Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 AM GMT

PDB ID	:	2ONE
Title	:	ASYMMETRIC YEAST ENOLASE DIMER COMPLEXED WITH RESOLVED 2'-PHOSPHOGLYCERATE AND PHOSPHOENOLPYRUVATE
Authors	:	Lebioda, L.
Deposited on	:	1997-09-08
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

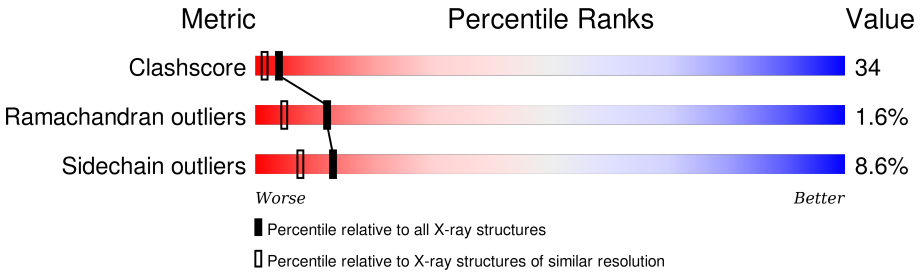
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	55% 31% 9% 5%
1	B	436	49% 37% 12% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6964 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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3292	2079	570	637	6			
1	B	436	Total	C	N	O	S	0	0	0
			3292	2079	570	637	6			

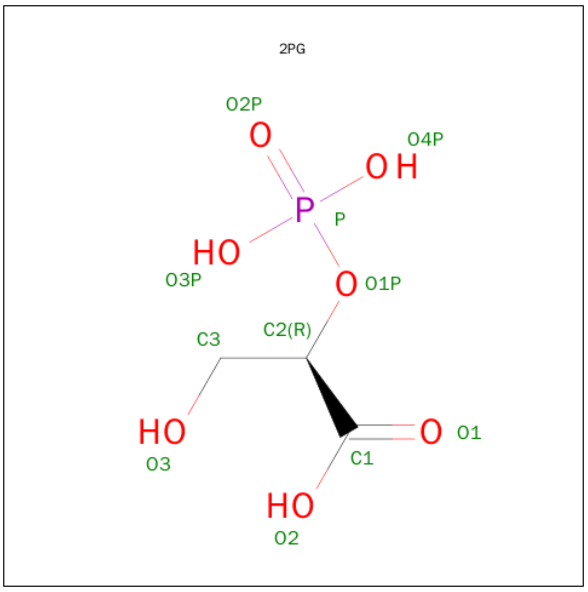
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is LITHIUM ION (three-letter code: LI) (formula: Li).

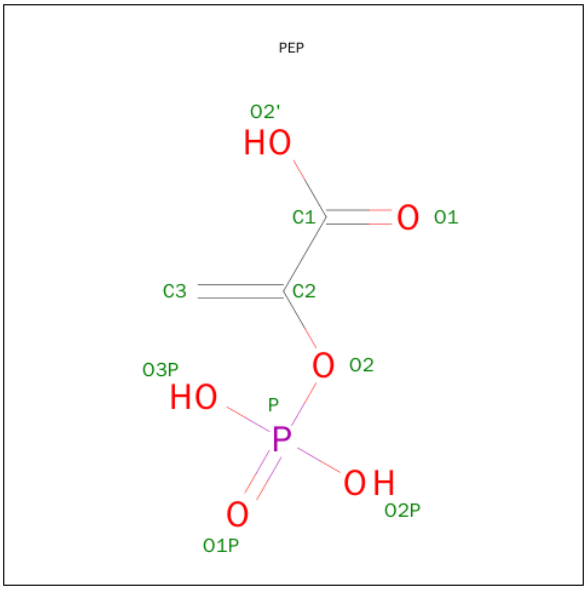
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Li	0	0
			1	1		

- Molecule 4 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	11	3	7	1	0	0

- Molecule 5 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	B	1	10	3	6	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	197	Total O 197 197	0	0
6	B	159	Total O 159 159	0	0

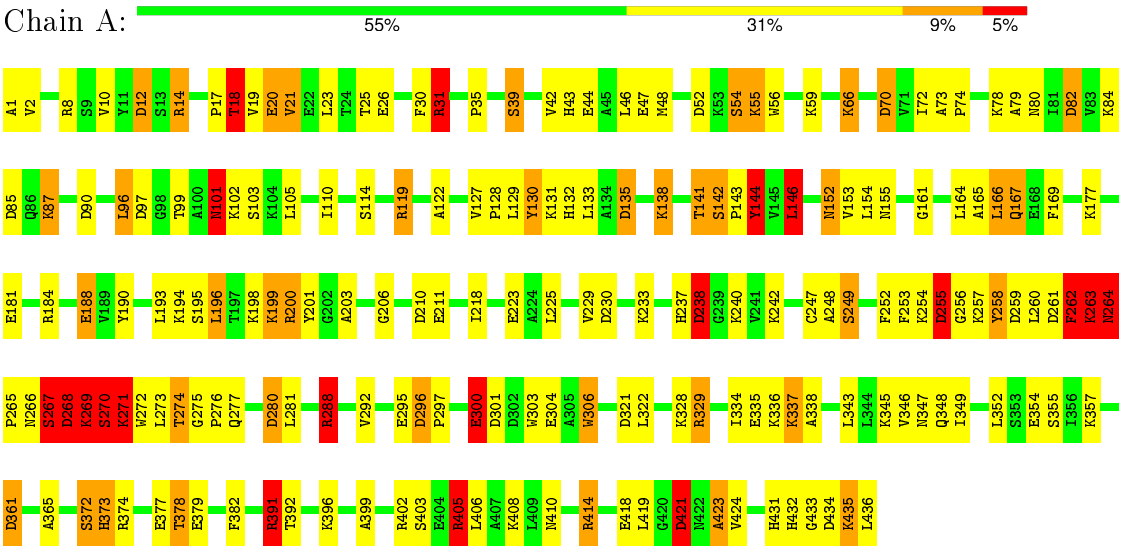
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

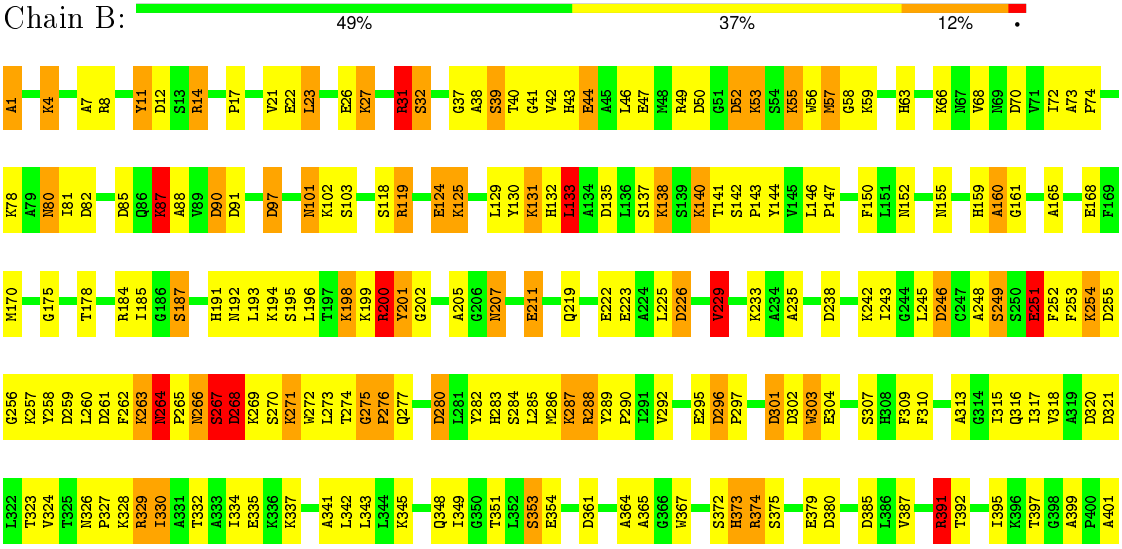
- Molecule 1: ENOLASE

Chain A:



