



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 AM UTC

PDB ID : 1JDY / pdb_00001jdy
Title : RABBIT MUSCLE PHOSPHOGLUCOMUTASE
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Deposited on : 1996-07-11
Resolution : 2.70 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

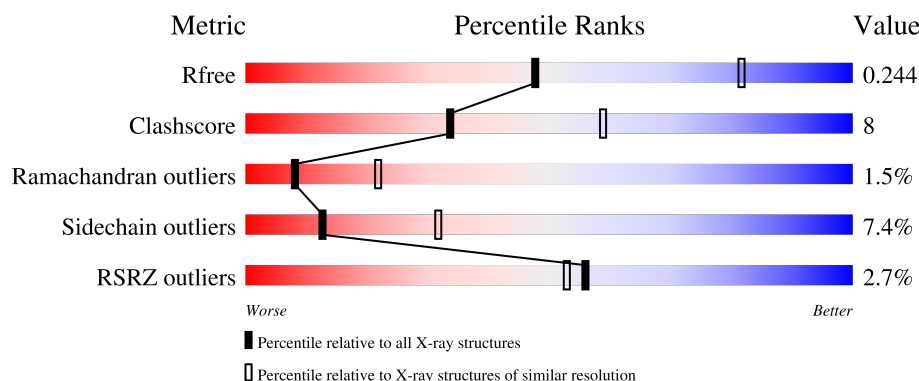
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	561	5% 56% 36% 7%
1	B	561	61% 32% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9010 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 PHOSPHOGLUCOMUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	P	S	0	0	0
			4333	2753	743	820	1	16			
1	B	561	Total	C	N	O	P	S	0	0	0
			4333	2753	743	820	1	16			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		
2	B	1	Total	Cd	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	196	Total	O	0	0
			196	196		

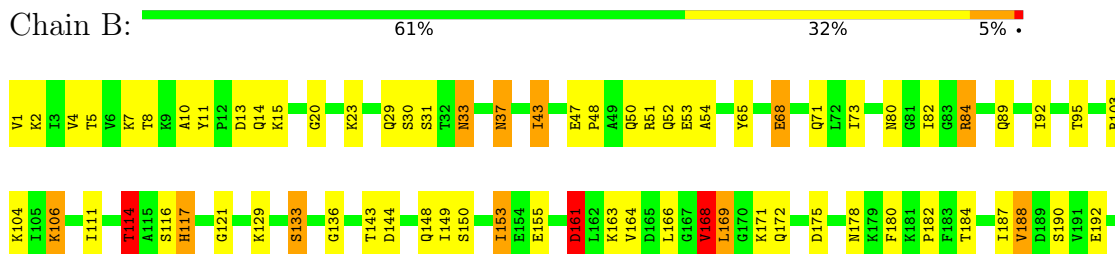
3 Residue-property plots

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: PHOSPHOGLUCOMUTASE



• Molecule 1: PHOSPHOGLUCOMUTASE



H476	R386	H280	R199
Q487	E387	D281	N200
G488	K388	F282	N205
L489	D389	G283	N205
R490	A396	A284	K208
A494	A402	A285	E209
I499	T403	G288	L210
I500	R404	D289	L211
F501	K405	G290	S212
S502	Q406	D291	G213
L503	E409	R292	P214
S504	D410	N293	N215
G505	I411	L296	R216
T506	L412	K218	L217
G507	K413	H299	K218
S508	D414	G300	I219
L515	H415	F301	R220
Y516	K416	F302	I221
Y517	H417	V311	D222
D518	K418	I312	H225
S519	F419	I315	G226
Y520	N422	I316	V227
E521	F423	F317	V232
D523	R426	S318	K233
N524	Y427	I319	K234
I527	D428	F322	I235
N528	Y429	Q323	L236
P531	R430	Q323	C237
Q532	E431	T325	E238
V533	V432	G326	E239
P537	E433	V327	L240
A542	A434	R328	G241
L543	A437	S337	A242
K544	D443	G338	P243
T558	M448	D341	A244
V559	F449	R342	N245
T560	D450	V343	N249
T561	R451	A344	C250
	S452	N345	V251
	F453	K348	P252
	K456	G357	L253
	Q457	K358	E254
	Y461	K359	H259
	D462	S358	P261
	K463	K369	D262
	D471	L370	P263
	N472	D383	N264
	F473	H364	Y267
		I385	D270
			L271
			E279

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.42Å 174.42Å 101.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.7 (6.00-2.70) 85.7 (6.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , 0.244 0.213 , 0.244	Depositor DCC
R_{free} test set	3802 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.1	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	9010	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, SO4, SEP

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	11/4409 (0.2%)	2.10	182/5958 (3.1%)
1	B	1.04	16/4409 (0.4%)	2.04	143/5958 (2.4%)
All	All	1.02	27/8818 (0.3%)	2.07	325/11916 (2.7%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	HIS	CD2-NE2	-7.22	1.29	1.37
1	A	117	HIS	CD2-NE2	-7.15	1.29	1.37
1	B	415	HIS	CD2-NE2	-7.05	1.30	1.37
1	A	415	HIS	CD2-NE2	-6.80	1.30	1.37
1	B	117	HIS	CD2-NE2	-6.76	1.30	1.37
1	B	299	HIS	CD2-NE2	-6.66	1.30	1.37
1	B	260	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	384	HIS	CD2-NE2	-6.58	1.30	1.37
1	B	500	ILE	CA-CB	6.43	1.64	1.54
1	A	280	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	417	HIS	CD2-NE2	-6.15	1.31	1.37
1	B	259	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	168	VAL	CA-CB	6.12	1.59	1.53
1	B	280	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	417	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	476	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	260	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	476	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	299	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	225	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	384	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	259	HIS	CD2-NE2	-5.60	1.31	1.37
1	B	68	GLU	CA-CB	-5.21	1.45	1.53
1	B	225	HIS	CG-ND1	-5.10	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	ILE	CA-CB	5.09	1.60	1.54
1	B	319	ILE	CA-CB	5.03	1.58	1.54
1	B	260	HIS	CG-ND1	-5.02	1.32	1.38

