Full wwPDB X-ray Structure Validation Report (i)

Feb 24, 2024 – 02:03 PM EST

PDB ID	:	7ENL
Title	:	MECHANISM OF ENOLASE: THE CRYSTAL STRUCTURE OF ENOLASE-MG2+-PHOSPHOGLYCERATE(SLASH) PHOSPHOENOLPYRUVATE COMPLEX AT 2.2-ANGSTROMS RESOLUTION
Authors	:	Lebioda, L.; Stec, B.
Deposited on	:	1990-11-13
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

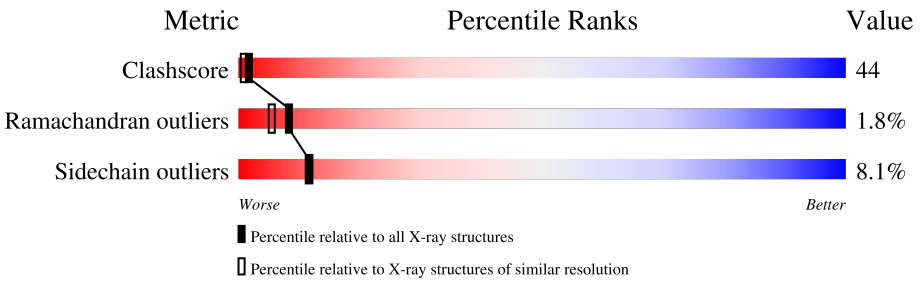
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	39% 45% 13% •

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
3	2PG	A	439	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3648 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
			Total	C	N	O	S			
1	A	436	3289	2076	569	638	6	0	0	0

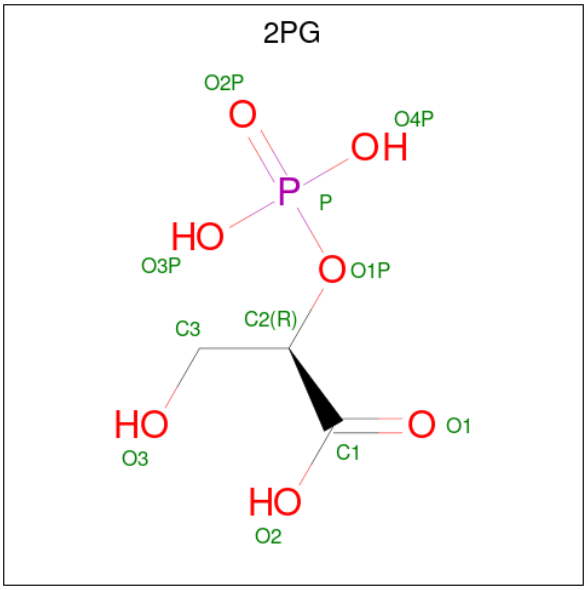
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	LYS	conflict	UNP P00924

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

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

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: $C_3H_7O_7P$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	347	347	347	0	0

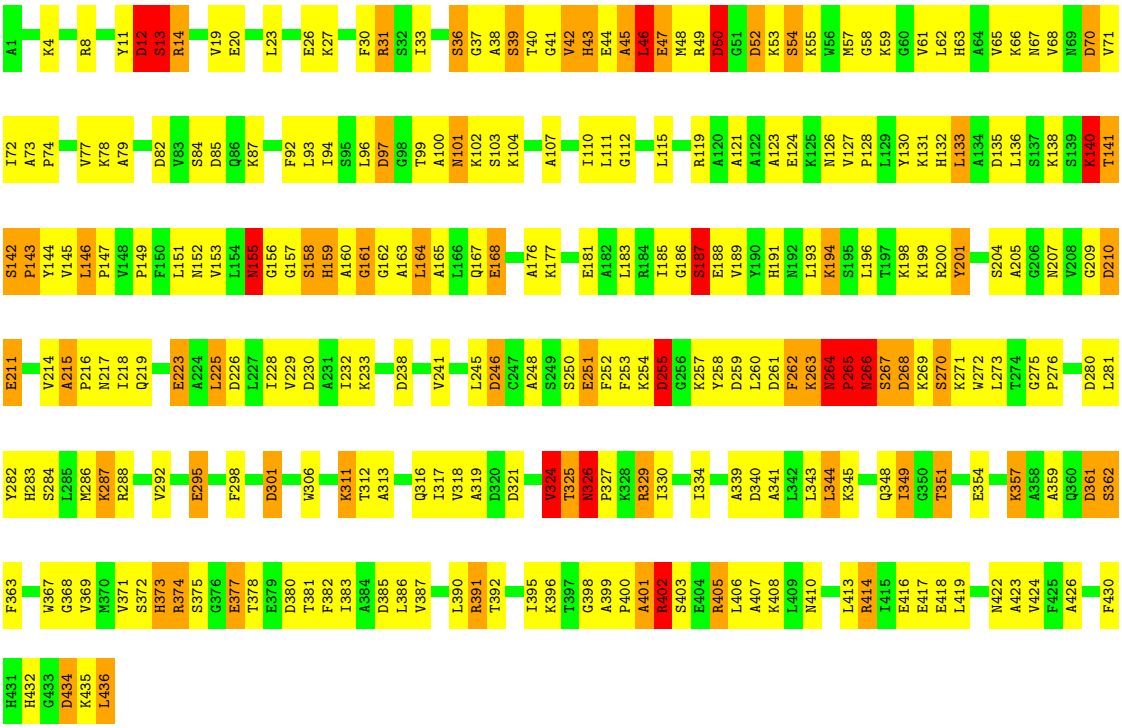
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 39% 45% 13% •



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.00Å 122.00Å 67.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3648	wwPDB-VP
Average B, all atoms ($Å^2$)	23.0	wwPDB-VP

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: MG, 2PG

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	2/3349 (0.1%)	2.31	171/4531 (3.8%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLU	CD-OE2	-5.69	1.19	1.25
1	A	47	GLU	CG-CD	-5.59	1.43	1.51

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	ARG	NE-CZ-NH1	18.70	129.65	120.30
1	A	329	ARG	NE-CZ-NH1	18.42	129.51	120.30
1	A	374	ARG	NE-CZ-NH1	18.04	129.32	120.30
1	A	14	ARG	NE-CZ-NH1	-16.65	111.97	120.30
1	A	265	PRO	CA-N-CD	-16.41	88.53	111.50
1	A	47	GLU	CB-CG-CD	15.12	155.03	114.20
1	A	49	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	391	ARG	NE-CZ-NH1	-14.25	113.17	120.30
1	A	130	TYR	CB-CG-CD2	-13.05	113.17	121.00
1	A	49	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	A	374	ARG	CD-NE-CZ	12.48	141.07	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	TYR	CB-CG-CD1	12.16	128.29	121.00
1	A	52	ASP	CB-CG-OD1	-11.46	107.98	118.30
1	A	417	GLU	OE1-CD-OE2	11.13	136.65	123.30