- Molecule 1: ENOLASE

Chain B:




R402
S403
E404
R405
L406
A407
K408
Q411
R414
I415
E416
E417
E418
L419
H431
D434
K435
L436

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.10Å 110.00Å 66.20Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	9.00 – 2.00	Depositor
% Data completeness (in resolution range)	83.3 (9.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.137 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEP, 2PG, LI

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	0.92	2/3352 (0.1%)	2.06	101/4534 (2.2%)
1	B	0.88	0/3352	2.01	104/4534 (2.3%)
All	All	0.90	2/6704 (0.0%)	2.04	205/9068 (2.3%)

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	A	0	17
1	B	0	7
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ASN	C-O	9.63	1.41	1.23
1	A	264	ASN	C-N	6.98	1.47	1.34

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ARG	NE-CZ-NH1	22.65	131.62	120.30
1	A	267	SER	C-N-CA	21.41	175.22	121.70
1	A	31	ARG	NE-CZ-NH1	18.10	129.35	120.30
1	B	391	ARG	CD-NE-CZ	17.56	148.19	123.60
1	B	391	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	B	405	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	A	82	ASP	CB-CG-OD1	15.13	131.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	ASN	CA-C-O	-14.28	90.11	120.10
1	A	264	ASN	O-C-N	-14.23	94.06	121.10
1	B	391	ARG	NE-CZ-NH1	14.15	127.38	120.30
1	A	405	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	A	190	TYR	CB-CG-CD2	13.89	129.33	121.00
1	B	301	ASP	CB-CG-OD2	11.92	129.03	118.30
1	B	14	ARG	NE-CZ-NH1	-11.81	114.39	120.30
1	A	238	ASP	CB-CG-OD1	11.70	128.83	118.30
1	B	49	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	A	190	TYR	CB-CG-CD1	-11.23	114.26	121.00
1	A	85	ASP	CB-CG-OD1	11.00	128.20	118.30
1	A	8	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	A	300	GLU	OE1-CD-OE2	10.05	135.36	123.30
1	A	264	ASN	N-CA-C	9.89	137.70	111.00
1	A	414	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	A	31	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	A	288	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	B	321	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	B	246	ASP	CB-CG-OD2	8.95	126.36	118.30
1	B	200	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	A	82	ASP	CB-CG-OD2	-8.82	110.37	118.30
1	A	181	GLU	OE1-CD-OE2	-8.78	112.76	123.30
1	B	329	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	96	LEU	CA-CB-CG	8.40	134.63	115.30
1	A	258	TYR	CB-CG-CD2	8.40	126.04	121.00
1	B	97	ASP	CB-CG-OD1	8.25	125.73	118.30
1	A	265	PRO	N-CA-CB	8.15	113.08	103.30
1	B	184	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	A	262	PHE	CA-C-O	8.09	137.09	120.10
1	B	187	SER	N-CA-CB	8.07	122.61	110.50
1	B	8	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	269	LYS	N-CA-CB	8.01	125.02	110.60
1	B	271	LYS	C-N-CA	7.86	141.34	121.70
1	A	119	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	296	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	A	329	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	8	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	4	LYS	N-CA-CB	7.65	124.37	110.60
1	B	245	LEU	CA-CB-CG	7.63	132.86	115.30
1	A	405	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	184	ARG	NH1-CZ-NH2	-7.57	111.07	119.40
1	A	379	GLU	CA-CB-CG	7.51	129.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	223	GLU	OE1-CD-OE2	7.48	132.28	123.30
1	A	135	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	B	246	ASP	N-CA-CB	7.44	123.99	110.60
1	B	14	ARG	CD-NE-CZ	-7.43	113.20	123.60
1	A	70	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	4	LYS	CA-CB-CG	7.39	129.67	113.40
1	B	380	ASP	CB-CG-OD1	7.26	124.84	118.30
1	B	201	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	B	296	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	258	TYR	CB-CG-CD1	-7.14	116.71	121.00
1	B	118	SER	N-CA-CB	7.13	121.20	110.50
1	A	414	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	A	130	TYR	CB-CG-CD1	-7.09	116.75	121.00
1	B	8	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	A	141	THR	CA-CB-CG2	7.01	122.22	112.40
1	B	52	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	97	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	264	ASN	CA-CB-CG	-6.98	98.04	113.40
1	B	14	ARG	NH1-CZ-NH2	6.87	126.95	119.40
1	B	124	GLU	CG-CD-OE1	-6.87	104.57	118.30
1	A	200	ARG	CD-NE-CZ	-6.82	114.05	123.60
1	A	280	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	B	414	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	B	367	TRP	CA-CB-CG	6.77	126.56	113.70
1	B	50	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	A	255	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	222	GLU	CG-CD-OE1	6.58	131.46	118.30
1	B	1	ALA	N-CA-CB	6.58	119.31	110.10
1	B	52	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	A	262	PHE	CA-C-N	-6.46	102.98	117.20
1	B	374	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	391	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	181	GLU	CG-CD-OE1	6.41	131.12	118.30
1	B	434	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	144	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	B	280	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	B	49	ARG	NH1-CZ-NH2	6.37	126.41	119.40
1	B	124	GLU	OE1-CD-OE2	6.37	130.94	123.30
1	A	264	ASN	CB-CA-C	-6.32	97.76	110.40
1	B	90	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	B	32	SER	CB-CA-C	-6.29	98.14	110.10
1	B	301	ASP	CB-CG-OD1	-6.27	112.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	296	ASP	OD1-CG-OD2	-6.23	111.46	123.30
1	A	230	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	12	ASP	O-C-N	6.16	132.55	122.70
1	B	207	ASN	CB-CA-C	6.15	122.71	110.40
1	A	335	GLU	OE1-CD-OE2	6.14	130.67	123.30
1	A	166	LEU	CB-CA-C	6.12	121.83	110.20
1	B	57	MET	CA-C-N	6.11	128.42	116.20
1	A	47	GLU	CG-CD-OE1	6.09	130.48	118.30
1	B	329	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	150	PHE	CB-CG-CD1	-6.06	116.56	120.80
1	B	296	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	32	SER	O-C-N	6.03	132.35	122.70
1	B	405	ARG	NH1-CZ-NH2	6.03	126.03	119.40
1	A	146	LEU	CB-CA-C	6.02	121.64	110.20
1	A	165	ALA	O-C-N	6.02	132.33	122.70
1	A	361	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	193	LEU	CB-CA-C	6.00	121.59	110.20
1	B	417	GLU	OE1-CD-OE2	5.98	130.48	123.30
1	A	101	ASN	CB-CG-OD1	5.98	133.56	121.60
1	B	85	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	80	ASN	CB-CA-C	5.95	122.29	110.40
1	B	335	GLU	CA-CB-CG	5.94	126.47	113.40
1	A	254	LYS	CA-CB-CG	5.90	126.39	113.40
1	A	54	SER	CB-CA-C	5.89	121.29	110.10
1	A	378	THR	O-C-N	5.85	132.06	122.70
1	B	87	LYS	CB-CG-CD	5.85	126.81	111.60
1	A	154	LEU	CB-CA-C	5.84	121.30	110.20
1	B	380	ASP	OD1-CG-OD2	-5.82	112.24	123.30
1	B	161	GLY	N-CA-C	5.82	127.65	113.10
1	A	101	ASN	N-CA-CB	-5.81	100.14	110.60
1	B	170	MET	CG-SD-CE	5.78	109.45	100.20
1	B	44	GLU	CG-CD-OE2	-5.76	106.78	118.30
1	B	254	LYS	C-N-CA	5.76	136.10	121.70
1	B	263	LYS	C-N-CA	5.76	136.10	121.70
1	B	385	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	271	LYS	CB-CA-C	-5.76	98.88	110.40
1	A	20	GLU	CG-CD-OE2	5.74	129.78	118.30
1	A	87	LYS	CA-CB-CG	5.73	126.01	113.40
1	A	402	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	200	ARG	CD-NE-CZ	-5.71	115.60	123.60
1	B	58	GLY	CA-C-O	5.68	130.82	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	266	ASN	C-N-CA	5.68	135.90	121.70
1	A	300	GLU	CG-CD-OE2	-5.58	107.15	118.30
1	A	300	GLU	CB-CA-C	-5.57	99.25	110.40
1	A	184	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	270	SER	CA-CB-OG	-5.54	96.25	111.20
1	A	421	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	14	ARG	O-C-N	-5.48	113.88	123.20
1	A	21	VAL	CA-CB-CG2	5.48	119.12	110.90
1	A	30	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	A	47	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	B	229	VAL	CB-CA-C	5.46	121.78	111.40
1	A	82	ASP	O-C-N	5.44	131.41	122.70
1	B	70	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	119	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	270	SER	N-CA-CB	5.42	118.64	110.50
1	A	141	THR	CA-CB-OG1	-5.42	97.62	109.00
1	A	52	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	226	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	31	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	32	SER	N-CA-CB	5.40	118.60	110.50
1	B	97	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	374	ARG	O-C-N	-5.39	114.08	122.70
1	A	20	GLU	CG-CD-OE1	-5.37	107.56	118.30
1	B	392	THR	CA-CB-OG1	-5.37	97.73	109.00
1	A	263	LYS	N-CA-C	-5.35	96.55	111.00
1	A	85	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	14	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	20	GLU	CA-CB-CG	5.31	125.09	113.40
1	B	379	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	B	23	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	18	THR	CA-CB-CG2	5.29	119.80	112.40
1	B	408	LYS	O-C-N	-5.27	114.27	122.70
1	A	306	TRP	CB-CG-CD2	5.27	133.45	126.60
1	B	81	ILE	CA-C-O	-5.26	109.05	120.10
1	B	284	SER	N-CA-CB	5.25	118.37	110.50
1	B	91	ASP	CA-C-O	5.23	131.09	120.10
1	A	90	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	80	ASN	CA-C-O	5.21	131.05	120.10
1	B	133	LEU	CB-CA-C	5.20	120.07	110.20
1	B	138	LYS	CB-CG-CD	5.20	125.11	111.60
1	B	223	GLU	CG-CD-OE2	-5.20	107.91	118.30
1	B	307	SER	CA-C-N	-5.19	105.79	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	72	ILE	O-C-N	5.18	130.99	122.70
1	A	210	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	404	GLU	CG-CD-OE2	-5.17	107.95	118.30
1	A	268	ASP	N-CA-C	5.17	124.95	111.00
1	B	82	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	19	VAL	O-C-N	5.15	130.95	122.70
1	B	175	GLY	C-N-CA	5.14	134.55	121.70
1	B	330	ILE	CB-CG1-CD1	5.14	128.29	113.90
1	B	335	GLU	N-CA-CB	-5.13	101.36	110.60
1	A	306	TRP	CA-CB-CG	5.13	123.44	113.70
1	B	380	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	262	PHE	C-N-CA	5.12	134.50	121.70
1	A	142	SER	N-CA-CB	5.11	118.17	110.50
1	B	406	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	392	THR	CA-CB-CG2	5.11	119.55	112.40
1	B	31	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	B	66	LYS	O-C-N	-5.10	114.53	122.70
1	A	300	GLU	CB-CG-CD	-5.10	100.44	114.20
1	A	391	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	423	ALA	O-C-N	5.09	130.84	122.70
1	A	181	GLU	CA-CB-CG	5.07	124.56	113.40
1	B	303	TRP	CA-CB-CG	5.06	123.32	113.70
1	B	187	SER	O-C-N	5.06	130.79	122.70
1	B	238	ASP	CA-CB-CG	-5.06	102.28	113.40
1	B	184	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	31	ARG	CB-CG-CD	5.04	124.69	111.60
1	A	188	GLU	OE1-CD-OE2	5.02	129.32	123.30
1	B	81	ILE	O-C-N	5.02	130.73	122.70
1	A	265	PRO	N-CA-C	-5.02	99.06	112.10
1	A	288	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LEU	Mainchain
1	A	119	ARG	Sidechain
1	A	14	ARG	Mainchain
1	A	144	TYR	Mainchain
1	A	152	ASN	Mainchain
1	A	167	GLN	Sidechain
1	A	201	TYR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	23	LEU	Mainchain
1	A	249	SER	Mainchain
1	A	264	ASN	Mainchain,Peptide
1	A	267	SER	Peptide
1	A	268	ASP	Mainchain
1	A	338	ALA	Mainchain
1	A	346	VAL	Mainchain
1	A	35	PRO	Mainchain
1	A	405	ARG	Sidechain
1	B	11	TYR	Sidechain
1	B	119	ARG	Sidechain
1	B	178	THR	Mainchain
1	B	200	ARG	Mainchain
1	B	39	SER	Mainchain
1	B	395	ILE	Mainchain
1	B	399	ALA	Mainchain