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	N-CA-C	11.39	123.26	111.07
1	A	37	ASN	OD1-CG-ND2	-11.15	111.45	122.60
1	A	532	GLN	OE1-CD-NE2	-10.83	111.77	122.60
1	A	10	ALA	N-CA-C	10.74	124.50	110.43
1	B	10	ALA	N-CA-C	10.70	124.14	110.24
1	A	529	GLN	OE1-CD-NE2	-10.50	112.10	122.60
1	A	205	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	B	168	VAL	N-CA-C	10.37	123.64	107.98
1	B	315	ASN	OD1-CG-ND2	-10.29	112.31	122.60
1	A	250	CYS	N-CA-C	10.23	124.13	112.57
1	A	291	ASP	CA-CB-CG	10.06	122.66	112.60
1	B	37	ASN	OD1-CG-ND2	-9.99	112.61	122.60
1	B	215	ASN	OD1-CG-ND2	-9.96	112.64	122.60
1	A	547	GLN	OE1-CD-NE2	-9.84	112.77	122.60
1	A	80	ASN	CA-CB-CG	-9.78	102.82	112.60
1	B	434	ALA	N-CA-C	9.64	121.79	111.28
1	B	524	ASN	OD1-CG-ND2	-9.58	113.02	122.60
1	A	178	ASN	OD1-CG-ND2	-9.51	113.09	122.60
1	A	383	ASP	CA-CB-CG	9.28	121.88	112.60
1	B	153	ILE	N-CA-C	9.27	121.53	107.99
1	A	527	ILE	N-CA-C	9.19	121.10	110.62
1	B	472	ASN	N-CA-C	-9.03	93.79	108.52
1	A	309	VAL	CB-CA-C	-8.98	100.02	112.14
1	A	168	VAL	N-CA-C	8.96	120.09	107.37
1	A	322	PHE	CA-CB-CG	-8.96	104.84	113.80
1	B	216	ARG	N-CA-C	8.85	123.06	110.23
1	A	13	ASP	N-CA-C	8.81	122.80	112.93
1	A	473	PHE	N-CA-C	8.79	123.48	110.30
1	B	180	PHE	N-CA-C	8.77	120.45	111.07
1	A	462	ASP	N-CA-C	8.74	120.89	111.36
1	A	180	PHE	N-CA-C	8.69	121.85	111.33
1	A	123	ASN	OD1-CG-ND2	-8.64	113.95	122.60
1	A	328	ARG	N-CA-C	8.59	122.52	112.72
1	A	461	ASN	OD1-CG-ND2	-8.57	114.03	122.60
1	B	291	ASP	CA-CB-CG	8.48	121.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	CYS	N-CA-C	8.45	121.93	112.97
1	A	33	ASN	OD1-CG-ND2	-8.45	114.16	122.60
1	B	532	GLN	OE1-CD-NE2	-8.39	114.21	122.60
1	B	29	GLN	OE1-CD-NE2	-8.33	114.27	122.60
1	B	192	GLU	N-CA-C	8.33	121.18	111.02
1	A	472	ASN	OD1-CG-ND2	-8.32	114.28	122.60
1	A	317	PHE	CA-CB-CG	-8.25	105.55	113.80
1	A	459	SER	N-CA-C	8.24	120.63	108.60
1	A	471	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	52	GLN	OE1-CD-NE2	-8.23	114.37	122.60
1	B	144	ASP	CA-CB-CG	8.22	120.82	112.60
1	B	168	VAL	N-CA-CB	-8.21	101.87	111.39
1	B	430	GLU	N-CA-C	8.15	128.15	110.80
1	A	264	ASN	CA-CB-CG	8.12	120.72	112.60
1	B	293	ASN	N-CA-C	8.01	121.56	108.99
1	B	345	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	B	211	LEU	N-CA-C	7.94	123.30	112.90
1	A	215	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	A	192	GLU	N-CA-C	7.88	120.64	111.02
1	B	200	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	457	GLN	OE1-CD-NE2	-7.87	114.73	122.60
1	B	178	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	A	50	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	A	360	PHE	CA-CB-CG	-7.73	106.07	113.80
1	B	358	TRP	N-CA-C	7.63	127.05	110.80
1	B	471	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	71	GLN	OE1-CD-NE2	-7.56	115.04	122.60
1	B	254	GLU	N-CA-C	7.55	121.42	111.75
1	A	304	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	B	13	ASP	N-CA-C	7.52	122.17	112.92
1	B	293	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	188	VAL	N-CA-CB	-7.47	95.52	111.37
1	B	490	ARG	N-CA-C	7.47	120.70	108.52
1	A	450	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	422	ASN	OD1-CG-ND2	-7.45	115.16	122.60
1	B	528	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	A	293	ASN	N-CA-C	7.40	120.70	109.23
1	A	260	HIS	CA-CB-CG	7.37	121.17	113.80
1	A	417	HIS	CA-CB-CG	-7.37	106.43	113.80
1	A	404	ARG	N-CA-C	7.35	119.29	111.28
1	B	260	HIS	CA-C-O	-7.30	113.92	119.32
1	A	227	VAL	N-CA-C	7.21	120.06	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	CB-CG-ND2	7.17	127.16	116.40
1	A	84	ARG	N-CA-C	7.17	121.25	109.06
1	A	549	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	B	337	SER	N-CA-C	7.17	119.82	110.43
1	B	463	LYS	N-CA-C	7.16	120.76	110.24
1	B	270	ASP	CA-CB-CG	-7.14	105.45	112.60
1	A	422	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	B	188	VAL	O-C-N	-7.14	115.55	122.98
1	A	524	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	A	205	ASN	CB-CG-ND2	7.11	127.07	116.40
1	B	524	ASN	CB-CG-ND2	7.10	127.05	116.40
1	A	315	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	A	5	THR	CA-CB-OG1	-7.05	99.02	109.60
1	B	389	ASP	N-CA-C	7.04	120.54	108.02
1	A	148	GLN	OE1-CD-NE2	-7.02	115.58	122.60
1	A	211	LEU	N-CA-C	6.99	121.56	112.89
1	A	490	ARG	N-CA-C	6.99	121.06	108.69
1	A	75	ARG	N-CA-C	6.97	118.88	111.28
1	B	84	ARG	N-CA-C	6.96	120.87	109.24
1	B	384	HIS	CB-CG-CD2	-6.96	122.16	131.20
1	A	14	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	A	471	ASP	N-CA-C	6.95	118.33	108.74
1	B	239	GLU	N-CA-C	6.95	119.45	111.11
1	A	503	LEU	N-CA-C	6.93	120.19	107.99
1	A	276	LYS	N-CA-C	6.92	118.83	111.28
1	A	245	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	B	317	PHE	CA-CB-CG	-6.91	106.89	113.80
1	A	254	GLU	N-CA-C	6.84	120.51	111.75
1	B	54	ALA	N-CA-C	6.83	120.82	109.95
1	B	117	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	168	VAL	N-CA-CB	-6.83	104.52	111.90