1	A	329	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	A	50	ASP	CB-CG-OD1	-9.91	109.38	118.30
1	A	168	GLU	OE1-CD-OE2	-9.84	111.49	123.30
1	A	85	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	A	414	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	A	251	GLU	CG-CD-OE1	-9.32	99.65	118.30
1	A	52	ASP	CB-CG-OD2	9.10	126.49	118.30
1	A	12	ASP	CB-CG-OD1	9.03	126.42	118.30
1	A	230	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	31	ARG	CD-NE-CZ	-8.84	111.22	123.60
1	A	255	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	A	246	ASP	N-CA-CB	8.72	126.29	110.60
1	A	31	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	31	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	A	301	ASP	O-C-N	8.54	136.36	122.70
1	A	268	ASP	CB-CG-OD1	-8.46	110.68	118.30
1	A	36	SER	CA-CB-OG	8.41	133.90	111.20
1	A	380	ASP	CB-CG-OD2	8.15	125.64	118.30
1	A	14	ARG	NH1-CZ-NH2	8.08	128.29	119.40
1	A	141	THR	CA-CB-CG2	8.06	123.69	112.40
1	A	48	MET	CA-CB-CG	-7.88	99.90	113.30
1	A	207	ASN	CB-CA-C	7.83	126.06	110.40
1	A	210	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	A	374	ARG	CG-CD-NE	7.82	128.21	111.80
1	A	49	ARG	CD-NE-CZ	7.79	134.51	123.60
1	A	142	SER	N-CA-CB	-7.65	99.02	110.50
1	A	140	LYS	CA-CB-CG	7.50	129.90	113.40
1	A	201	TYR	CB-CG-CD1	-7.49	116.51	121.00
1	A	264	ASN	CA-C-O	-7.41	104.53	120.10
1	A	340	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	42	VAL	N-CA-CB	-7.37	95.29	111.50
1	A	162	GLY	N-CA-C	-7.35	94.72	113.10
1	A	288	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	434	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	133	LEU	CB-CA-C	7.21	123.90	110.20
1	A	255	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	319	ALA	CB-CA-C	7.18	120.87	110.10
1	A	268	ASP	N-CA-CB	-7.15	97.73	110.60
1	A	8	ARG	NH1-CZ-NH2	-7.13	111.56	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	GLU	OE1-CD-OE2	7.13	131.85	123.30
1	A	361	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	124	GLU	CG-CD-OE1	-7.05	104.20	118.30
1	A	377	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	A	266	ASN	N-CA-CB	6.93	123.08	110.60
1	A	266	ASN	N-CA-C	-6.93	92.28	111.00
1	A	223	GLU	CG-CD-OE2	-6.88	104.54	118.30
1	A	316	GLN	O-C-N	6.87	133.70	122.70
1	A	133	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	351	THR	N-CA-CB	6.87	123.35	110.30
1	A	255	ASP	N-CA-CB	6.81	122.85	110.60
1	A	19	VAL	CA-CB-CG1	6.80	121.10	110.90
1	A	349	ILE	CB-CA-C	6.78	125.17	111.60
1	A	374	ARG	NH1-CZ-NH2	-6.78	111.94	119.40
