAL:HG12	1:B:7:ILE:HD11	1.66	0.78
1:A:169:LEU:HD22	1:A:254:TYR:HB2	1.67	0.77
1:B:187:THR:HG21	1:B:243:ILE:HG13	1.65	0.76
1:A:419:GLU:O	1:A:442:PRO:HB2	1.85	0.76
1:B:373:HIS:C	1:B:373:HIS:CD2	2.64	0.76
1:B:365:CYS:O	1:B:367:PRO:CD	2.34	0.75
1:A:181:ASN:HB2	1:B:181:ASN:HB2	1.66	0.75
1:B:266:ASP:OD1	1:B:266:ASP:C	2.30	0.75
1:A:315:LEU:O	1:A:315:LEU:HD12	1.88	0.73
1:B:301:ASN:O	1:B:331:ARG:NH1	2.21	0.73
1:B:151:MET:CE	1:B:254:TYR:CG	2.73	0.72
1:B:367:PRO:HB2	1:B:387:ILE:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:VAL:HG11	1:B:459:MET:HE1	1.69	0.72
1:A:381:THR:HG21	1:A:421:LEU:HD11	1.70	0.72
1:B:136:SER:HB2	6:B:1468:SO4:O1	1.88	0.72
1:A:283:GLU:CD	1:A:286:ARG:HH21	1.98	0.71
1:A:169:LEU:CD2	1:A:254:TYR:HB2	2.20	0.71
1:A:49:ARG:NE	1:A:256:ARG:HD3	2.04	0.71
1:B:263:ASP:HB2	9:B:2029:HOH:O	1.89	0.71
1:B:311:MET:HA	1:B:311:MET:HE2	1.72	0.71
1:B:250:LEU:HD12	1:B:250:LEU:C	2.12	0.70
1:A:417:VAL:HG12	1:A:437:GLU:HG3	1.73	0.70
1:A:165:ASP:O	1:A:168:ARG:HB2	1.91	0.70
1:A:284:ARG:CG	1:A:284:ARG:HH11	2.05	0.70
1:A:435:ARG:NH2	1:A:437:GLU:OE1	2.23	0.70
1:A:9:ILE:HG13	1:B:2:ASN:HA	1.74	0.70
1:A:342:LYS:O	1:A:346:LEU:HB2	1.91	0.70
1:B:281:ILE:HD11	1:B:296:ALA:HB2	1.73	0.70
1:B:151:MET:HE1	1:B:254:TYR:CG	2.27	0.70
1:A:126:ARG:HD2	1:A:409:HIS:HE1	1.57	0.70
1:A:264:GLY:HA2	1:A:267:GLY:O	1.91	0.69
1:A:21:ASP:OD2	1:A:22:LEU:HD13	1.93	0.69
1:A:30:LEU:HD12	1:A:256:ARG:CZ	2.22	0.69
1:A:91:PHE:CE2	1:A:171:ARG:HG2	2.29	0.68
1:B:2:ASN:OD1	1:B:2:ASN:C	2.36	0.68
1:B:151:MET:CE	1:B:254:TYR:CD2	2.76	0.68
1:A:148:ARG:HH11	1:A:148:ARG:CB	2.06	0.68
1:B:395:PHE:CD2	1:B:459:MET:HE3	2.30	0.67
1:A:60:VAL:HB	1:A:61:PRO:CD	2.25	0.67
1:A:382:ARG:NH1	1:A:411:GLU:OE1	2.24	0.67
1:B:251:VAL:HG12	1:B:254:TYR:H	1.59	0.67
1:A:60:VAL:HB	1:A:61:PRO:HD2	1.75	0.67
1:A:35:ALA:HB3	1:A:285:THR:HG22	1.77	0.67
1:A:96:GLU:OE2	1:A:100:ARG:NH2	2.27	0.67
1:A:183:VAL:O	1:A:187:THR:HG23	1.96	0.66
1:A:193:SER:O	1:A:197:VAL:HG23	1.95	0.66
1:B:194:LEU:CD1	1:B:238:LEU:HD22	2.24	0.66
1:B:228:MET:CE	1:B:238:LEU:CD1	2.71	0.66
1:B:428:SER:H	1:B:431:ASP:HB2	1.60	0.66
1:A:30:LEU:CD1	1:A:256:ARG:CZ	2.73	0.66
1:A:333:THR:HG23	1:A:362:ILE:HB	1.78	0.66
1:A:22:LEU:HD12	1:A:25:ARG:HE	1.59	0.66
1:A:65:VAL:O	1:A:69:GLU:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:OE1	8:B:1470:GOL:H2	1.96	0.66
1:B:136:SER:OG	1:B:284:ARG:NH1	2.28	0.66
1:B:432:LEU:O	1:B:436:TYR:HB2	1.96	0.66
1:A:365:CYS:HB2	1:A:394:PHE:CG	2.30	0.66
1:A:419:GLU:OE2	1:A:438:THR:N	2.29	0.66
1:B:99:ILE:HG21	1:B:182:LEU:HD23	1.78	0.65
1:A:281:ILE:HD13	1:A:292:HIS:HB3	1.79	0.65
1:A:165:ASP:C	1:A:165:ASP:OD1	2.40	0.64
1:B:104:ARG:HG2	1:B:104:ARG:HH11	1.62	0.64
1:B:264:GLY:O	1:B:267:GLY:N	2.30	0.64
1:A:22:LEU:CD1	1:A:25:ARG:HE	2.09	0.64
1:A:148:ARG:NH1	1:A:148:ARG:CB	2.54	0.64
1:A:364:GLN:NE2	1:A:409:HIS:HB2	2.12	0.64
1:A:393:GLY:O	1:A:397:VAL:HG23	1.97	0.64
1:A:445:ASN:OD1	1:A:445:ASN:C	2.39	0.64
1:B:391:VAL:CG1	1:B:459:MET:CE	2.54	0.64
1:A:60:VAL:HG22	1:A:63:GLU:HG3	1.80	0.63
1:B:165:ASP:O	1:B:168:ARG:HB2	1.98	0.63
1:A:84:GLY:HA2	1:A:410:VAL:O	1.99	0.62
1:A:36:GLN:O	1:A:148:ARG:NH2	2.32	0.62
1:A:381:THR:HG21	1:A:421:LEU:CD1	2.30	0.62
1:B:77:GLY:HA2	1:B:404:HIS:CD2	2.35	0.62