1	B	33	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	229	GLY	CA-C-N	6.80	127.07	119.32
1	A	229	GLY	C-N-CA	6.80	127.07	119.32
1	B	448	MET	N-CA-C	6.79	118.68	111.28
1	B	370	LEU	N-CA-C	6.77	119.45	108.34
1	B	520	TYR	N-CA-C	6.76	119.15	108.67
1	B	345	ASN	CB-CG-ND2	6.75	126.53	116.40
1	B	323	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	B	302	PHE	N-CA-C	6.73	119.48	109.59
1	B	428	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	172	GLN	OE1-CD-NE2	-6.70	115.90	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	PHE	CA-CB-CG	-6.66	107.14	113.80
1	B	415	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	A	476	HIS	CB-CG-CD2	-6.65	122.56	131.20
1	A	458	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	279	GLU	N-CA-C	6.62	119.33	111.71
1	A	264	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	B	472	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	462	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	245	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	B	4	VAL	N-CA-C	6.53	117.31	108.17
1	A	172	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	B	51	ARG	N-CA-C	6.51	118.17	111.14
1	B	114	THR	CB-CA-C	-6.49	96.12	109.94
1	B	205	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	B	240	LEU	N-CA-C	6.47	121.19	113.16
1	A	171	LYS	N-CA-C	6.43	120.13	109.46
1	B	558	THR	CA-C-O	6.42	127.37	120.24
1	A	32	THR	CA-CB-OG1	-6.39	100.02	109.60
1	A	289	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	29	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	B	236	LEU	N-CA-C	6.38	119.54	111.69
1	A	169	LEU	O-C-N	-6.38	114.97	122.81
1	A	323	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	B	487	GLN	N-CA-C	6.34	120.87	113.20
1	A	118	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	461	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	61	ASP	N-CA-C	6.30	120.43	112.87
1	A	189	ASP	O-C-N	-6.30	115.43	122.86
1	A	133	SER	N-CA-C	6.29	119.81	111.75
1	A	324	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	A	453	PHE	CA-CB-CG	-6.28	107.53	113.80
1	B	80	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	164	VAL	CA-C-O	-6.23	115.86	121.97
1	B	227	VAL	N-CA-C	6.21	119.74	111.17
1	B	171	LYS	N-CA-C	6.17	120.33	109.96
1	A	434	ALA	N-CA-C	6.17	123.94	110.80
1	B	527	ILE	N-CA-C	6.17	122.17	109.34
1	B	518	ASP	CA-C-O	6.16	127.09	120.32
1	B	302	PHE	CA-CB-CG	6.13	119.93	113.80
1	B	406	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	417	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	A	421	ARG	O-C-N	-6.10	116.09	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	HIS	CA-CB-CG	6.10	119.90	113.80
1	A	528	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	178	ASN	CB-CG-ND2	6.07	125.50	116.40
1	A	337	SER	CB-CA-C	-6.07	98.34	110.42
1	A	529	GLN	N-CA-C	6.05	118.34	110.53
1	B	50	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	155	GLU	N-CA-C	6.04	118.59	109.23
1	B	396	ALA	N-CA-C	-6.02	104.80	111.36
1	A	551	ARG	N-CA-C	6.01	120.16	112.34
1	A	54	ALA	N-CA-C	6.00	119.68	110.20
1	A	200	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	392	TRP	CG-CD2-CE3	5.98	139.88	133.90
1	A	163	LYS	O-C-N	-5.97	116.35	123.28
1	A	345	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	A	332	ARG	NE-CZ-NH2	5.95	124.55	119.20
1	A	131	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	506	THR	N-CA-C	5.90	118.29	108.20
1	B	414	ASP	N-CA-CB	-5.90	101.14	110.28
1	A	238	GLU	CA-CB-CG	-5.89	102.31	114.10
1	A	52	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	248	VAL	CB-CA-C	-5.88	102.91	111.68
1	A	235	ILE	N-CA-C	5.87	116.08	110.74
1	B	30	SER	CA-CB-OG	5.86	122.82	111.10
1	A	188	VAL	CB-CA-C	5.86	120.15	111.31
1	A	188	VAL	O-C-N	-5.85	116.02	122.69
1	A	350	ALA	N-CA-C	5.84	118.70	110.23
1	A	117	HIS	CB-CG-CD2	-5.83	123.61	131.20
1	A	463	LYS	N-CA-C	5.83	118.72	110.14
1	B	386	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	A	80	ASN	N-CA-C	5.80	120.20	113.18
1	B	523	ASP	CA-C-O	5.79	127.30	120.58
1	A	316	ILE	N-CA-CB	-5.78	101.69	111.23
1	B	299	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	216	ARG	N-CA-C	5.77	123.10	110.80
1	A	383	ASP	N-CA-C	5.77	120.02	113.15
1	A	476	HIS	CB-CG-ND1	5.76	131.35	122.70
1	A	14	GLN	CG-CD-NE2	5.76	125.04	116.40
1	B	221	ILE	CB-CG1-CD1	5.74	125.86	113.80
1	A	280	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	B	280	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	B	487	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	A	32	THR	CA-CB-CG2	5.71	120.22	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ILE	O-C-N	-5.71	116.48	122.81
1	B	219	ILE	N-CA-C	5.71	117.64	108.85
1	A	494	ALA	N-CA-C	5.70	119.49	112.54
1	B	312	ILE	CA-C-O	-5.69	115.20	121.29
1	A	333	SER	O-C-N	-5.69	116.36	122.85
1	A	5	THR	CA-CB-CG2	5.69	120.17	110.50
1	A	80	ASN	OD1-CG-ND2	-5.67	116.92	122.60
1	A	40	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	B	249	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	57	VAL	O-C-N	-5.64	115.56	122.61