1	A	201	TYR	CB-CG-CD2	6.75	125.05	121.00
1	A	391	ARG	CD-NE-CZ	-6.74	114.16	123.60
1	A	46	LEU	C-N-CA	6.74	138.55	121.70
1	A	280	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	168	GLU	CA-CB-CG	6.69	128.13	113.40
1	A	159	HIS	N-CA-C	6.69	129.06	111.00
1	A	405	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	326	ASN	OD1-CG-ND2	6.66	137.22	121.90
1	A	124	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	A	146	LEU	CB-CA-C	6.63	122.79	110.20
1	A	372	SER	CA-C-O	6.60	133.96	120.10
1	A	414	ARG	NH1-CZ-NH2	6.49	126.54	119.40
1	A	287	LYS	CA-CB-CG	-6.47	99.16	113.40
1	A	8	ARG	CD-NE-CZ	6.44	132.61	123.60
1	A	417	GLU	CG-CD-OE1	-6.39	105.52	118.30
1	A	161	GLY	N-CA-C	6.34	128.95	113.10
1	A	141	THR	CA-CB-OG1	-6.33	95.71	109.00
1	A	11	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	340	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	382	PHE	CB-CG-CD1	-6.25	116.43	120.80
1	A	301	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	406	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	A	161	GLY	CA-C-O	6.21	131.77	120.60
1	A	210	ASP	O-C-N	6.20	132.63	122.70
1	A	158	SER	N-CA-CB	-6.18	101.24	110.50
1	A	12	ASP	OD1-CG-OD2	-6.16	111.59	123.30
1	A	223	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	A	401	ALA	C-N-CA	6.09	136.92	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	405	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	368	GLY	N-CA-C	-6.08	97.91	113.10
1	A	341	ALA	N-CA-CB	6.07	118.59	110.10
1	A	226	ASP	CA-CB-CG	6.04	126.68	113.40
1	A	402	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	A	47	GLU	N-CA-CB	-6.03	99.75	110.60
1	A	418	GLU	CA-CB-CG	6.00	126.61	113.40
1	A	357	LYS	N-CA-CB	5.96	121.33	110.60
1	A	266	ASN	CA-C-N	-5.92	104.17	117.20
1	A	400	PRO	O-C-N	-5.91	113.24	122.70
1	A	252	PHE	CB-CA-C	5.87	122.14	110.40
1	A	145	VAL	CG1-CB-CG2	5.85	120.25	110.90
1	A	84	SER	N-CA-CB	5.84	119.26	110.50
1	A	30	PHE	CB-CG-CD1	-5.83	116.72	120.80
1	A	226	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	19	VAL	CG1-CB-CG2	-5.80	101.61	110.90
1	A	27	LYS	CA-CB-CG	-5.77	100.70	113.40
1	A	187	SER	CB-CA-C	5.73	120.99	110.10
1	A	295	GLU	CG-CD-OE1	-5.72	106.86	118.30
1	A	156	GLY	N-CA-C	-5.70	98.85	113.10
1	A	362	SER	O-C-N	5.70	131.81	122.70
1	A	344	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	385	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	280	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	162	GLY	O-C-N	5.54	131.56	122.70