1:A:381:THR:HG23	1:A:382:ARG:N	2.14	0.62
1:A:168:ARG:NH1	1:A:168:ARG:CG	2.62	0.62
1:B:87:CYS:SG	1:B:441:ASP:HB2	2.40	0.62
1:B:104:ARG:HG2	1:B:104:ARG:NH1	2.13	0.62
1:B:347:LEU:O	1:B:351:VAL:HG23	1.99	0.62
1:A:40:TRP:HB2	1:A:41:PRO:HD2	1.81	0.62
1:A:83:GLN:HA	1:A:124:VAL:O	2.01	0.61
1:B:210:ALA:O	1:B:211:GLY:C	2.44	0.61
1:A:140:ASP:C	1:A:140:ASP:OD1	2.40	0.61
1:A:5:VAL:CG2	1:A:5:VAL:O	2.47	0.61
1:B:228:MET:HE3	1:B:238:LEU:CD1	2.14	0.61
1:B:260:ARG:HG3	1:B:274:LEU:HD12	1.83	0.61
1:A:194:LEU:CD2	1:A:225:LEU:HD21	2.29	0.60
1:B:256:ARG:HG3	2:B:1466:TYR:O	2.01	0.60
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.02	0.60
1:A:419:GLU:OE1	1:A:438:THR:HB	2.02	0.60
1:B:191:LEU:CD1	1:B:200:TRP:HH2	2.15	0.60
1:B:18:LEU:HD21	1:B:271:LEU:HD21	1.84	0.60
1:B:395:PHE:HD2	1:B:459:MET:HE3	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASP:N	1:A:385:ASP:OD1	2.34	0.59
1:A:68:GLN:HE21	1:A:68:GLN:C	2.11	0.59
1:A:141:ALA:C	1:A:143:GLY:H	2.10	0.59
1:B:248:GLU:HG2	1:B:250:LEU:HB2	1.85	0.59
1:B:419:GLU:OE2	1:B:438:THR:N	2.34	0.59
1:B:348:PRO:HG3	1:B:397:VAL:HG13	1.84	0.59
1:A:347:LEU:HB3	1:A:348:PRO:HD3	1.85	0.58
1:B:264:GLY:O	1:B:267:GLY:HA2	2.04	0.58
1:B:399:ARG:NH2	1:B:459:MET:O	2.36	0.58
1:B:94:ASN:ND2	1:B:175:ASN:HB3	2.19	0.58
1:A:5:VAL:CG1	1:B:7:ILE:HD11	2.34	0.58
1:A:222:ASP:OD2	1:A:226:ARG:NH1	2.37	0.58
1:A:306:LYS:C	1:A:307:LEU:HD23	2.29	0.58
1:B:115:TYR:CE2	1:B:220:GLU:HG2	2.39	0.58
1:A:264:GLY:O	1:A:267:GLY:O	2.22	0.58
1:A:364:GLN:HE21	1:A:408:ILE:C	2.12	0.57
1:B:203:GLU:OE1	1:B:206:ARG:NH1	2.37	0.57
1:B:373:HIS:HD2	1:B:374:GLU:N	2.01	0.57
1:B:264:GLY:O	1:B:267:GLY:CA	2.52	0.57
1:A:48:MET:HE2	1:A:167:SER:CA	2.29	0.57
1:A:133:LYS:CE	1:A:440:CYS:SG	2.93	0.57
1:B:49:ARG:O	1:B:53:GLU:HG3	2.04	0.57
1:B:194:LEU:HD22	1:B:225:LEU:CD1	2.35	0.57
1:B:389:ASP:O	1:B:392:GLN:HB3	2.04	0.57
1:B:204:PHE:CG	1:B:450:LEU:HD23	2.39	0.57
1:A:68:GLN:O	1:A:68:GLN:NE2	2.30	0.57
1:A:348:PRO:N	1:A:349:PRO:CD	2.68	0.57
1:B:450:LEU:O	1:B:453:ALA:HB3	2.05	0.57
1:A:133:LYS:O	1:A:148:ARG:NH1	2.33	0.57
1:B:283:GLU:OE2	1:B:308:GLY:HA3	2.05	0.57
1:A:60:VAL:CG2	1:A:63:GLU:HG3	2.34	0.56
1:A:87:CYS:SG	1:A:441:ASP:HB2	2.44	0.56
1:B:37:GLN:HA	1:B:37:GLN:NE2	2.20	0.56
1:A:98:HIS:ND1	1:A:415:GLU:OE2	2.32	0.56
1:A:233:VAL:O	1:A:233:VAL:HG23	2.03	0.56
1:B:457:ALA:O	1:B:461:ARG:HG2	2.06	0.56
1:A:30:LEU:HD12	1:A:256:ARG:HH21	1.61	0.56
1:B:7:ILE:O	1:B:9:ILE:CD1	2.53	0.56
1:A:68:GLN:OE1	1:A:331:ARG:HA	2.05	0.56
1:A:74:VAL:HG22	1:A:79:ALA:C	2.31	0.56
1:B:217:LEU:HD12	1:B:217:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ASP:OD1	1:B:366:ASP:C	2.49	0.56
1:A:286:ARG:NH1	1:A:311:MET:CE	2.68	0.56
1:A:428:SER:O	1:A:431:ASP:N	2.37	0.56
1:B:307:LEU:HD11	1:B:334:LEU:CD2	2.26	0.56
1:A:39:THR:H	1:A:164:HIS:HD2	1.53	0.56
1:B:283:GLU:OE1	1:B:286:ARG:NH1	2.38	0.56
1:A:49:ARG:CZ	1:A:256:ARG:HD3	2.37	0.55
1:A:287:GLN:CD	1:A:287:GLN:H	2.12	0.55
1:A:315:LEU:HD12	1:A:315:LEU:C	2.30	0.55
1:A:452:LEU:O	1:A:452:LEU:HG	2.06	0.55
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.42	0.55
1:B:151:MET:O	1:B:151:MET:HG2	2.05	0.55
1:B:147:TYR:HE1	1:B:153:ASN:O	1.89	0.55
1:B:294:ALA:HA	1:B:297:GLN:HG3	1.89	0.55