1	A	126	PHE	O-C-N	-5.64	116.48	123.36
1	A	486	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	A	392	TRP	CE2-CD2-CG	-5.63	100.44	107.20
1	A	238	GLU	N-CA-C	5.61	117.07	111.07
1	A	456	LYS	N-CA-C	5.60	118.57	110.28
1	A	22	ARG	NH1-CZ-NH2	-5.59	112.04	119.30
1	A	287	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	357	GLY	N-CA-C	5.58	126.40	113.18
1	A	71	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	164	VAL	N-CA-C	5.57	116.78	109.21
1	B	169	LEU	N-CA-C	5.57	117.48	110.24
1	A	177	GLU	CA-CB-CG	5.56	125.22	114.10
1	B	473	PHE	N-CA-C	5.55	118.38	110.10
1	B	92	ILE	N-CA-C	5.55	116.36	107.98
1	A	406	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	397	TRP	CE2-CD2-CG	-5.54	100.55	107.20
1	B	241	GLY	N-CA-C	5.54	123.00	115.30
1	A	495	ASP	CA-C-O	5.53	126.17	119.31
1	A	309	VAL	N-CA-CB	5.53	118.06	110.54
1	B	65	TYR	N-CA-CB	-5.52	107.87	114.17
1	B	103	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	B	47	GLU	CA-C-N	5.52	126.74	119.84
1	B	47	GLU	C-N-CA	5.52	126.74	119.84
1	A	358	TRP	N-CA-C	5.51	120.46	111.37
1	B	43	ILE	CB-CA-C	-5.51	104.70	112.14
1	B	343	VAL	N-CA-C	-5.50	105.48	110.82
1	B	188	VAL	N-CA-CB	-5.49	98.85	111.81
1	B	404	ARG	N-CA-C	5.49	119.15	112.23
1	A	144	ASP	CA-CB-CG	-5.48	107.12	112.60
1	A	293	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	528	ASN	N-CA-C	5.47	119.95	113.16
1	A	163	LYS	N-CA-C	5.46	116.33	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	THR	N-CA-C	5.46	118.44	109.76
1	A	21	LEU	N-CA-C	5.43	117.32	108.63
1	B	271	LEU	N-CA-C	-5.43	105.25	111.07
1	A	222	ASP	CA-C-O	5.43	126.17	120.36
1	B	89	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	415	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	B	121	GLY	CA-C-N	5.42	124.87	119.24
1	B	121	GLY	C-N-CA	5.42	124.87	119.24
1	B	415	HIS	CB-CG-ND1	5.42	130.82	122.70
1	A	370	LEU	N-CA-C	5.41	117.44	108.13
1	B	23	LYS	O-C-N	-5.41	116.59	122.92
1	B	234	LYS	N-CA-C	5.38	117.14	111.28
1	A	173	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	431	GLU	N-CA-C	5.36	122.22	110.80
1	A	316	ILE	N-CA-C	5.36	120.49	109.34
1	A	169	LEU	N-CA-C	5.36	117.64	110.35
1	B	52	GLN	CG-CD-NE2	5.35	124.42	116.40
1	A	36	GLU	CB-CA-C	-5.34	102.27	110.81
1	A	8	THR	O-C-N	-5.33	116.97	122.84
1	B	384	HIS	CB-CG-ND1	5.33	130.70	122.70
1	A	328	ARG	CB-CG-CD	-5.32	99.07	111.30
1	A	153	ILE	N-CA-C	5.31	116.10	108.93
1	A	59	GLY	CA-C-O	-5.31	116.55	121.96
1	A	187	ILE	CA-C-O	5.30	126.86	120.65
1	B	133	SER	N-CA-C	5.30	122.09	110.80
1	A	93	LEU	O-C-N	-5.30	116.08	123.34
1	A	304	ASN	CB-CG-ND2	5.29	124.33	116.40
1	B	559	VAL	N-CA-C	5.28	116.32	108.46
1	A	94	SER	N-CA-C	5.28	116.90	110.41
1	B	430	GLU	O-C-N	-5.28	115.57	122.59
1	B	5	THR	CA-CB-OG1	-5.27	101.70	109.60
1	A	219	ILE	N-CA-C	5.25	116.71	109.46
1	B	419	PHE	N-CA-C	5.25	119.78	112.90
1	B	188	VAL	N-CA-C	5.25	116.87	108.89
1	B	328	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	B	433	GLU	CA-CB-CG	5.23	124.57	114.10
1	A	392	TRP	CB-CG-CD1	-5.23	119.05	126.90
1	B	443	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	532	GLN	CG-CD-NE2	5.22	124.24	116.40
1	B	279	GLU	N-CA-C	5.22	116.97	111.28
1	B	383	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	416	TRP	O-C-N	-5.20	115.88	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	TYR	N-CA-C	5.20	118.78	112.23
1	A	178	ASN	CA-CB-CG	5.19	117.79	112.60
1	B	190	SER	N-CA-C	5.19	117.61	111.33
1	B	533	VAL	O-C-N	-5.18	116.49	121.83
1	A	375	GLU	O-C-N	-5.18	116.95	123.27
1	B	239	GLU	O-C-N	-5.18	116.70	122.09
1	A	259	HIS	CA-CB-CG	5.17	118.97	113.80
1	B	144	ASP	N-CA-C	-5.16	105.56	111.14
1	B	184	THR	N-CA-C	5.16	117.89	109.59
1	B	29	GLN	N-CA-C	5.15	119.42	113.18
1	A	397	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	B	161	ASP	N-CA-C	5.15	118.82	112.54
1	B	311	VAL	N-CA-C	-5.15	105.83	110.82
1	A	526	LYS	N-CA-C	5.14	117.78	111.82
1	B	95	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	212	SER	N-CA-C	5.13	120.38	113.72
1	B	171	LYS	N-CA-CB	-5.12	101.93	110.23
1	A	63	ARG	N-CA-C	5.12	117.13	110.43
1	A	358	TRP	CA-CB-CG	-5.12	103.88	113.60
1	B	494	ALA	N-CA-C	5.11	118.98	112.34
1	A	123	ASN	CB-CG-ND2	5.10	124.06	116.40
1	A	389	ASP	CA-C-N	5.08	125.58	119.94
1	A	389	ASP	C-N-CA	5.08	125.58	119.94
1	B	148	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	173	GLN	CG-CD-NE2	5.07	124.00	116.40
1	A	162	LEU	N-CA-C	5.06	117.77	110.28
1	B	215	ASN	CB-CG-ND2	5.05	123.98	116.40
1	B	214	PRO	CA-C-O	5.05	127.06	119.74
1	A	430	GLU	N-CA-C	5.04	117.61	110.10
1	A	520	TYR	N-CA-C	5.04	116.96	109.25
1	B	8	THR	N-CA-C	5.04	117.77	110.17
1	A	475	TYR	N-CA-C	5.03	117.60	109.40
1	A	387	GLU	CB-CA-C	-5.03	101.90	110.95
1	A	337	SER	N-CA-C	5.01	121.48	110.80
1	B	136	GLY	CA-C-N	5.01	124.78	119.76
1	B	136	GLY	C-N-CA	5.01	124.78	119.76
1	A	319	ILE	CA-C-N	5.01	126.11	119.84
1	A	319	ILE	C-N-CA	5.01	126.11	119.84