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	3292	0	3300	217	0
1	B	3292	0	3300	242	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	11	0	4	1	0
5	B	10	0	2	3	0
6	A	197	0	0	42	1
6	B	159	0	0	36	0
All	All	6964	0	6606	453	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:H	1:A:277:GLN:NE2	1.28	1.32
1:B:257:LYS:HB3	1:B:273:LEU:O	1.26	1.28
1:A:261:ASP:OD2	1:A:271:LYS:HB3	1.38	1.21
1:A:122:ALA:HB2	6:A:811:HOH:O	1.37	1.18
1:A:54:SER:C	6:A:621:HOH:O	1.80	1.17
1:B:415:ILE:HG22	6:B:881:HOH:O	1.43	1.15
1:B:74:PRO:O	1:B:78:LYS:HD3	1.48	1.12
1:A:432:HIS:HD2	6:A:726:HOH:O	1.33	1.08
1:A:238:ASP:HB2	6:A:614:HOH:O	1.53	1.08
1:A:114:SER:HB2	6:A:865:HOH:O	1.54	1.07
1:A:432:HIS:CD2	6:A:726:HOH:O	2.07	1.06
1:A:48:MET:HE2	6:A:798:HOH:O	1.54	1.06
1:A:252:PHE:CE2	6:A:866:HOH:O	2.08	1.05
1:B:257:LYS:HD2	1:B:272:TRP:O	1.55	1.05
1:B:235:ALA:HB2	6:B:777:HOH:O	1.57	1.04
1:A:274:THR:N	1:A:277:GLN:HE21	1.54	1.04
1:B:406:LEU:HD23	6:B:793:HOH:O	0.86	1.02
1:A:122:ALA:CB	6:A:811:HOH:O	1.96	1.02
1:A:255:ASP:HB3	1:A:257:LYS:NZ	1.76	1.01
1:B:415:ILE:CG2	6:B:881:HOH:O	1.99	1.00
1:A:274:THR:N	1:A:277:GLN:NE2	2.10	0.99
1:A:274:THR:HG23	1:A:277:GLN:NE2	1.76	0.99
1:A:268:ASP:O	1:A:270:SER:N	1.97	0.98
1:A:261:ASP:OD2	1:A:271:LYS:CB	2.10	0.97
1:A:110:ILE:O	6:A:865:HOH:O	1.82	0.95
1:B:219:GLN:HG2	6:B:870:HOH:O	1.66	0.95
1:B:14:ARG:HH22	1:B:38:ALA:HB2	1.32	0.95
1:A:132:HIS:CB	6:A:811:HOH:O	2.15	0.94
1:A:337:LYS:HE3	1:A:337:LYS:HA	1.47	0.93
1:A:264:ASN:C	1:A:264:ASN:OD1	2.07	0.92
1:A:39:SER:HB3	6:A:604:HOH:O	1.69	0.92
1:A:195:SER:O	1:A:199:LYS:HE2	1.69	0.92
1:B:192:ASN:ND2	6:B:777:HOH:O	2.03	0.91
1:A:255:ASP:HB3	1:A:257:LYS:HZ2	1.32	0.91
1:B:419:LEU:HD11	6:B:881:HOH:O	1.72	0.90
1:A:132:HIS:HB3	6:A:811:HOH:O	1.71	0.88
1:B:87:LYS:HG2	1:B:88:ALA:N	1.87	0.87
1:B:252:PHE:HB2	1:B:259:ASP:O	1.73	0.87
1:A:198:LYS:HG2	1:A:203:ALA:HA	1.53	0.87
1:A:257:LYS:HD2	1:A:257:LYS:N	1.91	0.85
1:B:251:GLU:HG2	6:B:597:HOH:O	1.74	0.85
1:A:252:PHE:CD2	6:A:866:HOH:O	2.26	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LYS:HE2	1:B:272:TRP:CH2	2.12	0.85
1:B:288:ARG:NH2	6:B:673:HOH:O	2.09	0.84
1:A:233:LYS:HG3	1:A:238:ASP:OD1	1.77	0.84
1:B:14:ARG:NH2	1:B:38:ALA:HB2	1.92	0.84
1:A:46:LEU:HD22	1:A:103:SER:HA	1.60	0.84
1:B:101:ASN:H	1:B:101:ASN:HD22	1.26	0.83
1:B:419:LEU:CD1	6:B:881:HOH:O	2.23	0.83
1:A:261:ASP:HB3	1:A:271:LYS:HB2	1.61	0.83
1:B:192:ASN:CG	6:B:777:HOH:O	2.15	0.82
1:B:274:THR:N	1:B:277:GLN:OE1	2.13	0.82
1:A:432:HIS:HA	6:A:701:HOH:O	1.77	0.82
1:A:131:LYS:NZ	1:A:141:THR:HG21	1.94	0.82
1:A:55:LYS:N	6:A:621:HOH:O	2.02	0.81
1:A:196:LEU:O	1:A:200:ARG:HG3	1.80	0.81
1:B:168:GLU:HG2	6:B:644:HOH:O	1.79	0.81
1:A:432:HIS:HB3	1:A:435:LYS:HG3	1.62	0.80
1:B:264:ASN:C	1:B:264:ASN:OD1	2.14	0.80
1:B:254:LYS:HD3	1:B:259:ASP:OD2	1.80	0.80
1:B:40:THR:CG2	6:B:792:HOH:O	2.31	0.79
1:B:286:MET:CE	1:B:309:PHE:HZ	1.95	0.79
1:B:235:ALA:CB	6:B:777:HOH:O	2.22	0.79
1:B:42:VAL:HA	6:B:823:HOH:O	1.81	0.79
1:B:254:LYS:HB3	1:B:272:TRP:CZ3	2.18	0.79
1:B:101:ASN:N	1:B:101:ASN:HD22	1.79	0.78
1:A:262:PHE:CD2	6:A:648:HOH:O	2.38	0.77
1:B:261:ASP:OD1	1:B:264:ASN:HA	1.85	0.77
1:A:20:GLU:CD	1:A:31:ARG:HD3	2.05	0.77
1:B:274:THR:O	1:B:277:GLN:HG3	1.85	0.76
1:A:373:HIS:HD2	1:A:405:ARG:HH11	1.33	0.76
1:A:262:PHE:HD2	6:A:648:HOH:O	1.67	0.76
1:B:391:ARG:NH2	1:B:436:LEU:O	2.17	0.75
1:A:188:GLU:OE1	1:A:237:HIS:NE2	2.14	0.75
1:B:254:LYS:N	1:B:257:LYS:O	2.20	0.75
1:B:273:LEU:HA	1:B:277:GLN:OE1	1.88	0.74
1:A:274:THR:H	1:A:277:GLN:HE21	0.74	0.74
1:A:198:LYS:HD2	1:A:206:GLY:HA3	1.70	0.74
1:B:40:THR:HG23	6:B:792:HOH:O	1.87	0.74
1:B:22:GLU:OE2	1:B:31:ARG:NH2	2.19	0.74
1:A:131:LYS:HG2	1:A:144:TYR:OH	1.88	0.73
1:B:257:LYS:CD	1:B:272:TRP:O	2.36	0.73
1:B:252:PHE:O	1:B:259:ASP:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:HIS:O	1:B:160:ALA:HB2	1.89	0.73
1:A:256:GLY:N	1:A:257:LYS:HD2	2.04	0.72
1:B:219:GLN:HG2	6:B:734:HOH:O	1.88	0.72
1:B:286:MET:HE3	1:B:309:PHE:HZ	1.54	0.72
1:B:159:HIS:O	1:B:160:ALA:CB	2.38	0.72
1:A:101:ASN:ND2	1:A:101:ASN:H	1.86	0.72
1:A:101:ASN:C	1:A:101:ASN:HD22	1.94	0.71
1:B:315:ILE:O	1:B:317:ILE:HD12	1.91	0.71
1:A:130:TYR:OH	1:A:418:GLU:OE1	2.05	0.71
1:A:255:ASP:C	1:A:257:LYS:H	1.93	0.71
1:A:274:THR:HG23	1:A:277:GLN:CD	2.10	0.70
1:A:271:LYS:O	1:A:271:LYS:HG3	1.91	0.70
1:B:235:ALA:CA	6:B:777:HOH:O	2.38	0.70
1:A:132:HIS:HB2	6:A:811:HOH:O	1.87	0.70
1:B:313:ALA:HB1	1:B:317:ILE:HD11	1.73	0.70
1:B:152:ASN:HD21	1:B:155:ASN:HD21	1.39	0.70
1:A:372:SER:HB2	1:A:396:LYS:HG2	1.74	0.70
1:B:264:ASN:ND2	1:B:267:SER:HA	2.07	0.69
1:A:233:LYS:CG	1:A:238:ASP:OD1	2.40	0.69
1:A:43:HIS:ND1	1:A:329:ARG:NH1	2.41	0.69
1:B:257:LYS:HB3	1:B:273:LEU:C	2.11	0.69
1:A:131:LYS:HD3	1:A:131:LYS:O	1.93	0.69
1:B:269:LYS:NZ	1:B:270:SER:OG	2.25	0.69
1:A:264:ASN:HD21	1:A:267:SER:HB2	1.58	0.69
1:B:42:VAL:O	6:B:823:HOH:O	2.09	0.69
1:A:403:SER:HB2	1:B:404:GLU:HB3	1.74	0.69
1:A:391:ARG:HH22	1:A:436:LEU:C	1.95	0.68