1:B:151:MET:HE2	1:B:254:TYR:CD1	2.41	0.55
1:B:183:VAL:O	1:B:187:THR:HG23	2.07	0.55
1:B:80:PHE:O	1:B:121:VAL:HA	2.07	0.55
1:B:96:GLU:HB3	1:B:97:PRO:HD3	1.89	0.55
1:B:450:LEU:O	1:B:451:GLU:C	2.47	0.55
1:B:383:HIS:HD2	1:B:385:ASP:H	1.54	0.55
1:A:233:VAL:O	1:A:233:VAL:CG2	2.54	0.54
1:A:145:ARG:NH2	6:A:1467:SO4:O4	2.28	0.54
1:A:445:ASN:OD1	1:A:448:GLN:N	2.37	0.54
1:A:51:VAL:O	1:A:55:VAL:HG13	2.07	0.54
1:A:415:GLU:HB2	1:A:417:VAL:HG13	1.90	0.54
1:A:147:TYR:OH	1:A:150:ASP:OD1	2.23	0.54
1:A:264:GLY:CA	1:A:267:GLY:O	2.55	0.54
1:A:461:ARG:O	1:A:462:ASP:OD1	2.25	0.54
1:B:115:TYR:OH	1:B:220:GLU:HG3	2.08	0.54
1:B:180:MET:SD	1:B:245:ALA:HB2	2.48	0.54
1:B:191:LEU:HD11	1:B:200:TRP:HH2	1.73	0.54
1:B:447:GLN:HB3	9:B:2045:HOH:O	2.08	0.54
1:A:63:GLU:HG2	1:B:189:SER:OG	2.08	0.53
1:A:282:GLY:O	1:A:286:ARG:HB3	2.09	0.53
1:A:186:LEU:HD13	1:A:191:LEU:HD22	1.90	0.53
1:B:373:HIS:CD2	1:B:374:GLU:N	2.76	0.53
4:A:1464:TRP:CE3	4:A:1464:TRP:OXT	2.61	0.53
1:B:90:THR:OG1	1:B:93:ASP:HB2	2.07	0.53
1:A:5:VAL:O	1:A:5:VAL:HG22	2.07	0.53
1:A:103:VAL:O	1:A:104:ARG:C	2.49	0.53
1:A:22:LEU:HD12	1:A:25:ARG:NE	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:VAL:HG21	1:B:173:TYR:CE1	2.43	0.53
1:A:80:PHE:CZ	1:A:407:GLY:HA2	2.43	0.53
1:A:191:LEU:HD12	1:A:200:TRP:HH2	1.72	0.53
1:A:288:ILE:HG13	1:A:322:ARG:NH1	2.23	0.53
1:B:311:MET:HE2	1:B:311:MET:CA	2.37	0.53
1:A:286:ARG:O	1:A:287:GLN:C	2.50	0.53
1:A:439:ALA:O	1:A:440:CYS:HB2	2.08	0.52
1:B:32:LYS:HB3	1:B:33:PRO:HD2	1.92	0.52
1:B:286:ARG:NH2	1:B:311:MET:HE1	2.24	0.52
1:A:417:VAL:HB	1:A:419:GLU:HG3	1.90	0.52
1:B:457:ALA:O	1:B:460:LEU:HB2	2.09	0.52
1:A:284:ARG:HG3	1:A:284:ARG:NH1	2.23	0.52
1:A:303:VAL:CG2	1:A:331:ARG:NH1	2.71	0.52
1:B:273:ASP:C	1:B:273:ASP:OD1	2.51	0.52
1:A:91:PHE:CZ	1:A:172:ALA:HA	2.44	0.52
1:B:331:ARG:HD2	1:B:331:ARG:O	2.10	0.52
1:B:373:HIS:C	1:B:373:HIS:HD2	2.17	0.52
1:A:148:ARG:HB3	1:A:148:ARG:CZ	2.37	0.51
1:A:194:LEU:HD23	1:A:225:LEU:CD2	2.34	0.51
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.75	0.51
1:B:333:THR:HG21	1:B:364:GLN:OE1	2.11	0.51
1:B:366:ASP:OD2	1:B:369:HIS:ND1	2.42	0.51
1:B:341:HIS:CD2	1:B:342:LYS:HG3	2.45	0.51
1:B:344:ARG:CD	9:B:2037:HOH:O	2.58	0.51
1:A:332:LEU:CD2	1:A:334:LEU:HD21	2.25	0.51
1:B:71:LEU:HB3	1:B:362:ILE:HD11	1.93	0.51
1:B:412:ILE:CG2	1:B:449:SER:HB3	2.41	0.51
1:A:256:ARG:NH1	9:A:2024:HOH:O	2.43	0.51
1:A:328:LYS:O	1:A:331:ARG:HB3	2.11	0.51
1:A:365:CYS:O	1:A:367:PRO:HD3	2.11	0.51
1:B:83:GLN:HA	1:B:124:VAL:O	2.11	0.51
1:B:367:PRO:HD2	1:B:409:HIS:O	2.10	0.51
1:A:281:ILE:CD1	1:A:292:HIS:HB3	2.41	0.51
1:B:458:GLU:HA	1:B:461:ARG:HG3	1.92	0.50
1:A:387:ILE:O	1:A:388:VAL:C	2.53	0.50
1:B:180:MET:O	1:B:181:ASN:C	2.52	0.50
1:A:96:GLU:N	1:A:97:PRO:CD	2.74	0.50
1:B:348:PRO:HB2	1:B:349:PRO:HD3	1.92	0.50
1:A:61:PRO:O	1:A:65:VAL:CG1	2.60	0.50
1:A:384:PHE:O	1:A:388:VAL:HG23	2.12	0.50
4:B:1464:TRP:CD1	4:B:1464:TRP:N	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:VAL:O	1:B:357:THR:OG1	2.22	0.50
1:A:264:GLY:C	1:A:267:GLY:O	2.55	0.50
1:A:294:ALA:O	1:A:297:GLN:HB2	2.12	0.50
1:A:419:GLU:O	1:A:442:PRO:CB	2.58	0.50
1:B:457:ALA:HA	1:B:460:LEU:HD12	1.93	0.50
1:A:284:ARG:CG	1:A:284:ARG:NH1	2.68	0.50