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	4333	0	4331	76	0
1	B	4333	0	4331	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	136	0	0	7	0
4	B	196	0	0	8	0
All	All	9010	0	8662	133	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 8.

All (133) 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:114:THR:HG21	1:B:289:ASP:HB3	1.46	0.94
1:A:14:GLN:HE21	1:A:150:SER:HB2	1.52	0.73
1:A:505:GLY:HA2	1:A:511:ALA:HA	1.71	0.73
1:B:33:ASN:HB3	1:B:37:ASN:ND2	2.03	0.73
1:A:357:GLY:HA3	1:A:359:LYS:HE3	1.78	0.66
1:B:68:GLU:HB2	4:B:715:HOH:O	1.98	0.63
1:B:271:LEU:HD13	1:B:296:LEU:HD12	1.80	0.63
1:A:519:SER:HB3	1:A:538:LEU:HD12	1.80	0.62
1:A:301:PHE:HE2	1:A:412:LEU:HD12	1.66	0.61
1:A:426:ARG:HG3	1:A:516:TYR:CD1	2.35	0.61
1:B:473:PHE:HB2	1:B:490:ARG:HD2	1.82	0.60
1:B:368:SER:HA	4:B:653:HOH:O	2.00	0.60
1:A:440:MET:O	1:A:444:LEU:HB2	2.03	0.59
1:A:164:VAL:HG21	1:A:185:VAL:HG11	1.84	0.58
1:A:449:PHE:HE1	1:A:471:ASP:HA	1.69	0.58
1:B:426:ARG:HG3	1:B:516:TYR:CD1	2.38	0.58
1:A:453:PHE:HA	1:A:456:LYS:NZ	2.17	0.58
1:A:63:ARG:HB3	1:A:256:PHE:CE1	2.40	0.57
1:A:193:ALA:HB2	4:A:682:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.53	0.56
1:B:114:THR:CG2	1:B:289:ASP:HB3	2.30	0.56
1:A:218:LYS:HB2	1:A:218:LYS:NZ	2.21	0.56
1:A:210:LEU:HD22	1:A:217:LEU:HB2	1.87	0.55
1:B:359:LYS:H	1:B:359:LYS:HD3	1.72	0.55
1:A:453:PHE:HA	1:A:456:LYS:HZ1	1.70	0.55
1:B:243:PRO:HB2	1:B:245:ASN:OD1	2.07	0.55
1:B:423:PHE:HD2	1:B:531:PRO:HB3	1.72	0.55
1:A:268:ALA:O	1:A:272:VAL:HG23	2.07	0.54
1:A:459:SER:OG	1:A:464:VAL:HA	2.07	0.54
1:A:306:SER:HB3	1:A:337:SER:HB2	1.87	0.54
1:A:219:ILE:HG22	1:A:282:PHE:HB3	1.88	0.54
1:A:382:SER:OG	1:A:384:HIS:HD2	1.91	0.54
1:A:311:VAL:HG11	1:A:397:TRP:CH2	2.44	0.53
1:B:43:ILE:HG23	1:B:82:ILE:HD11	1.91	0.52
1:A:220:ARG:NH1	1:A:274:THR:HG21	2.25	0.52
1:A:432:VAL:HG22	1:A:511:ALA:O	2.09	0.52
1:A:1:VAL:HG11	1:A:162:LEU:HD12	1.91	0.52
1:A:437:ALA:O	1:A:441:MET:HG2	2.10	0.51
1:B:33:ASN:HB3	1:B:37:ASN:HD22	1.76	0.51
1:A:440:MET:HE1	1:A:513:ILE:HD13	1.93	0.51
1:B:451:ARG:HD3	1:B:451:ARG:H	1.75	0.51
1:A:497:SER:HB3	1:A:538:LEU:HD11	1.91	0.51
1:A:61:ASP:HA	1:A:227:VAL:HB	1.94	0.50
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.77	0.50
1:A:16:PRO:HB2	1:A:143:THR:HG22	1.93	0.50
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.94	0.50
1:A:151:LYS:HG2	4:A:566:HOH:O	2.11	0.49
1:A:182:PRO:HA	4:A:652:HOH:O	2.12	0.49
1:A:239:GLU:HB2	1:B:168:VAL:HG21	1.94	0.49
1:A:69:ALA:O	1:A:72:LEU:HB2	2.12	0.49
1:A:365:MET:HG3	1:A:370:LEU:HD23	1.95	0.49
1:A:526:LYS:HD2	1:A:534:MET:HE1	1.94	0.49
1:A:301:PHE:CE2	1:A:412:LEU:HD12	2.48	0.49
1:B:106:LYS:NZ	4:B:721:HOH:O	2.40	0.49
1:B:220:ARG:O	1:B:283:GLY:HA2	2.13	0.49
1:B:129:LYS:NZ	1:B:387:GLU:OE1	2.46	0.49
1:A:14:GLN:NE2	1:A:150:SER:HB2	2.23	0.49
1:A:384:HIS:CE1	1:A:385:ILE:HG12	2.47	0.49
1:A:549:GLN:O	1:A:553:GLY:HA2	2.13	0.49
1:B:232:VAL:HG13	1:B:236:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ARG:NH2	4:A:659:HOH:O	2.47	0.48
1:A:388:LYS:NZ	4:A:579:HOH:O	2.47	0.48
1:A:24:ARG:HA	1:A:125:ASP:HA	1.96	0.48
1:B:216:ARG:NH2	1:B:243:PRO:HG3	2.29	0.47
1:A:29:GLN:HE22	1:A:64:PHE:HE2	1.62	0.47
1:B:544:LYS:HE2	4:B:677:HOH:O	2.15	0.46
1:B:432:VAL:CG1	1:B:437:ALA:HB2	2.45	0.46