1:B:434:ASP:OD2	1:B:435:LYS:HD2	1.94	0.68
1:B:257:LYS:HD2	1:B:272:TRP:C	2.13	0.68
1:A:43:HIS:CE1	1:A:329:ARG:NH1	2.62	0.67
1:B:40:THR:CG2	1:B:41:GLY:N	2.58	0.67
1:A:194:LYS:HE3	6:A:859:HOH:O	1.95	0.67
1:B:286:MET:CE	1:B:309:PHE:CZ	2.77	0.67
1:A:264:ASN:HD21	1:A:267:SER:CB	2.07	0.67
1:B:316:GLN:OE1	1:B:431:HIS:HD2	1.78	0.66
1:B:264:ASN:HD22	1:B:267:SER:HA	1.61	0.66
1:B:42:VAL:CA	6:B:823:HOH:O	2.41	0.66
1:A:357:LYS:HE2	1:A:361:ASP:OD1	1.95	0.66
1:B:41:GLY:O	6:B:792:HOH:O	2.12	0.66
1:A:259:ASP:OD2	1:A:262:PHE:HB3	1.96	0.66
1:A:268:ASP:C	1:A:270:SER:H	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:PRO:HD2	1:B:266:ASN:H	1.61	0.66
1:A:146:LEU:HD23	1:A:423:ALA:HB1	1.76	0.66
1:B:265:PRO:CD	1:B:266:ASN:H	2.06	0.66
1:A:59:LYS:HG2	6:A:575:HOH:O	1.97	0.65
1:B:257:LYS:HD3	1:B:274:THR:HG23	1.77	0.65
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.32	0.65
1:B:264:ASN:HB3	1:B:265:PRO:CA	2.28	0.64
1:B:248:ALA:O	1:B:251:GLU:HB2	1.98	0.64
1:A:74:PRO:O	1:A:78:LYS:HG3	1.98	0.64
1:A:1:ALA:HB1	1:A:26:GLU:OE1	1.97	0.64
1:B:165:ALA:HB2	1:B:260:LEU:O	1.97	0.64
1:B:39:SER:O	1:B:40:THR:HB	1.98	0.64
1:B:274:THR:O	1:B:277:GLN:N	2.27	0.64
1:B:37:GLY:HA3	1:B:374:ARG:NH2	2.13	0.64
1:B:194:LYS:O	1:B:198:LYS:HG2	1.97	0.64
1:A:131:LYS:HZ2	1:A:141:THR:HG21	1.63	0.63
1:A:114:SER:CB	6:A:865:HOH:O	2.24	0.63
1:B:187:SER:O	1:B:191:HIS:ND1	2.31	0.63
1:A:66:LYS:HD2	1:A:70:ASP:OD2	1.98	0.63
1:B:275:GLY:O	1:B:277:GLN:N	2.32	0.63
1:B:264:ASN:OD1	1:B:264:ASN:O	2.16	0.63
1:B:251:GLU:OE1	1:B:251:GLU:CA	2.44	0.62
1:A:264:ASN:ND2	1:A:267:SER:CB	2.62	0.62
1:A:114:SER:N	6:A:865:HOH:O	2.20	0.62
1:A:260:LEU:HB2	1:A:271:LYS:HD3	1.82	0.62
1:B:39:SER:HB2	5:B:440:PEP:O3P	1.99	0.62
1:B:74:PRO:HA	1:B:78:LYS:HZ3	1.63	0.62
1:B:74:PRO:HA	1:B:78:LYS:NZ	2.15	0.62
1:B:301:ASP:OD1	1:B:329:ARG:NH2	2.32	0.61
1:A:72:ILE:HA	1:A:96:LEU:HD21	1.81	0.61
1:B:274:THR:OG1	1:B:277:GLN:HG3	2.00	0.61
1:B:286:MET:HE3	1:B:309:PHE:CZ	2.34	0.61
1:B:257:LYS:CB	1:B:273:LEU:O	2.23	0.61
1:A:248:ALA:HB1	6:A:668:HOH:O	2.01	0.61
1:A:242:LYS:HD3	1:A:292:VAL:HG11	1.82	0.61
1:A:264:ASN:C	1:A:266:ASN:H	2.03	0.61
1:A:274:THR:O	1:A:277:GLN:HB2	2.01	0.61
1:B:411:GLN:O	1:B:415:ILE:HG13	2.01	0.61
1:A:225:LEU:O	1:A:229:VAL:HG13	2.00	0.60
1:A:131:LYS:HZ3	1:A:141:THR:HG21	1.62	0.60
1:A:274:THR:HG23	1:A:277:GLN:HE22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:HA	6:B:627:HOH:O	2.01	0.60
1:A:161:GLY:H	1:B:207:ASN:HD21	1.50	0.60
1:A:406:LEU:HD13	1:B:12:ASP:O	2.02	0.60
1:A:261:ASP:H	1:A:271:LYS:HG2	1.66	0.59
1:A:373:HIS:HD2	1:A:405:ARG:NH1	2.00	0.59
1:B:373:HIS:ND1	1:B:405:ARG:NH1	2.50	0.59
1:A:240:LYS:NZ	6:A:833:HOH:O	2.25	0.59
1:B:53:LYS:HD2	1:B:53:LYS:N	2.17	0.59
1:A:349:ILE:HG12	1:A:354:GLU:HB3	1.83	0.59
1:A:101:ASN:ND2	1:A:103:SER:OG	2.36	0.59
1:B:226:ASP:OD1	1:B:289:TYR:OH	2.11	0.59
1:A:403:SER:CB	1:B:404:GLU:HB3	2.33	0.59
1:B:140:LYS:HE3	1:B:434:ASP:O	2.03	0.59
1:B:202:GLY:O	1:B:205:ALA:HB3	2.02	0.59
1:B:313:ALA:CB	1:B:317:ILE:HD11	2.31	0.59
1:A:42:VAL:HG22	1:A:300:GLU:OE2	2.03	0.59
1:B:235:ALA:HA	6:B:777:HOH:O	2.03	0.59
1:A:433:GLY:HA2	1:A:436:LEU:HD13	1.85	0.58
1:A:73:ALA:N	1:A:74:PRO:HD2	2.18	0.58
1:A:372:SER:HB2	1:A:396:LYS:CG	2.33	0.58
1:B:313:ALA:HB3	1:B:317:ILE:HD13	1.85	0.58
1:A:260:LEU:CD1	1:A:273:LEU:HD12	2.34	0.58
1:B:269:LYS:C	1:B:271:LYS:H	2.07	0.58
1:A:281:LEU:O	1:A:281:LEU:HD12	2.03	0.58
1:B:46:LEU:HD23	1:B:103:SER:HB3	1.86	0.58
1:B:102:LYS:HE2	1:B:351:THR:HG23	1.85	0.57
1:B:334:ILE:HD13	1:B:365:ALA:HB2	1.86	0.57
1:B:39:SER:HB2	5:B:440:PEP:P	2.44	0.57
1:B:40:THR:HG22	1:B:41:GLY:N	2.20	0.57
1:B:101:ASN:ND2	1:B:101:ASN:N	2.52	0.57
1:A:255:ASP:CB	1:A:257:LYS:NZ	2.62	0.57
1:A:101:ASN:HD22	1:A:102:LYS:N	2.01	0.57
1:B:53:LYS:CD	1:B:53:LYS:N	2.66	0.57
1:A:255:ASP:HB3	1:A:257:LYS:HZ3	1.68	0.57
1:A:66:LYS:O	1:A:66:LYS:HG3	2.04	0.57
1:A:378:THR:O	1:A:408:LYS:NZ	2.38	0.56
1:B:152:ASN:HD21	1:B:155:ASN:ND2	2.02	0.56
1:B:313:ALA:CB	1:B:317:ILE:CD1	2.83	0.56
1:A:300:GLU:O	1:A:322:LEU:HD12	2.06	0.56
1:A:432:HIS:HB3	1:A:435:LYS:CG	2.35	0.56
1:A:46:LEU:CD2	1:A:103:SER:HA	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:O	1:B:280:ASP:OD2	2.23	0.56
1:B:55:LYS:HB3	1:B:56:TRP:CE3	2.40	0.56
1:A:274:THR:OG1	1:A:276:PRO:HD2	2.06	0.56
1:B:53:LYS:H	1:B:53:LYS:CD	2.16	0.56
1:B:53:LYS:HE2	6:B:848:HOH:O	2.05	0.56
1:A:391:ARG:NH2	1:A:436:LEU:OXT	2.39	0.56
1:A:264:ASN:ND2	1:A:267:SER:HB3	2.21	0.56
1:A:349:ILE:HG12	1:A:354:GLU:CB	2.35	0.56
1:B:229:VAL:O	1:B:233:LYS:HG3	2.06	0.56
1:A:260:LEU:HD11	1:A:273:LEU:HD12	1.88	0.55
1:B:14:ARG:HH22	1:B:38:ALA:CB	2.11	0.55
1:B:269:LYS:HG2	1:B:270:SER:N	2.22	0.55
1:B:271:LYS:HG2	1:B:271:LYS:O	2.07	0.55
1:A:101:ASN:HD22	1:A:103:SER:H	1.54	0.55
1:A:144:TYR:CD2	1:A:419:LEU:HD22	2.41	0.55
1:A:253:PHE:CE1	1:A:255:ASP:O	2.60	0.55
1:A:255:ASP:C	1:A:257:LYS:N	2.60	0.55
1:B:269:LYS:HG2	1:B:270:SER:H	1.71	0.55
1:A:1:ALA:HB3	6:A:679:HOH:O	2.07	0.55