1:B:15:LEU:N	1:B:16:PRO:CD	2.75	0.50
1:A:239:GLN:C	1:A:240:THR:HG23	2.37	0.49
1:A:450:LEU:O	1:A:453:ALA:N	2.40	0.49
1:A:68:GLN:NE2	1:A:68:GLN:HA	2.26	0.49
1:B:99:ILE:CG2	1:B:182:LEU:HD23	2.42	0.49
1:A:52:LEU:HB2	1:A:257:ALA:HB1	1.92	0.49
1:B:140:ASP:CB	1:B:144:LEU:O	2.60	0.49
1:B:155:PHE:O	1:B:156:ALA:C	2.54	0.49
1:B:417:VAL:CG2	1:B:419:GLU:HG3	2.42	0.49
1:A:68:GLN:NE2	1:A:68:GLN:CA	2.74	0.49
1:B:80:PHE:CE1	1:B:407:GLY:HA2	2.48	0.49
1:A:419:GLU:CD	1:A:438:THR:HB	2.38	0.49
1:B:207:THR:O	1:B:208:SER:C	2.52	0.49
1:A:119:MET:HB2	1:A:120:PRO:HD2	1.94	0.49
1:B:49:ARG:O	1:B:53:GLU:CG	2.60	0.49
1:B:285:THR:HB	1:B:292:HIS:ND1	2.27	0.49
1:B:348:PRO:N	1:B:349:PRO:HD2	2.27	0.49
1:B:281:ILE:HD11	1:B:296:ALA:CB	2.43	0.49
1:A:139:ILE:HG22	1:A:140:ASP:O	2.13	0.49
1:A:150:ASP:HB3	1:A:168:ARG:HH12	1.78	0.49
1:B:151:MET:HE1	1:B:254:TYR:CE2	2.45	0.49
1:B:282:GLY:O	1:B:286:ARG:HG2	2.14	0.48
1:B:395:PHE:CD2	1:B:459:MET:CE	2.95	0.48
1:A:386:ARG:NH1	9:A:2033:HOH:O	2.46	0.48
1:B:412:ILE:HG21	1:B:449:SER:HB3	1.95	0.48
1:B:456:VAL:O	1:B:459:MET:HB2	2.13	0.48
1:B:37:GLN:NE2	1:B:37:GLN:CA	2.76	0.48
1:B:194:LEU:HD22	1:B:225:LEU:HD13	1.94	0.48
1:B:247:HIS:HD2	1:B:248:GLU:O	1.95	0.48
1:A:340:ASN:OD1	1:A:340:ASN:N	2.47	0.48
1:A:445:ASN:OD1	1:A:448:GLN:HG3	2.14	0.48
1:B:61:PRO:O	1:B:62:SER:C	2.57	0.48
1:B:147:TYR:CZ	1:B:149:GLY:HA2	2.49	0.48
1:B:316:ALA:O	1:B:320:VAL:HG23	2.14	0.48
1:B:450:LEU:O	1:B:453:ALA:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:NH2	1:B:311:MET:CE	2.77	0.48
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.54	0.48
1:A:212:ALA:O	1:A:213:ARG:C	2.57	0.47
1:A:383:HIS:O	1:A:387:ILE:HG13	2.13	0.47
1:A:66:ARG:O	1:A:70:GLN:HG3	2.13	0.47
1:A:151:MET:O	1:A:168:ARG:HB3	2.14	0.47
1:A:13:PRO:HG2	1:B:92:MET:HG3	1.95	0.47
1:A:286:ARG:HH12	1:A:311:MET:HE1	1.77	0.47
1:B:158:ASP:O	1:B:159:ALA:C	2.58	0.47
1:B:251:VAL:O	1:B:255:GLU:HG2	2.14	0.47
1:B:148:ARG:CB	1:B:152:ILE:HD12	2.45	0.47
1:A:69:GLU:O	1:A:72:ALA:HB3	2.15	0.47
1:B:391:VAL:O	1:B:394:PHE:HB3	2.15	0.47
1:B:16:PRO:O	2:B:1466:TYR:OH	2.32	0.46
1:A:77:GLY:HA2	1:A:404:HIS:CG	2.48	0.46
1:A:288:ILE:CG2	1:A:289:ASP:N	2.77	0.46
1:A:40:TRP:HD1	1:A:40:TRP:O	1.98	0.46
1:A:235:ASP:O	1:A:238:LEU:HB2	2.15	0.46
1:A:82:LEU:HD12	1:A:83:GLN:N	2.30	0.46
1:B:151:MET:HE2	1:B:254:TYR:CG	2.48	0.46
1:B:419:GLU:OE1	1:B:438:THR:HB	2.15	0.46
1:A:243:ILE:O	8:A:1469:GOL:O2	2.33	0.46
1:A:364:GLN:CD	1:A:409:HIS:HB2	2.39	0.46
1:A:61:PRO:O	1:A:65:VAL:HG13	2.16	0.46
1:B:66:ARG:CZ	1:B:70:GLN:HE21	2.28	0.46
1:A:284:ARG:HH11	1:A:284:ARG:HG3	1.77	0.46
1:B:2:ASN:OD1	1:B:2:ASN:O	2.34	0.46
1:B:151:MET:O	1:B:168:ARG:HB3	2.16	0.46
1:A:109:MET:HE3	1:A:449:SER:O	2.15	0.46
1:B:309:PRO:HA	1:B:346:LEU:HD13	1.97	0.46
1:B:344:ARG:HD2	9:B:2037:HOH:O	2.16	0.46
1:A:132:ALA:HA	1:A:149:GLY:HA3	1.98	0.46
1:A:335:VAL:HA	1:A:364:GLN:O	2.16	0.46
1:B:117:ALA:HA	1:B:460:LEU:HD22	1.97	0.46
1:B:264:GLY:C	1:B:267:GLY:H	2.22	0.46
1:A:365:CYS:HB2	1:A:394:PHE:CD1	2.51	0.45
1:A:382:ARG:NH1	1:A:441:ASP:HB3	2.30	0.45
1:B:1:MET:HB3	1:B:2:ASN:H	1.54	0.45
1:B:266:ASP:OD1	1:B:267:GLY:N	2.49	0.45
1:A:341:HIS:ND1	1:A:341:HIS:N	2.63	0.45
1:A:91:PHE:CD2	1:A:171:ARG:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:HA	1:A:287:GLN:HE22	1.80	0.45