1	A	215	ALA	CB-CA-C	5.53	118.39	110.10
1	A	187	SER	N-CA-CB	-5.52	102.22	110.50
1	A	115	LEU	CB-CA-C	5.52	120.69	110.20
1	A	97	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	13	SER	CB-CA-C	-5.48	99.69	110.10
1	A	168	GLU	CB-CG-CD	5.46	128.95	114.20
1	A	416	GLU	CG-CD-OE2	-5.45	107.39	118.30
1	A	155	ASN	CA-C-N	-5.44	105.32	116.20
1	A	288	ARG	CB-CG-CD	5.44	125.73	111.60
1	A	45	ALA	N-CA-CB	5.41	117.67	110.10
1	A	186	GLY	C-N-CA	5.40	135.21	121.70
1	A	47	GLU	CG-CD-OE2	5.39	129.08	118.30
1	A	70	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	161	GLY	CA-C-N	-5.36	105.48	116.20
1	A	126	ASN	O-C-N	5.36	131.28	122.70
1	A	405	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	42	VAL	CA-CB-CG1	5.31	118.87	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	ASN	O-C-N	5.31	132.23	123.20
1	A	250	SER	CA-C-O	5.31	131.24	120.10
1	A	377	GLU	CG-CD-OE2	5.30	128.90	118.30
1	A	211	GLU	CG-CD-OE2	-5.28	107.73	118.30
1	A	188	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	A	416	GLU	OE1-CD-OE2	5.28	129.63	123.30
1	A	20	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	A	385	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	14	ARG	CD-NE-CZ	-5.26	116.23	123.60
1	A	380	ASP	OD1-CG-OD2	-5.26	113.31	123.30
1	A	85	ASP	CA-C-O	5.22	131.05	120.10
1	A	371	VAL	CB-CA-C	5.21	121.30	111.40
1	A	426	ALA	CB-CA-C	5.21	117.91	110.10
1	A	262	PHE	CA-CB-CG	5.19	126.36	113.90
1	A	402	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	A	47	GLU	CA-C-N	5.19	128.61	117.20
1	A	264	ASN	C-N-CD	-5.19	109.19	120.60
1	A	351	THR	O-C-N	5.17	130.98	122.70
1	A	436	LEU	CB-CA-C	5.17	120.03	110.20
1	A	436	LEU	N-CA-CB	-5.14	100.12	110.40
1	A	258	TYR	O-C-N	5.14	130.92	122.70
1	A	211	GLU	OE1-CD-OE2	5.13	129.45	123.30
1	A	138	LYS	CA-CB-CG	5.12	124.66	113.40
1	A	265	PRO	N-CA-C	5.12	125.41	112.10
1	A	340	ASP	CA-CB-CG	5.11	124.64	113.40
1	A	225	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	402	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	430	PHE	CB-CG-CD1	-5.08	117.25	120.80
1	A	326	ASN	CB-CG-OD1	-5.08	111.45	121.60
1	A	262	PHE	CB-CA-C	5.07	120.54	110.40
1	A	251	GLU	CG-CD-OE2	5.07	128.43	118.30
1	A	92	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	A	329	ARG	CD-NE-CZ	-5.06	116.52	123.60
1	A	414	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	ASN	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3289	0	3291	288	2