1:A:373:HIS:CD2	1:A:405:ARG:HH11	2.20	0.54
1:B:46:LEU:HD23	1:B:103:SER:CB	2.36	0.54
1:A:43:HIS:HE1	1:A:301:ASP:OD2	1.91	0.54
1:B:401:ALA:O	1:B:402:ARG:HB2	2.06	0.54
1:B:152:ASN:HB2	6:B:893:HOH:O	2.07	0.54
1:A:272:TRP:CD1	1:A:272:TRP:N	2.74	0.54
1:B:274:THR:O	1:B:275:GLY:C	2.46	0.54
1:A:273:LEU:HA	1:A:277:GLN:NE2	2.23	0.54
1:B:273:LEU:HB3	1:B:277:GLN:HB2	1.89	0.54
1:B:40:THR:HA	1:B:44:GLU:OE2	2.08	0.54
1:B:349:ILE:HG12	1:B:354:GLU:HB3	1.90	0.54
1:A:261:ASP:N	1:A:271:LYS:HG2	2.23	0.53
1:A:261:ASP:OD1	1:A:267:SER:O	2.27	0.53
1:A:166:LEU:HD22	1:A:247:CYS:HB3	1.89	0.53
1:A:249:SER:HA	1:A:252:PHE:CE2	2.44	0.53
1:B:283:HIS:O	1:B:287:LYS:HG3	2.09	0.53
1:A:373:HIS:CD2	1:A:405:ARG:NH1	2.76	0.53
1:A:59:LYS:CD	6:A:750:HOH:O	2.55	0.53
1:B:269:LYS:O	1:B:271:LYS:N	2.37	0.52
1:B:304:GLU:HG3	6:B:741:HOH:O	2.10	0.52
1:B:27:LYS:HD3	1:B:124:GLU:HA	1.90	0.52
1:B:243:ILE:HD12	1:B:290:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:OE2	1:A:343:LEU:HD22	2.10	0.52
1:B:275:GLY:C	1:B:277:GLN:N	2.62	0.52
1:B:219:GLN:CG	6:B:734:HOH:O	2.51	0.52
1:B:43:HIS:ND1	1:B:329:ARG:NH1	2.58	0.52
1:A:261:ASP:HB3	1:A:271:LYS:CB	2.37	0.52
1:B:267:SER:O	1:B:269:LYS:N	2.43	0.52
1:B:264:ASN:HD21	1:B:268:ASP:CG	2.12	0.52
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.92	0.52
1:B:38:ALA:N	5:B:440:PEP:O1P	2.36	0.51
1:B:301:ASP:O	1:B:303:TRP:N	2.35	0.51
1:B:273:LEU:CA	1:B:277:GLN:OE1	2.56	0.51
1:B:137:SER:O	1:B:138:LYS:HB2	2.09	0.51
1:B:265:PRO:CD	1:B:266:ASN:N	2.70	0.51
1:B:90:ASP:OD2	1:B:353:SER:OG	2.22	0.51
1:B:42:VAL:C	6:B:823:HOH:O	2.46	0.51
1:B:261:ASP:O	1:B:262:PHE:C	2.46	0.51
1:A:127:VAL:HB	1:A:128:PRO:HD2	1.91	0.51
1:B:253:PHE:CD1	1:B:258:TYR:CE1	2.99	0.51
1:B:254:LYS:HE2	1:B:272:TRP:HH2	1.67	0.51
1:B:275:GLY:C	1:B:277:GLN:H	2.13	0.51
1:B:274:THR:H	1:B:277:GLN:CD	2.11	0.51
1:A:42:VAL:HG23	1:A:43:HIS:CE1	2.46	0.50
1:B:43:HIS:CE1	1:B:329:ARG:NH1	2.80	0.50
1:B:147:PRO:HG3	1:B:387:VAL:CG1	2.41	0.50
1:A:262:PHE:HA	1:A:264:ASN:HB3	1.92	0.50
1:A:143:PRO:O	1:A:391:ARG:NH1	2.42	0.50
1:B:251:GLU:N	1:B:251:GLU:OE1	2.44	0.50
1:B:269:LYS:CE	1:B:270:SER:OG	2.60	0.50
1:A:262:PHE:CG	1:A:263:LYS:N	2.79	0.49
1:A:337:LYS:HA	1:A:337:LYS:CE	2.21	0.49
1:B:249:SER:HB2	1:B:296:ASP:O	2.11	0.49
1:B:252:PHE:O	1:B:258:TYR:HA	2.12	0.49
1:A:12:ASP:O	1:B:406:LEU:HD13	2.11	0.49
1:A:127:VAL:O	6:A:699:HOH:O	2.19	0.49
1:B:74:PRO:CA	1:B:78:LYS:HZ3	2.25	0.49
1:A:277:GLN:O	1:A:280:ASP:HB3	2.12	0.49
1:A:233:LYS:HA	6:A:614:HOH:O	2.12	0.49
1:B:194:LYS:NZ	1:B:194:LYS:HB3	2.28	0.49
1:B:53:LYS:H	1:B:53:LYS:HZ3	1.61	0.49
1:A:132:HIS:O	1:A:135:ASP:HB2	2.12	0.49
1:B:406:LEU:CD2	6:B:793:HOH:O	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HB3	1:B:265:PRO:C	2.33	0.48
1:B:152:ASN:ND2	1:B:155:ASN:HD21	2.08	0.48
1:B:253:PHE:HA	1:B:257:LYS:O	2.13	0.48
1:A:102:LYS:NZ	1:A:354:GLU:OE1	2.29	0.48
1:A:253:PHE:CZ	1:A:255:ASP:O	2.66	0.48
1:A:300:GLU:HG3	1:A:321:ASP:HB3	1.95	0.48
1:B:323:THR:HB	1:B:330:ILE:CD1	2.43	0.48
1:A:17:PRO:HG3	1:A:56:TRP:CD1	2.49	0.48
1:B:39:SER:O	1:B:40:THR:CB	2.62	0.48
1:B:97:ASP:OD2	1:B:102:LYS:HA	2.13	0.48
1:B:274:THR:O	1:B:277:GLN:CG	2.58	0.48
1:B:130:TYR:CE1	1:B:419:LEU:HD21	2.49	0.48
1:B:192:ASN:O	1:B:195:SER:HB2	2.14	0.48
1:B:147:PRO:HG3	1:B:387:VAL:HG11	1.95	0.48
1:B:101:ASN:ND2	1:B:103:SER:OG	2.46	0.47
1:A:271:LYS:O	1:A:271:LYS:CG	2.61	0.47
1:A:131:LYS:HD3	1:A:131:LYS:C	2.35	0.47
1:B:282:TYR:O	1:B:286:MET:HG3	2.14	0.47
1:A:374:ARG:O	1:A:377:GLU:HG2	2.13	0.47
1:A:99:THR:CB	1:A:101:ASN:HD21	2.27	0.47
1:A:257:LYS:N	1:A:257:LYS:CD	2.68	0.47
1:B:132:HIS:O	1:B:135:ASP:HB2	2.13	0.47
1:A:261:ASP:OD2	1:A:271:LYS:HB2	2.08	0.47
1:B:257:LYS:HD3	1:B:274:THR:CG2	2.44	0.47
1:B:264:ASN:HB3	1:B:265:PRO:HA	1.97	0.47
1:A:43:HIS:CE1	1:A:329:ARG:HH12	2.32	0.47
1:A:421:ASP:N	1:A:421:ASP:OD1	2.46	0.47
1:A:79:ALA:O	1:A:80:ASN:C	2.53	0.47
1:A:258:TYR:HB2	1:A:273:LEU:O	2.15	0.47
1:B:46:LEU:HD12	1:B:47:GLU:O	2.14	0.47
1:A:82:ASP:OD1	1:A:84:LYS:HB2	2.14	0.47
1:A:391:ARG:NH2	1:A:436:LEU:C	2.65	0.47
1:A:10:VAL:C	6:A:695:HOH:O	2.53	0.47
1:B:74:PRO:CA	1:B:78:LYS:NZ	2.78	0.46
1:B:196:LEU:O	1:B:200:ARG:HG3	2.15	0.46
1:A:101:ASN:ND2	1:A:103:SER:H	2.12	0.46
1:B:330:ILE:HD12	1:B:342:LEU:HD13	1.97	0.46
1:B:296:ASP:N	1:B:297:PRO:CD	2.78	0.46
1:B:52:ASP:OD1	1:B:52:ASP:C	2.54	0.46
1:A:261:ASP:CB	1:A:271:LYS:HB2	2.37	0.46
1:A:274:THR:CG2	1:A:277:GLN:NE2	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:HB	1:A:101:ASN:HD21	1.81	0.46
1:B:269:LYS:CG	1:B:270:SER:N	2.78	0.46
1:B:269:LYS:HZ3	1:B:270:SER:HG	1.55	0.46
1:A:42:VAL:N	1:A:300:GLU:OE2	2.44	0.46
1:B:304:GLU:HB2	6:B:741:HOH:O	2.16	0.46
1:B:7:ALA:HB2	1:B:68:VAL:HG11	1.97	0.46
1:A:101:ASN:ND2	1:A:101:ASN:C	2.65	0.46
1:B:283:HIS:CE1	1:B:309:PHE:CE1	3.04	0.46
1:B:303:TRP:CH2	1:B:332:THR:HB	2.50	0.46
1:A:268:ASP:OD1	1:A:268:ASP:C	2.54	0.46
1:A:42:VAL:CG2	1:A:43:HIS:CE1	2.99	0.46
1:A:10:VAL:O	1:A:18:THR:N	2.39	0.46