1:B:80:PHE:CZ	1:B:407:GLY:HA2	2.51	0.45
1:B:410:VAL:HG23	1:B:412:ILE:HG23	1.98	0.45
1:B:194:LEU:HD22	1:B:225:LEU:HD11	1.97	0.45
1:A:348:PRO:HB2	1:A:349:PRO:HD3	1.99	0.45
1:A:396:GLU:HA	1:A:399:ARG:HD2	1.98	0.45
1:A:458:GLU:O	1:A:459:MET:C	2.59	0.45
1:B:368:MET:HE3	1:B:368:MET:HB3	1.91	0.45
1:A:7:ILE:HG21	1:B:3:TRP:CZ2	2.51	0.45
1:A:286:ARG:HG3	1:A:319:TYR:OH	2.17	0.45
1:B:94:ASN:HD22	1:B:175:ASN:HB3	1.82	0.45
1:B:104:ARG:O	1:B:108:GLN:HG3	2.17	0.45
1:B:191:LEU:HD12	1:B:191:LEU:HA	1.74	0.45
1:A:5:VAL:HG12	1:B:7:ILE:CD1	2.44	0.45
1:A:5:VAL:HG23	1:A:7:ILE:CD1	2.47	0.45
1:A:135:ARG:HG2	1:A:148:ARG:HD2	1.99	0.45
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.56	0.44
1:B:228:MET:HE1	1:B:238:LEU:CD1	2.47	0.44
1:B:436:TYR:CE1	1:B:438:THR:HG22	2.52	0.44
1:B:102:ASN:ND2	9:B:2009:HOH:O	2.49	0.44
1:B:348:PRO:N	1:B:349:PRO:CD	2.80	0.44
1:A:2:ASN:O	1:A:4:THR:HG23	2.17	0.44
1:A:130:GLN:OE1	1:A:247:HIS:HA	2.17	0.44
1:B:445:ASN:C	1:B:445:ASN:OD1	2.60	0.44
1:A:256:ARG:HG2	1:A:257:ALA:N	2.30	0.44
1:A:135:ARG:CG	1:A:146:SER:HB3	2.47	0.44
1:B:382:ARG:NH1	1:B:411:GLU:OE1	2.39	0.44
1:A:44:GLN:O	1:A:45:ALA:C	2.57	0.44
1:A:119:MET:HB2	1:A:120:PRO:CD	2.48	0.44
1:B:55:VAL:HB	1:B:173:TYR:CZ	2.52	0.44
1:A:150:ASP:O	1:A:168:ARG:NH1	2.51	0.43
1:A:422:GLY:H	1:A:427:ILE:HB	1.83	0.43
1:B:23:ARG:HA	1:B:23:ARG:HD3	1.73	0.43
1:B:191:LEU:HD12	1:B:200:TRP:HH2	1.81	0.43
1:B:203:GLU:O	1:B:207:THR:HG23	2.18	0.43
1:B:259:LEU:HD23	1:B:273:ASP:HA	1.98	0.43
1:A:365:CYS:HB2	1:A:394:PHE:CD2	2.52	0.43
1:B:116:GLY:O	1:B:117:ALA:C	2.60	0.43
1:B:386:ARG:NH1	9:B:2042:HOH:O	2.50	0.43
1:A:185:ALA:HB2	1:B:184:ARG:CZ	2.48	0.43
1:B:104:ARG:HH11	1:B:104:ARG:CG	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:VAL:HG11	1:B:363:TRP:CZ2	2.53	0.43
1:A:52:LEU:CB	1:A:257:ALA:HB1	2.48	0.43
1:A:193:SER:HG	1:A:196:LEU:H	1.66	0.43
1:A:461:ARG:HG2	1:A:461:ARG:HH11	1.83	0.43
1:B:110:ALA:CB	1:B:123:LYS:HD3	2.48	0.43
1:B:368:MET:H	1:B:368:MET:HG2	1.54	0.43
1:B:242:GLU:HG2	8:B:1469:GOL:H32	2.00	0.43
1:B:367:PRO:HA	1:B:390:GLU:HG2	2.00	0.43
1:A:140:ASP:OD1	1:A:142:LEU:N	2.44	0.43
1:A:426:ASP:O	1:A:427:ILE:C	2.61	0.43
1:B:95:THR:OG1	1:B:97:PRO:HD2	2.18	0.43
1:A:288:ILE:HG23	1:A:289:ASP:N	2.33	0.43
1:B:63:GLU:O	1:B:66:ARG:HB3	2.18	0.43
1:B:395:PHE:CE2	1:B:459:MET:HE2	2.52	0.43
1:B:115:TYR:OH	1:B:220:GLU:CG	2.67	0.43
1:B:193:SER:O	1:B:197:VAL:HG23	2.19	0.43
1:B:415:GLU:HB2	1:B:417:VAL:HG13	1.99	0.43
1:A:304:GLY:HA2	1:A:333:THR:O	2.19	0.43
1:A:211:GLY:O	1:A:212:ALA:C	2.62	0.42
1:A:212:ALA:C	1:A:214:TYR:H	2.27	0.42
1:A:316:ALA:O	1:A:319:TYR:HB2	2.18	0.42
1:B:412:ILE:HG22	1:B:444:LEU:HB2	2.00	0.42
1:A:40:TRP:CD1	1:A:40:TRP:C	2.96	0.42
1:A:247:HIS:HE1	1:A:275:SER:HB2	1.85	0.42
1:B:6:ASP:N	1:B:6:ASP:OD1	2.48	0.42
1:B:148:ARG:HB2	1:B:152:ILE:HD12	2.01	0.42
1:B:191:LEU:HD11	1:B:200:TRP:CH2	2.52	0.42
1:A:95:THR:HB	1:A:97:PRO:HD2	2.01	0.42
1:A:337:ARG:O	1:A:337:ARG:NH1	2.52	0.42
1:A:74:VAL:O	1:A:75:ALA:C	2.60	0.42
1:A:147:TYR:HE1	1:A:153:ASN:O	2.03	0.42
1:A:181:ASN:HB2	1:B:181:ASN:CB	2.44	0.42
1:A:288:ILE:HG13	1:A:322:ARG:HH12	1.84	0.42
1:B:110:ALA:HB1	1:B:123:LYS:HD3	2.01	0.42