1:B:261:PRO:HB2	1:B:288:GLY:N	2.31	0.46
1:A:36:GLU:HG2	1:A:156:TYR:CZ	2.51	0.46
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.97	0.46
1:B:456:LYS:NZ	1:B:457:GLN:O	2.49	0.46
1:A:438:THR:O	1:A:442:LYS:HG2	2.16	0.46
1:B:73:ILE:HD13	1:B:111:ILE:HG21	1.97	0.46
1:A:236:LEU:HD23	1:A:240:LEU:HD12	1.97	0.46
1:A:71:GLN:HB3	1:A:75:ARG:HH12	1.79	0.45
1:B:338:GLY:HA2	1:B:341:ASP:OD1	2.16	0.45
1:A:298:LYS:HG3	4:A:606:HOH:O	2.16	0.45
1:A:439:LYS:HE3	1:A:439:LYS:HB2	1.78	0.45
1:B:149:ILE:O	1:B:153:ILE:HB	2.16	0.45
1:A:147:PHE:CZ	1:A:151:LYS:HD2	2.50	0.45
1:B:501:PHE:CE1	1:B:515:LEU:HD13	2.51	0.45
1:A:473:PHE:HA	4:A:697:HOH:O	2.16	0.45
1:A:539:ILE:O	1:A:543:LEU:HD23	2.15	0.45
1:A:14:GLN:O	1:A:16:PRO:HD3	2.16	0.45
1:A:431:GLU:O	1:A:554:ARG:NH2	2.50	0.45
1:B:383:ASP:O	1:B:386:ARG:NH2	2.50	0.45
1:A:275:MET:HG3	1:A:296:LEU:HD13	1.97	0.45
1:B:348:LYS:HA	4:B:647:HOH:O	2.16	0.44
1:B:499:ILE:HD13	1:B:542:ALA:HB2	1.98	0.44
1:A:440:MET:HG3	1:A:546:SER:O	2.18	0.44
1:A:504:SER:HB2	1:A:512:THR:HB	2.00	0.44
1:B:426:ARG:HG3	1:B:516:TYR:CE1	2.52	0.44
1:A:15:LYS:HA	1:A:16:PRO:HD3	1.83	0.44
1:B:520:TYR:OH	1:B:522:LYS:HD3	2.17	0.44
1:B:262:ASP:HA	1:B:263:PRO:HD2	1.91	0.43
1:A:343:VAL:HA	1:A:419:PHE:CE1	2.53	0.43
1:B:449:PHE:HE1	1:B:471:ASP:HA	1.82	0.43
1:A:33:ASN:HB3	1:A:37:ASN:HD22	1.82	0.43
1:A:198:LEU:HD13	1:A:395:LEU:HD12	2.01	0.43
1:B:453:PHE:O	1:B:456:LYS:HB3	2.19	0.43
1:A:286:PHE:CZ	1:A:394:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:HG	1:A:352:TYR:N	2.31	0.43
1:A:71:GLN:HB3	1:A:75:ARG:NH1	2.34	0.42
1:B:463:LYS:HE3	4:B:678:HOH:O	2.18	0.42
1:A:20:GLY:HA3	1:A:129:LYS:HA	2.00	0.42
1:B:117:HIS:HB3	1:B:292:ARG:NH2	2.34	0.42
1:B:322:PHE:HA	1:B:325:THR:HG22	2.01	0.42
1:A:384:HIS:HE1	1:A:389:ASP:OD2	2.02	0.42
1:B:388:LYS:NZ	4:B:753:HOH:O	2.53	0.42
1:A:276:LYS:HA	1:A:299:HIS:C	2.45	0.42
1:B:20:GLY:HA3	1:B:129:LYS:HA	2.02	0.42
1:A:144:ASP:O	1:A:147:PHE:HB3	2.19	0.42
1:B:222:ASP:O	1:B:285:ALA:HA	2.19	0.42
1:A:56:LEU:HD23	1:A:108:ILE:HG22	2.00	0.42
1:A:102:ILE:HD11	1:A:110:GLY:HA3	2.01	0.41
1:B:1:VAL:N	1:B:175:ASP:O	2.52	0.41
1:B:358:TRP:CD1	1:B:388:LYS:HG3	2.54	0.41
1:A:429:TYR:HB2	1:A:513:ILE:HB	2.02	0.41
1:A:546:SER:O	1:A:551:ARG:NH1	2.53	0.41
1:B:218:LYS:HZ1	1:B:279:GLU:CD	2.28	0.41
1:B:325:THR:HG23	1:B:326:GLY:O	2.20	0.41
1:B:489:LEU:O	1:B:500:ILE:HA	2.20	0.41
1:B:104:LYS:HD2	4:B:575:HOH:O	2.21	0.41
1:B:410:ASP:O	1:B:414:ASP:HB3	2.20	0.41
1:A:459:SER:HG	1:A:464:VAL:HA	1.85	0.41
1:B:2:LYS:HZ3	1:B:161:ASP:CG	2.29	0.41
1:A:334:MET:HE3	1:A:334:MET:HB3	1.85	0.41
1:B:11:TYR:OH	1:B:31:SER:HB3	2.21	0.41
1:B:84:ARG:HH11	1:B:84:ARG:HD2	1.74	0.41
1:A:418:LYS:HE3	1:A:418:LYS:HB2	1.57	0.40
1:B:503:LEU:HD12	1:B:503:LEU:HA	1.90	0.40
1:B:427:TYR:HB2	1:B:515:LEU:HB3	2.02	0.40
1:B:199:ARG:NH1	1:B:239:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/561 (100%)	505 (90%)	44 (8%)	9 (2%)	7	20
1	B	558/561 (100%)	530 (95%)	20 (4%)	8 (1%)	9	23
All	All	1116/1122 (100%)	1035 (93%)	64 (6%)	17 (2%)	8	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	431	GLU
1	B	358	TRP
1	A	224	MET
1	A	301	PHE
1	A	434	ALA
1	A	467	VAL
1	B	133	SER
1	B	238	GLU
1	B	461	ASN
1	B	508	SER
1	A	508	SER
1	B	462	ASP
1	A	337	SER
1	B	430	GLU
1	B	301	PHE
1	A	316	ILE