1:B:185:ILE:HG21	1:B:185:ILE:HD13	1.56	0.46
1:A:138:LYS:HB2	1:A:138:LYS:HE3	1.26	0.45
1:A:406:LEU:HD22	1:B:11:TYR:HB2	1.98	0.45
1:A:44:GLU:HG2	1:A:348:GLN:HG2	1.98	0.45
1:A:2:VAL:HA	1:A:25:THR:HG22	1.99	0.45
1:B:57:MET:CE	1:B:59:LYS:NZ	2.80	0.45
1:B:252:PHE:CB	1:B:259:ASP:O	2.54	0.45
1:B:316:GLN:OE1	1:B:431:HIS:CD2	2.63	0.45
1:A:252:PHE:HE2	6:A:866:HOH:O	1.73	0.45
1:B:21:VAL:O	1:B:31:ARG:HA	2.17	0.45
1:A:177:LYS:HG2	6:A:833:HOH:O	2.16	0.45
1:A:55:LYS:HE2	6:A:787:HOH:O	2.16	0.45
1:A:262:PHE:CE2	6:A:616:HOH:O	2.67	0.45
1:B:73:ALA:HB3	1:B:74:PRO:HD3	1.97	0.45
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.51	0.45
1:B:44:GLU:OE1	6:B:577:HOH:O	2.21	0.44
1:B:323:THR:HA	1:B:329:ARG:HB2	1.99	0.44
1:A:296:ASP:HA	1:A:306:TRP:HH2	1.81	0.44
1:B:361:ASP:O	1:B:364:ALA:HB3	2.16	0.44
1:B:1:ALA:N	1:B:26:GLU:OE1	2.47	0.44
1:A:259:ASP:CG	1:A:262:PHE:HB3	2.37	0.44
1:A:431:HIS:CD2	1:A:432:HIS:CE1	3.06	0.44
1:A:303:TRP:CE3	1:A:336:LYS:HD2	2.52	0.44
1:A:55:LYS:CE	6:A:787:HOH:O	2.65	0.44
1:B:419:LEU:HD12	6:B:881:HOH:O	2.06	0.44
1:B:131:LYS:C	1:B:131:LYS:HD2	2.38	0.44
1:A:59:LYS:HD3	6:A:858:HOH:O	2.17	0.44
1:B:254:LYS:O	1:B:256:GLY:N	2.50	0.44
1:B:248:ALA:HA	6:B:615:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:C	1:B:263:LYS:N	2.70	0.44
1:B:261:ASP:OD1	1:B:264:ASN:N	2.51	0.44
1:B:246:ASP:HA	1:B:295:GLU:HB3	1.99	0.44
1:A:262:PHE:O	1:A:263:LYS:HB2	2.18	0.44
1:B:296:ASP:OD2	1:B:320:ASP:HB3	2.17	0.44
1:B:125:LYS:HB3	1:B:125:LYS:NZ	2.32	0.44
1:B:274:THR:OG1	1:B:277:GLN:CG	2.65	0.43
1:A:349:ILE:CG2	1:A:355:SER:OG	2.66	0.43
1:B:211:GLU:HG2	6:B:772:HOH:O	2.17	0.43
1:A:268:ASP:C	1:A:270:SER:N	2.54	0.43
1:B:264:ASN:CB	1:B:265:PRO:CA	2.97	0.43
1:A:275:GLY:N	1:A:276:PRO:HD2	2.34	0.43
1:A:54:SER:CA	6:A:621:HOH:O	2.52	0.43
1:B:269:LYS:HD3	1:B:270:SER:HB2	2.00	0.43
1:B:131:LYS:HD2	1:B:131:LYS:O	2.19	0.43
1:A:334:ILE:HG12	1:A:365:ALA:HB1	2.00	0.43
1:A:256:GLY:C	1:A:257:LYS:HD2	2.39	0.43
1:B:287:LYS:HE3	1:B:287:LYS:HB3	1.83	0.43
1:B:313:ALA:HB1	1:B:317:ILE:CD1	2.46	0.43
1:A:255:ASP:O	1:A:257:LYS:N	2.52	0.42
1:A:152:ASN:ND2	1:A:155:ASN:ND2	2.67	0.42
1:B:345:LYS:O	1:B:348:GLN:HB2	2.18	0.42
1:A:372:SER:OG	1:A:373:HIS:O	2.35	0.42
1:B:43:HIS:HB2	1:B:324:VAL:HG21	2.01	0.42
1:B:17:PRO:HG3	1:B:56:TRP:CD1	2.55	0.42
1:B:74:PRO:O	1:B:78:LYS:CD	2.41	0.42
1:B:261:ASP:O	1:B:264:ASN:N	2.49	0.42
1:B:286:MET:HE1	1:B:309:PHE:CZ	2.55	0.42
1:B:129:LEU:HG	1:B:133:LEU:HD22	2.00	0.42
1:B:318:VAL:HG22	1:B:341:ALA:HB3	2.00	0.42
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.50	0.42
1:A:218:ILE:HG21	1:A:218:ILE:HD13	1.74	0.42
1:B:251:GLU:HA	1:B:251:GLU:OE1	2.18	0.42
1:A:43:HIS:CE1	1:A:301:ASP:OD2	2.71	0.42
1:B:401:ALA:O	1:B:402:ARG:CB	2.66	0.42
1:A:129:LEU:HD21	1:A:382:PHE:CE1	2.54	0.42
1:A:272:TRP:HD1	1:A:272:TRP:N	2.17	0.42
1:B:310:PHE:CD2	1:B:337:LYS:O	2.73	0.42
1:B:343:LEU:HD11	1:B:372:SER:HB2	2.01	0.42
1:A:84:LYS:HE2	1:A:84:LYS:HB2	1.88	0.42
1:A:211:GLU:OE2	4:A:441:2PG:O3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASP:O	1:B:263:LYS:N	2.52	0.42
1:B:141:THR:HG22	1:B:144:TYR:CZ	2.55	0.42
1:A:271:LYS:HE2	1:A:271:LYS:O	2.20	0.41
1:B:168:GLU:CG	6:B:644:HOH:O	2.52	0.41
1:A:21:VAL:O	1:A:31:ARG:HA	2.20	0.41
1:B:326:ASN:OD1	1:B:327:PRO:N	2.53	0.41
1:B:261:ASP:O	1:B:261:ASP:OD1	2.37	0.41
1:A:142:SER:HA	1:A:143:PRO:HA	1.78	0.41
1:A:146:LEU:HA	1:A:146:LEU:HD13	1.84	0.41
1:A:343:LEU:CD2	1:A:345:LYS:HE3	2.50	0.41
1:B:63:HIS:CE1	6:B:856:HOH:O	2.74	0.41
1:B:140:LYS:HD3	1:B:391:ARG:NH2	2.34	0.41
1:B:130:TYR:CE2	1:B:418:GLU:OE2	2.74	0.41
1:B:201:TYR:CD1	1:B:201:TYR:N	2.88	0.41
1:B:225:LEU:HD12	1:B:285:LEU:HD22	2.03	0.41
1:A:262:PHE:HB2	6:A:648:HOH:O	2.20	0.41
1:A:59:LYS:HD3	6:A:750:HOH:O	2.19	0.41
1:A:54:SER:HB2	6:A:621:HOH:O	2.20	0.41
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.47	0.41
1:A:258:TYR:O	1:A:272:TRP:HA	2.21	0.41
1:B:27:LYS:HB3	1:B:27:LYS:HE2	1.30	0.41
1:B:326:ASN:C	1:B:328:LYS:H	2.23	0.41
1:B:274:THR:O	1:B:277:GLN:CB	2.69	0.41
1:B:130:TYR:HE2	1:B:418:GLU:OE2	2.03	0.41
1:B:269:LYS:HD3	1:B:270:SER:CB	2.50	0.41
1:A:42:VAL:HG23	1:A:43:HIS:CD2	2.56	0.41
1:B:146:LEU:HA	1:B:147:PRO:HD3	1.96	0.41
1:A:352:LEU:HA	1:A:352:LEU:HD12	1.95	0.41
1:A:255:ASP:CB	1:A:257:LYS:HZ3	2.31	0.40
1:B:142:SER:HA	1:B:143:PRO:HA	1.86	0.40
1:A:164:LEU:HD21	1:A:169:PHE:CE1	2.56	0.40
1:B:40:THR:HG23	1:B:41:GLY:N	2.36	0.40
1:A:152:ASN:O	1:A:399:ALA:HB2	2.21	0.40
1:A:410:ASN:O	1:A:414:ARG:HG3	2.21	0.40
1:A:54:SER:CB	6:A:621:HOH:O	2.68	0.40
1:B:56:TRP:O	1:B:59:LYS:HB2	2.21	0.40
1:A:167:GLN:HB2	6:A:529:HOH:O	2.20	0.40
1:A:273:LEU:HD22	1:A:277:GLN:HB3	2.04	0.40
1:B:373:HIS:CG	1:B:397:THR:HA	2.57	0.40
1:B:211:GLU:HG2	1:B:211:GLU:H	1.67	0.40
1:B:225:LEU:HA	1:B:225:LEU:HD23	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LYS:HD2	1:B:292:VAL:CG1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:ND2	6:A:520:HOH:O[1_556]	1.99	0.21