2	A	1	0	0	0	0
3	A	11	0	3	4	0
4	A	347	0	0	93	2
All	All	3648	0	3294	291	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (291) 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:158:SER:HB2	4:A:576:HOH:O	1.14	1.24
1:A:47:GLU:HG3	1:A:47:GLU:O	1.42	1.14
1:A:57:MET:O	4:A:471:HOH:O	1.68	1.10
1:A:66:LYS:HE2	4:A:504:HOH:O	1.51	1.09
1:A:140:LYS:HB3	1:A:391:ARG:NH1	1.75	1.01
1:A:57:MET:SD	4:A:692:HOH:O	2.21	0.99
1:A:73:ALA:HB1	4:A:619:HOH:O	1.64	0.98
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.45	0.96
1:A:47:GLU:O	1:A:47:GLU:CG	2.08	0.96
1:A:152:ASN:ND2	1:A:168:GLU:HB3	1.81	0.95
1:A:46:LEU:HD13	1:A:103:SER:CB	1.97	0.95
1:A:62:LEU:O	4:A:571:HOH:O	1.85	0.94
1:A:14:ARG:NH1	1:A:375:SER:OG	2.01	0.94
1:A:391:ARG:NH2	1:A:436:LEU:OXT	2.01	0.94
1:A:325:THR:O	1:A:349:ILE:HD12	1.68	0.93
1:A:348:GLN:NE2	4:A:644:HOH:O	1.96	0.93
1:A:155:ASN:ND2	4:A:621:HOH:O	2.00	0.93
1:A:37:GLY:HA2	1:A:374:ARG:HB3	1.52	0.91
1:A:301:ASP:OD2	4:A:515:HOH:O	1.89	0.90
1:A:152:ASN:OD1	1:A:155:ASN:ND2	2.05	0.89
1:A:152:ASN:O	1:A:399:ALA:HB2	1.72	0.88
1:A:71:VAL:O	1:A:74:PRO:HG2	1.73	0.88
1:A:43:HIS:HE1	4:A:515:HOH:O	1.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:O	1:A:269:LYS:HD3	1.71	0.88
1:A:142:SER:HA	4:A:586:HOH:O	1.73	0.87
1:A:41:GLY:HA2	4:A:613:HOH:O	1.75	0.86
1:A:4:LYS:HE2	4:A:600:HOH:O	1.76	0.86
1:A:155:ASN:OD1	1:A:209:GLY:HA3	1.76	0.86
1:A:199:LYS:HG3	4:A:669:HOH:O	1.76	0.86
1:A:163:ALA:HB1	1:A:261:ASP:HA	1.60	0.83
1:A:41:GLY:O	1:A:44:GLU:OE2	1.95	0.83
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.07	0.83
1:A:46:LEU:HD13	1:A:103:SER:HB3	1.61	0.83
1:A:435:LYS:HE2	4:A:694:HOH:O	1.78	0.83
1:A:152:ASN:HD21	1:A:168:GLU:HB3	1.44	0.82
1:A:164:LEU:N	1:A:219:GLN:O	2.12	0.82
1:A:264:ASN:CG	1:A:266:ASN:H	1.83	0.82
1:A:54:SER:O	1:A:55:LYS:HG3	1.79	0.81
1:A:168:GLU:OE2	4:A:525:HOH:O	1.96	0.81
1:A:158:SER:HB3	4:A:523:HOH:O	1.80	0.81
1:A:251:GLU:OE1	4:A:522:HOH:O	1.98	0.81
1:A:41:GLY:O	1:A:44:GLU:HG2	1.80	0.80
1:A:13:SER:HB2	4:A:524:HOH:O	1.81	0.80
1:A:82:ASP:HB2	4:A:557:HOH:O	1.82	0.80
1:A:39:SER:O	1:A:40:THR:HG23	1.81	0.80
1:A:257:LYS:CE	4:A:614:HOH:O	2.30	0.79
1:A:387:VAL:HG23	1:A:392:THR:OG1	1.82	0.78
1:A:38:ALA:HB1	4:A:760:HOH:O	1.83	0.78
1:A:63:HIS:CD2	4:A:688:HOH:O	2.36	0.78
1:A:260:LEU:HD12	1:A:273:LEU:HD11	1.66	0.77
1:A:264:ASN:ND2	1:A:266:ASN:O	2.18	0.77
1:A:257:LYS:HE2	4:A:614:HOH:O	1.85	0.77
1:A:264:ASN:CB	1:A:266:ASN:H	1.98	0.76