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.81	0.42
1:B:286:ARG:O	1:B:287:GLN:C	2.61	0.42
1:A:212:ALA:C	1:A:214:TYR:N	2.75	0.42
1:B:194:LEU:HD13	1:B:225:LEU:HD11	2.01	0.42
1:A:217:LEU:HD12	1:A:217:LEU:O	2.20	0.42
1:A:332:LEU:HD21	1:A:334:LEU:CD2	2.26	0.42
4:A:1464:TRP:OXT	4:A:1464:TRP:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:O	1:A:10:ASP:C	2.63	0.41
1:B:212:ALA:C	1:B:214:TYR:H	2.29	0.41
1:A:6:ASP:O	1:A:8:PRO:HD3	2.20	0.41
1:A:17:PRO:C	1:A:18:LEU:O	2.62	0.41
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.86	0.41
1:A:213:ARG:HB2	1:A:213:ARG:NH1	2.35	0.41
1:A:419:GLU:HG2	1:A:436:TYR:HA	2.01	0.41
1:A:430:THR:O	1:A:430:THR:HG22	2.18	0.41
1:B:258:MET:HE3	1:B:258:MET:HB3	1.70	0.41
1:A:248:GLU:HB2	1:A:280:TRP:CE2	2.55	0.41
1:B:194:LEU:HD13	1:B:225:LEU:CD1	2.50	0.41
1:B:458:GLU:HA	1:B:458:GLU:OE1	2.21	0.41
1:A:7:ILE:HG21	1:B:3:TRP:CE2	2.56	0.41
1:A:268:GLU:HA	1:A:269:PRO:HD3	1.95	0.41
1:A:395:PHE:O	1:A:399:ARG:HG3	2.20	0.41
1:A:456:VAL:O	1:A:457:ALA:C	2.63	0.41
1:B:392:GLN:O	1:B:396:GLU:HG3	2.20	0.41
1:A:346:LEU:HA	1:A:346:LEU:HD23	1.68	0.41
1:B:5:VAL:CG1	1:B:6:ASP:N	2.80	0.41
1:A:319:TYR:HD1	1:A:319:TYR:HA	1.73	0.41
1:A:461:ARG:HG2	1:A:461:ARG:NH1	2.36	0.41
1:A:220:GLU:O	1:A:221:ILE:C	2.61	0.41
1:A:236:ARG:C	1:A:238:LEU:N	2.79	0.41
1:A:412:ILE:HG22	1:A:444:LEU:HB2	2.01	0.41
1:B:272:PHE:CD2	1:B:300:ALA:HB3	2.55	0.41
1:A:91:PHE:CE1	1:A:172:ALA:HA	2.56	0.41
1:A:137:ALA:O	1:A:146:SER:OG	2.38	0.41
1:A:348:PRO:O	1:A:352:GLU:HG2	2.21	0.41
1:B:69:GLU:O	1:B:72:ALA:HB3	2.21	0.41
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.65	0.41
1:A:171:ARG:O	1:A:172:ALA:C	2.64	0.41
1:A:355:GLN:HA	1:A:355:GLN:NE2	2.36	0.41
1:B:159:ALA:O	1:B:160:ALA:C	2.62	0.41
1:B:246:SER:HB3	1:B:278:THR:HG23	2.03	0.41
1:B:318:GLU:O	1:B:319:TYR:C	2.62	0.41
1:A:300:ALA:O	1:A:301:ASN:C	2.62	0.40
1:A:347:LEU:C	1:A:349:PRO:HD2	2.46	0.40
1:B:390:GLU:O	1:B:390:GLU:HG3	2.18	0.40
1:B:27:ASP:O	1:B:28:ALA:C	2.63	0.40
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.77	0.40
1:B:455:LEU:HA	1:B:455:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:C	1:A:238:LEU:H	2.29	0.40
1:B:306:LYS:NZ	1:B:366:ASP:OD2	2.43	0.40
1:A:368:MET:HE3	1:A:368:MET:HB3	1.92	0.40
1:B:235:ASP:HB2	1:B:236:ARG:H	1.54	0.40
1:B:457:ALA:O	1:B:461:ARG:CG	2.69	0.40
1:A:107:LEU:HD13	1:A:192:ALA:HA	2.04	0.40
1:A:158:ASP:O	1:A:159:ALA:C	2.64	0.40
1:B:305:VAL:HG12	1:B:306:LYS:O	2.21	0.40
1:B:446:THR:CG2	1:B:447:GLN:N	2.84	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	456/462 (99%)	430 (94%)	25 (6%)	1 (0%)	43	64
1	B	453/462 (98%)	418 (92%)	34 (8%)	1 (0%)	43	64
All	All	909/924 (98%)	848 (93%)	59 (6%)	2 (0%)	43	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	CYS
1	B	440	CYS

5.3.2 Protein sidechains [i](#)

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	366/376 (97%)	305 (83%)	61 (17%)	2	3
1	B	369/376 (98%)	319 (86%)	50 (14%)	3	6
All	All	735/752 (98%)	624 (85%)	111 (15%)	3	4

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	VAL
1	A	6	ASP
1	A	22	LEU
1	A	54	SER
1	A	64	ILE
1	A	65	VAL
1	A	68	GLN
1	A	73	GLN
1	A	92	MET
1	A	96	GLU
1	A	104	ARG
1	A	111	VAL
1	A	133	LYS
1	A	135	ARG
1	A	136	SER