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	434/436 (100%)	407 (94%)	23 (5%)	4 (1%)	21 13
1	B	434/436 (100%)	394 (91%)	30 (7%)	10 (2%)	8 3
All	All	868/872 (100%)	801 (92%)	53 (6%)	14 (2%)	12 5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	LYS
1	B	160	ALA
1	B	255	ASP
1	B	264	ASN
1	B	267	SER
1	B	268	ASP
1	A	268	ASP
1	B	251	GLU
1	B	275	GLY
1	A	263	LYS
1	B	276	PRO
1	A	300	GLU

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Mol	Chain	Res	Type
1	B	302	ASP
1	B	402	ARG

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	344/344 (100%)	313 (91%)	31 (9%)	12 7
1	B	344/344 (100%)	316 (92%)	28 (8%)	15 9
All	All	688/688 (100%)	629 (91%)	59 (9%)	13 7

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	31	ARG
1	A	39	SER
1	A	55	LYS
1	A	66	LYS
1	A	87	LYS
1	A	101	ASN
1	A	133	LEU
1	A	138	LYS
1	A	146	LEU
1	A	196	LEU
1	A	199	LYS
1	A	238	ASP
1	A	255	ASP
1	A	262	PHE
1	A	269	LYS
1	A	270	SER
1	A	271	LYS
1	A	274	THR
1	A	288	ARG
1	A	304	GLU