3:A:439:2PG:O1	3:A:439:2PG:O3	2.01	0.76
1:A:4:LYS:CE	4:A:600:HOH:O	2.32	0.76
1:A:164:LEU:HB3	4:A:702:HOH:O	1.85	0.75
1:A:361:ASP:OD1	4:A:735:HOH:O	2.04	0.75
1:A:327:PRO:HG2	4:A:648:HOH:O	1.87	0.75
1:A:66:LYS:HE3	4:A:688:HOH:O	1.87	0.75
1:A:62:LEU:O	1:A:66:LYS:HG3	1.87	0.74
1:A:52:ASP:C	1:A:52:ASP:OD1	2.27	0.73
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.71	0.73
1:A:100:ALA:O	4:A:736:HOH:O	2.05	0.73
1:A:348:GLN:OE1	4:A:644:HOH:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HG2	4:A:571:HOH:O	1.88	0.72
1:A:283:HIS:HA	1:A:286:MET:HE3	1.71	0.72
1:A:262:PHE:O	1:A:263:LYS:HB2	1.89	0.72
1:A:4:LYS:HE3	4:A:764:HOH:O	1.90	0.71
1:A:348:GLN:CD	4:A:644:HOH:O	2.28	0.71
1:A:200:ARG:O	4:A:765:HOH:O	2.06	0.71
1:A:37:GLY:CA	1:A:374:ARG:HB3	2.20	0.70
1:A:46:LEU:C	1:A:46:LEU:HD23	2.12	0.70
1:A:264:ASN:HB3	1:A:266:ASN:H	1.57	0.69
1:A:50:ASP:N	1:A:50:ASP:OD1	2.17	0.69
1:A:94:ILE:HG23	4:A:684:HOH:O	1.92	0.68
1:A:176:ALA:O	4:A:670:HOH:O	2.11	0.68
1:A:260:LEU:HD11	1:A:281:LEU:HD23	1.75	0.68
1:A:45:ALA:HB1	1:A:107:ALA:HB2	1.76	0.67
1:A:313:ALA:CB	1:A:317:ILE:CD1	2.73	0.67
1:A:111:LEU:HB2	4:A:754:HOH:O	1.95	0.67
1:A:264:ASN:HB3	1:A:265:PRO:HA	1.75	0.67
1:A:73:ALA:N	1:A:74:PRO:HD2	2.10	0.67
1:A:257:LYS:HE3	4:A:614:HOH:O	1.94	0.67
1:A:283:HIS:HE1	1:A:312:THR:O	1.77	0.66
1:A:326:ASN:C	1:A:326:ASN:HD22	1.98	0.66
1:A:325:THR:OG1	1:A:348:GLN:NE2	2.28	0.66
1:A:259:ASP:OD1	1:A:272:TRP:NE1	2.29	0.66
1:A:301:ASP:OD1	4:A:510:HOH:O	2.14	0.66
1:A:43:HIS:CE1	4:A:515:HOH:O	2.38	0.66
1:A:131:LYS:NZ	1:A:135:ASP:OD2	2.30	0.65
1:A:214:VAL:HG23	1:A:216:PRO:HD3	1.79	0.65
1:A:419:LEU:O	4:A:560:HOH:O	2.13	0.65
1:A:196:LEU:O	1:A:200:ARG:HG3	1.96	0.65
1:A:268:ASP:O	1:A:272:TRP:NE1	2.30	0.65
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.27	0.65
1:A:238:ASP:HB2	4:A:695:HOH:O	1.98	0.64
1:A:119:ARG:O	4:A:508:HOH:O	2.15	0.63
1:A:4:LYS:CE	4:A:764:HOH:O	2.46	0.63
1:A:391:ARG:HG2	1:A:434:ASP:HA	1.80	0.62
1:A:123:ALA:HB1	4:A:663:HOH:O	1.99	0.62
1:A:4:LYS:NZ	4:A:600:HOH:O	2.24	0.62
1:A:262:PHE:O	1:A:263:LYS:CB	2.48	0.61
1:A:4:LYS:NZ	4:A:764:HOH:O	2.23	0.61
1:A:12:ASP:OD2	1:A:36:SER:HB2	2.01	0.61
1:A:136:LEU:O	4:A:770:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG12	4:A:761:HOH:O	2.01	0.61
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.83	0.61
1:A:266:ASN:O	1:A:268:ASP:N	2.34	0.61
1:A:283:HIS:HA	1:A:286:MET:CE	2.31	0.60
1:A:41:GLY:HA3	1:A:324:VAL:HG11	1.83	0.60