1	A	148	ARG
1	A	167	SER
1	A	168	ARG
1	A	177	SER
1	A	193	SER
1	A	203	GLU
1	A	215	GLU
1	A	219	THR
1	A	236	ARG
1	A	243	ILE
1	A	256	ARG
1	A	275	SER
1	A	281	ILE
1	A	284	ARG
1	A	285	THR
1	A	297	GLN
1	A	302	PRO

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Mol	Chain	Res	Type
1	A	306	LYS
1	A	315	LEU
1	A	331	ARG
1	A	332	LEU
1	A	334	LEU
1	A	336	SER
1	A	337	ARG
1	A	341	HIS
1	A	342	LYS
1	A	344	ARG
1	A	350	ILE
1	A	352	GLU
1	A	353	LYS
1	A	360	GLN
1	A	362	ILE
1	A	367	PRO
1	A	381	THR
1	A	383	HIS
1	A	385	ASP
1	A	386	ARG
1	A	401	LEU
1	A	412	ILE
1	A	420	CYS
1	A	428	SER
1	A	437	GLU
1	A	443	ARG
1	A	450	LEU
1	A	461	ARG
1	B	7	ILE
1	B	9	ILE
1	B	23	ARG
1	B	25	ARG
1	B	37	GLN
1	B	43	ASP
1	B	44	GLN
1	B	73	GLN
1	B	104	ARG
1	B	111	VAL
1	B	119	MET
1	B	123	LYS
1	B	127	ILE
1	B	133	LYS

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Mol	Chain	Res	Type
1	B	135	ARG
1	B	136	SER
1	B	168	ARG
1	B	170	VAL
1	B	193	SER
1	B	194	LEU
1	B	207	THR
1	B	215	GLU
1	B	228	MET
1	B	229	SER
1	B	235	ASP
1	B	243	ILE
1	B	250	LEU
1	B	256	ARG
1	B	262	SER
1	B	266	ASP
1	B	268	GLU
1	B	286	ARG
1	B	310	ASN
1	B	336	SER
1	B	337	ARG
1	B	353	LYS
1	B	360	GLN
1	B	372	THR
1	B	373	HIS
1	B	376	SER
1	B	386	ARG
1	B	390	GLU
1	B	403	THR
1	B	408	ILE
1	B	426	ASP
1	B	430	THR
1	B	446	THR
1	B	449	SER
1	B	459	MET
1	B	461	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	195	HIS

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Mol	Chain	Res	Type
1	A	198	HIS
1	A	292	HIS
1	A	359	HIS
1	A	364	GLN
1	A	373	HIS
1	A	409	HIS
1	A	416	ASN
1	B	68	GLN
1	B	297	GLN
1	B	310	ASN
1	B	341	HIS
1	B	373	HIS
1	B	383	HIS
1	B	404	HIS

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](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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
4	TRP	A	1464	-	15,16,16	1.68	5 (33%)	18,22,22	1.09	1 (5%)
5	PO4	A	1466	-	4,4,4	1.31	0	6,6,6	1.13	0
2	TYR	B	1465	-	12,13,13	0.87	0	13,17,17	0.88	0
8	GOL	A	1469	-	5,5,5	0.47	0	5,5,5	0.57	0
4	TRP	B	1464	-	15,16,16	1.92	2 (13%)	18,22,22	1.49	3 (16%)
8	GOL	B	1469	-	5,5,5	0.77	0	5,5,5	0.83	0
2	TYR	A	1465	-	12,13,13	0.91	1 (8%)	13,17,17	1.26	2 (15%)
2	TYR	B	1466	-	12,13,13	1.12	1 (8%)	13,17,17	1.66	2 (15%)
5	PO4	B	1467	-	4,4,4	0.96	0	6,6,6	2.54	2 (33%)
8	GOL	B	1470	-	5,5,5	1.21	0	5,5,5	1.47	1 (20%)
8	GOL	B	1471	-	5,5,5	0.59	0	5,5,5	1.49	2 (40%)
6	SO4	A	1467	-	4,4,4	0.81	0	6,6,6	2.08	3 (50%)
6	SO4	B	1468	-	4,4,4	0.70	0	6,6,6	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRP	A	1464	-	-	1/8/8/8	0/2/2/2
2	TYR	B	1465	-	-	0/8/8/8	0/1/1/1
8	GOL	A	1469	-	-	4/4/4/4	-
4	TRP	B	1464	-	-	0/8/8/8	0/2/2/2
8	GOL	B	1469	-	-	4/4/4/4	-
2	TYR	A	1465	-	-	3/8/8/8	0/1/1/1
2	TYR	B	1466	-	-	0/8/8/8	0/1/1/1
8	GOL	B	1470	-	-	4/4/4/4	-
8	GOL	B	1471	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1464	TRP	CD2-CE2	5.21	1.47	1.41
4	A	1464	TRP	CE3-CD2	-3.44	1.34	1.39
4	B	1464	TRP	CE2-NE1	-3.22	1.32	1.37
4	A	1464	TRP	OXT-C	-3.11	1.20	1.30
2	B	1466	TYR	OXT-C	-2.76	1.21	1.30
4	A	1464	TRP	CD2-CE2	2.73	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1465	TYR	OXT-C	-2.50	1.22	1.30
4	A	1464	TRP	CE2-NE1	-2.26	1.34	1.37