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	461/461 (100%)	428 (93%)	33 (7%)	13	32
1	B	461/461 (100%)	426 (92%)	35 (8%)	12	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	922/922 (100%)	854 (93%)	68 (7%)	13	32

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	47	GLU
1	A	48	PRO
1	A	92	ILE
1	A	125	ASP
1	A	143	THR
1	A	144	ASP
1	A	163	LYS
1	A	199	ARG
1	A	208	LYS
1	A	210	LEU
1	A	218	LYS
1	A	227	VAL
1	A	230	PRO
1	A	234	LYS
1	A	243	PRO
1	A	248	VAL
1	A	291	ASP
1	A	309	VAL
1	A	358	TRP
1	A	359	LYS
1	A	380	THR
1	A	386	ARG
1	A	388	LYS
1	A	431	GLU
1	A	442	LYS
1	A	451	ARG
1	A	456	LYS
1	A	459	SER
1	A	527	ILE
1	A	544	LYS
1	A	548	LEU
1	A	549	GLN
1	B	7	LYS
1	B	15	LYS
1	B	48	PRO
1	B	53	GLU

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Mol	Chain	Res	Type
1	B	106	LYS
1	B	114	THR
1	B	143	THR
1	B	155	GLU
1	B	161	ASP
1	B	163	LYS
1	B	166	LEU
1	B	168	VAL
1	B	169	LEU
1	B	182	PRO
1	B	188	VAL
1	B	208	LYS
1	B	209	GLU
1	B	227	VAL
1	B	233	LYS
1	B	252	PRO
1	B	271	LEU
1	B	281	ASP
1	B	316	ILE
1	B	358	TRP
1	B	359	LYS
1	B	405	LYS
1	B	409	GLU
1	B	412	LEU
1	B	430	GLU
1	B	432	VAL
1	B	451	ARG
1	B	461	ASN
1	B	490	ARG
1	B	524	ASN
1	B	537	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	GLN
1	A	33	ASN
1	A	37	ASN
1	A	71	GLN
1	A	215	ASN
1	A	280	HIS