1:A:143:PRO:HG3	1:A:424:VAL:CG1	2.32	0.60
1:A:163:ALA:O	1:A:164:LEU:C	2.40	0.60
1:A:101:ASN:ND2	4:A:728:HOH:O	2.35	0.60
1:A:343:LEU:HD23	1:A:345:LYS:HE3	1.84	0.59
1:A:260:LEU:CD1	1:A:273:LEU:HD11	2.32	0.59
1:A:41:GLY:C	1:A:42:VAL:O	2.39	0.59
1:A:104:LYS:HG3	4:A:677:HOH:O	2.03	0.59
1:A:31:ARG:NH1	4:A:486:HOH:O	2.34	0.59
1:A:102:LYS:NZ	1:A:354:GLU:OE1	2.29	0.59
1:A:155:ASN:CG	4:A:621:HOH:O	2.38	0.59
1:A:141:THR:HG22	4:A:484:HOH:O	2.02	0.58
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.33	0.58
1:A:232:ILE:HD13	1:A:241:VAL:HG12	1.84	0.58
1:A:225:LEU:HD21	1:A:245:LEU:HD21	1.86	0.58
1:A:82:ASP:HA	4:A:503:HOH:O	2.03	0.58
1:A:157:GLY:HA3	4:A:521:HOH:O	2.03	0.58
1:A:168:GLU:OE1	1:A:396:LYS:HE3	2.03	0.58
1:A:143:PRO:HG3	1:A:424:VAL:HG13	1.86	0.58
1:A:391:ARG:CG	1:A:391:ARG:O	2.52	0.57
1:A:111:LEU:O	1:A:112:GLY:C	2.41	0.57
1:A:152:ASN:HB2	4:A:753:HOH:O	2.02	0.57
1:A:52:ASP:O	1:A:58:GLY:HA2	2.05	0.57
1:A:141:THR:HB	1:A:144:TYR:CZ	2.39	0.57
1:A:391:ARG:HG2	1:A:391:ARG:O	2.04	0.57
1:A:41:GLY:O	1:A:44:GLU:CG	2.51	0.57
1:A:46:LEU:HD13	1:A:103:SER:HB2	1.86	0.57
1:A:255:ASP:HB3	4:A:708:HOH:O	2.05	0.57
1:A:283:HIS:CE1	1:A:312:THR:O	2.56	0.57
1:A:164:LEU:HD23	4:A:702:HOH:O	2.05	0.56
1:A:62:LEU:O	1:A:66:LYS:CG	2.53	0.56
1:A:311:LYS:HB3	1:A:312:THR:HG23	1.86	0.56
1:A:321:ASP:OD1	4:A:464:HOH:O	2.17	0.56
1:A:47:GLU:HB2	4:A:440:HOH:O	2.04	0.56
1:A:47:GLU:O	1:A:47:GLU:HG2	2.02	0.56
1:A:163:ALA:O	1:A:165:ALA:N	2.39	0.55
1:A:295:GLU:OE1	1:A:396:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:CD2	1:A:345:LYS:HE3	2.37	0.55
1:A:50:ASP:OD2	1:A:62:LEU:HB2	2.06	0.55
1:A:61:VAL:O	1:A:65:VAL:HG23	2.06	0.55
1:A:369:VAL:O	1:A:392:THR:HB	2.07	0.55
1:A:215:ALA:N	4:A:512:HOH:O	2.36	0.55
1:A:232:ILE:HD13	1:A:241:VAL:CG1	2.36	0.55
1:A:228:ILE:O	1:A:232:ILE:HG13	2.06	0.54
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.90	0.54
1:A:44:GLU:HA	4:A:465:HOH:O	2.08	0.54
1:A:233:LYS:HE3	1:A:238:ASP:OD2	2.07	0.54
1:A:330:ILE:HG22	1:A:334:ILE:HD12	1.89	0.54
1:A:327:PRO:HD3	1:A:349:ILE:CD1	2.38	0.53
1:A:93:LEU:HB3	1:A:110:ILE:HG23	1.90	0.53
1:A:183:LEU:O	1:A:187:SER:HB3	2.08	0.53
1:A:269:LYS:O	1:A:269:LYS:CD	2.50	0.53
1:A:4:LYS:HG2	4:A:470:HOH:O	2.09	0.53
1:A:4:LYS:HB3	4:A:763:HOH:O	2.09	0.53
1:A:282:TYR:O	1:A:286:MET:HE3	2.09	0.52
1:A:282:TYR:C	1:A:286:MET:HE3	2.29	0.52
1:A:140:LYS:HB3	1:A:391:ARG:HH12	1.71	0.52
1:A:283:HIS:CA	1:A:286:MET:HE3	2.37	0.52