4	A	1464	TRP	CD2-CG	2.09	1.47	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1466	TYR	OXT-C-O	-4.84	113.09	124.08
4	B	1464	TRP	CA-CB-CG	-4.10	105.71	113.49
5	B	1467	PO4	O4-P-O3	3.94	120.18	107.91
5	B	1467	PO4	O2-P-O1	-3.77	97.60	110.95
2	A	1465	TYR	CG-CB-CA	-3.33	107.31	114.13
6	A	1467	SO4	O3-S-O2	2.74	123.87	109.56
2	A	1465	TYR	OXT-C-O	-2.71	117.94	124.08
6	A	1467	SO4	O4-S-O3	-2.71	93.61	108.54
4	A	1464	TRP	CE2-NE1-CD1	2.68	111.46	109.08
6	A	1467	SO4	O4-S-O1	2.59	123.12	109.56
4	B	1464	TRP	CZ3-CH2-CZ2	2.53	123.36	120.24
2	B	1466	TYR	CG-CB-CA	2.47	119.18	114.13
4	B	1464	TRP	CE2-NE1-CD1	2.39	111.20	109.08
8	B	1471	GOL	O2-C2-C3	-2.26	99.81	109.18
8	B	1471	GOL	C3-C2-C1	2.25	120.04	111.80
8	B	1470	GOL	O2-C2-C3	2.03	117.58	109.18

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1469	GOL	O1-C1-C2-C3
8	A	1469	GOL	C1-C2-C3-O3
8	B	1469	GOL	O1-C1-C2-C3
8	B	1469	GOL	C1-C2-C3-O3
8	B	1470	GOL	O1-C1-C2-C3
8	B	1470	GOL	C1-C2-C3-O3
8	A	1469	GOL	O1-C1-C2-O2
8	A	1469	GOL	O2-C2-C3-O3
8	B	1469	GOL	O1-C1-C2-O2
8	B	1469	GOL	O2-C2-C3-O3
8	B	1470	GOL	O1-C1-C2-O2
8	B	1470	GOL	O2-C2-C3-O3
2	A	1465	TYR	OXT-C-CA-N
2	A	1465	TYR	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	A	1465	TYR	O-C-CA-N
4	A	1464	TRP	OXT-C-CA-CB

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1464	TRP	2	0
8	A	1469	GOL	1	0
4	B	1464	TRP	1	0
8	B	1469	GOL	1	0
2	B	1466	TYR	2	0
8	B	1470	GOL	2	0
6	A	1467	SO4	1	0
6	B	1468	SO4	2	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	460/462 (99%)	0.08	21 (4%) 37 36	16, 39, 73, 121	1 (0%)
1	B	457/462 (98%)	0.02	19 (4%) 40 39	7, 35, 70, 120	2 (0%)
All	All	917/924 (99%)	0.05	40 (4%) 39 38	7, 37, 71, 121	3 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ASP	7.2
1	A	3	TRP	5.8
1	B	148	ARG	4.3
1	A	189	SER	4.1
1	A	266	ASP	4.1
1	B	9	ILE	3.9
1	A	2	ASN	3.9
1	B	266	ASP	3.7
1	B	370	GLY	3.6
1	B	15	LEU	3.6
1	B	264	GLY	3.5
1	B	3	TRP	3.5
1	B	267	GLY	3.4
1	A	15	LEU	3.3
1	A	138	ASP	3.2
1	A	265	ASP	3.0
1	A	234	ALA	3.0
1	A	383	HIS	2.9
1	B	234	ALA	2.8
1	A	136	SER	2.7
1	A	1	MET	2.7
1	A	399	ARG	2.6
1	B	141	ALA	2.5
1	A	30	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2	ASN	2.4
1	B	426	ASP	2.4
1	B	236	ARG	2.4
1	B	399	ARG	2.4
1	B	137	ALA	2.3
1	A	13	PRO	2.2
1	A	31	ALA	2.2
1	A	14	SER	2.2
1	A	372	THR	2.1
1	A	416	ASN	2.1
1	A	263	ASP	2.1
1	A	233	VAL	2.1
1	B	140	ASP	2.0
1	B	327	ASN	2.0
1	B	462	ASP	2.0
1	B	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	B	1471	6/6	0.78	0.24	54,72,78,82	0
8	GOL	B	1469	6/6	0.81	0.31	50,69,93,105	0
6	SO4	A	1467	5/5	0.85	0.13	52,58,74,92	0
8	GOL	B	1470	6/6	0.85	0.20	54,57,80,86	0
7	CL	A	1468	1/1	0.85	0.13	80,80,80,80	0
7	CL	A	1500	1/1	0.87	0.13	73,73,73,73	0
2	TYR	B	1465	13/13	0.89	0.14	35,47,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	1468	5/5	0.92	0.12	55,77,84,120	0
3	MN	B	1463	1/1	0.92	0.13	29,29,29,29	1
2	TYR	B	1466	13/13	0.92	0.10	26,37,52,54	0
2	TYR	A	1465	13/13	0.93	0.13	32,47,60,65	0
8	GOL	A	1469	6/6	0.94	0.14	50,65,69,71	0
4	TRP	A	1464	15/15	0.97	0.06	17,32,40,41	0
5	PO4	A	1466	5/5	0.97	0.09	23,39,47,54	0
4	TRP	B	1464	15/15	0.98	0.06	16,27,35,37	0
5	PO4	B	1467	5/5	0.98	0.08	34,36,40,59	0
3	MN	A	1463	1/1	0.99	0.05	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.