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Mol	Chain	Res	Type
1	A	328	LYS
1	A	337	LYS
1	A	347	ASN
1	A	372	SER
1	A	373	HIS
1	A	391	ARG
1	A	421	ASP
1	A	424	VAL
1	A	434	ASP
1	A	435	LYS
1	B	4	LYS
1	B	23	LEU
1	B	27	LYS
1	B	31	ARG
1	B	32	SER
1	B	53	LYS
1	B	55	LYS
1	B	80	ASN
1	B	87	LYS
1	B	101	ASN
1	B	125	LYS
1	B	131	LYS
1	B	133	LEU
1	B	140	LYS
1	B	198	LYS
1	B	199	LYS
1	B	211	GLU
1	B	229	VAL
1	B	249	SER
1	B	251	GLU
1	B	267	SER
1	B	268	ASP
1	B	287	LYS
1	B	288	ARG
1	B	353	SER
1	B	373	HIS
1	B	375	SER
1	B	391	ARG

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	101	ASN
1	A	207	ASN
1	A	219	GLN
1	A	264	ASN
1	A	277	GLN
1	A	373	HIS
1	A	432	HIS
1	B	63	HIS
1	B	101	ASN
1	B	152	ASN
1	B	207	ASN
1	B	266	ASN
1	B	348	GLN
1	B	422	ASN
1	B	431	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	$\#\|Z\|>2$
4	2PG	A	441	3,2	6,10,10	2.05	2 (33%)	5,14,14	2.06	2 (40%)
5	PEP	B	440	2	5,9,9	0.97	0	8,13,13	1.82	3 (37%)

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	2PG	A	441	3,2	-	0/7/11/11	0/0/0/0
5	PEP	B	440	2	-	0/5/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	441	2PG	P-O1P	2.79	1.68	1.60
4	A	441	2PG	C3-C2	3.80	1.60	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	441	2PG	O3P-P-O2P	-2.88	101.32	110.58
5	B	440	PEP	O3P-P-O2	-2.43	97.31	105.25
5	B	440	PEP	P-O2-C2	2.08	127.58	122.96
5	B	440	PEP	O3P-P-O1P	3.04	120.35	110.58
4	A	441	2PG	O4P-P-O3P	3.18	119.50	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	441	2PG	1	0
5	B	440	PEP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.