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	384	HIS
1	A	461	ASN
1	B	14	GLN
1	B	71	GLN
1	B	89	GLN
1	B	173	GLN
1	B	417	HIS
1	B	476	HIS
1	B	487	GLN
1	B	549	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	SEP	A	116	1,2	8,9,10	1.63	1 (12%)	7,12,14	3.34	1 (14%)
1	SEP	B	116	1,2	8,9,10	1.75	1 (12%)	7,12,14	2.97	1 (14%)

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
1	SEP	A	116	1,2	-	2/6/8/10	-
1	SEP	B	116	1,2	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	SEP	P-OG	-3.73	1.48	1.60
1	A	116	SEP	P-OG	-2.98	1.50	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	SEP	OG-CB-CA	8.58	116.49	108.14
1	B	116	SEP	OG-CB-CA	7.51	115.45	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	116	SEP	N-CA-CB-OG
1	A	116	SEP	C-CA-CB-OG
1	B	116	SEP	N-CA-CB-OG
1	B	116	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	SO4	B	563	-	4,4,4	0.38	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	563	-	4,4,4	0.43	0	6,6,6	0.41	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	560/561 (99%)	0.02	28 (5%) 34 30	0, 34, 88, 98	0
1	B	560/561 (99%)	-0.54	2 (0%) 88 87	3, 25, 58, 89	0
All	All	1120/1122 (99%)	-0.26	30 (2%) 56 53	0, 28, 79, 98	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ASP	11.2
1	A	507	GLY	9.5
1	A	461	ASN	9.3
1	A	509	ALA	8.6
1	A	528	ASN	8.6
1	A	508	SER	8.2
1	A	529	GLN	6.3
1	A	530	ASP	5.9
1	A	446	ALA	5.7
1	A	463	LYS	5.7
1	A	506	THR	5.1
1	B	505	GLY	4.1
1	B	507	GLY	4.1
1	A	510	GLY	4.1
1	A	437	ALA	3.8
1	A	443	ASP	3.6
1	A	450	ASP	3.5
1	A	452	SER	3.4
1	A	434	ALA	3.2
1	A	460	ALA	3.2
1	A	459	SER	3.1
1	A	464	VAL	3.1
1	A	453	PHE	2.9
1	A	552	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	532	GLN	2.4
1	A	555	THR	2.3
1	A	543	LEU	2.1
1	A	414	ASP	2.1
1	A	536	ALA	2.0
1	A	547	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	SEP	B	116	10/11	0.73	0.15	19,29,47,49	0
1	SEP	A	116	10/11	0.89	0.12	23,30,44,46	0

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(Å ²)	Q<0.9
3	SO4	A	563	5/5	0.86	0.13	95,95,96,96	0
3	SO4	B	563	5/5	0.86	0.16	90,90,90,91	0
2	CD	A	562	1/1	0.92	0.27	2,2,2,2	0
2	CD	B	562	1/1	0.97	0.23	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.