1:A:63:HIS:O	1:A:66:LYS:N	2.43	0.52
1:A:63:HIS:O	1:A:67:ASN:N	2.41	0.52
1:A:292:VAL:O	4:A:639:HOH:O	2.19	0.52
1:A:327:PRO:HD3	1:A:349:ILE:HD11	1.92	0.52
1:A:410:ASN:O	1:A:414:ARG:HG3	2.09	0.52
1:A:146:LEU:CD1	1:A:423:ALA:HB1	2.39	0.52
1:A:152:ASN:HD22	1:A:168:GLU:HB3	1.70	0.51
1:A:87:LYS:HE2	4:A:733:HOH:O	2.09	0.51
1:A:422:ASN:HB2	4:A:560:HOH:O	2.09	0.51
1:A:185:ILE:O	1:A:189:VAL:HG23	2.11	0.51
1:A:37:GLY:O	1:A:38:ALA:C	2.49	0.51
1:A:282:TYR:HB3	1:A:286:MET:HE2	1.92	0.50
1:A:63:HIS:HB2	4:A:569:HOH:O	2.10	0.50
1:A:363:PHE:HZ	1:A:392:THR:HG22	1.76	0.50
1:A:43:HIS:CE1	1:A:329:ARG:NH2	2.80	0.50
1:A:435:LYS:CE	4:A:694:HOH:O	2.44	0.50
1:A:260:LEU:CD1	1:A:281:LEU:HD23	2.40	0.50
1:A:211:GLU:HB2	4:A:621:HOH:O	2.10	0.50
1:A:264:ASN:HB3	1:A:266:ASN:N	2.25	0.50
1:A:383:ILE:HG13	1:A:395:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:NZ	4:A:748:HOH:O	2.27	0.49
1:A:4:LYS:HD3	4:A:469:HOH:O	2.10	0.49
1:A:57:MET:HB2	4:A:555:HOH:O	2.13	0.49
1:A:111:LEU:HD22	4:A:754:HOH:O	2.11	0.49
1:A:102:LYS:HE2	1:A:351:THR:HG23	1.94	0.49
1:A:253:PHE:C	1:A:254:LYS:HG3	2.32	0.49
1:A:362:SER:O	1:A:367:TRP:HB2	2.12	0.49
1:A:187:SER:O	1:A:191:HIS:ND1	2.45	0.49
1:A:74:PRO:O	1:A:78:LYS:HD2	2.12	0.49
1:A:432:HIS:HD2	4:A:671:HOH:O	1.96	0.49
1:A:41:GLY:HA3	1:A:324:VAL:CG1	2.42	0.48
1:A:46:LEU:C	1:A:46:LEU:CD2	2.81	0.48
1:A:131:LYS:NZ	1:A:135:ASP:CG	2.66	0.48
1:A:218:ILE:HG23	1:A:223:GLU:HG2	1.94	0.48
1:A:403:SER:O	1:A:407:ALA:CB	2.61	0.48
1:A:398:GLY:HA3	1:A:405:ARG:HD2	1.95	0.48
1:A:73:ALA:HB3	1:A:74:PRO:HD2	1.95	0.48
1:A:45:ALA:CB	1:A:107:ALA:HB2	2.43	0.47
1:A:57:MET:CB	4:A:555:HOH:O	2.63	0.47
1:A:260:LEU:CD1	1:A:273:LEU:CD1	2.92	0.47
1:A:158:SER:CB	4:A:576:HOH:O	2.00	0.47
1:A:131:LYS:NZ	1:A:135:ASP:OD1	2.41	0.47
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.59	0.47
1:A:374:ARG:O	1:A:377:GLU:HG2	2.14	0.47
1:A:152:ASN:O	1:A:399:ALA:CB	2.53	0.47
1:A:264:ASN:ND2	1:A:266:ASN:C	2.68	0.47
1:A:66:LYS:CE	4:A:688:HOH:O	2.57	0.47
1:A:161:GLY:O	1:A:217:ASN:OD1	2.32	0.46
1:A:357:LYS:O	1:A:357:LYS:HG2	2.15	0.46
1:A:196:LEU:HD22	1:A:200:ARG:NH2	2.30	0.46
1:A:225:LEU:O	1:A:229:VAL:HG22	2.15	0.46
1:A:248:ALA:HB1	4:A:654:HOH:O	2.16	0.46
1:A:66:LYS:CE	4:A:504:HOH:O	2.30	0.46
1:A:144:TYR:O	1:A:423:ALA:HA	2.16	0.46
1:A:275:GLY:N	1:A:276:PRO:CD	2.79	0.46
1:A:326:ASN:C	1:A:326:ASN:ND2	2.67	0.46
1:A:312:THR:CG2	4:A:623:HOH:O	2.64	0.45
1:A:101:ASN:ND2	1:A:103:SER:HB3	2.32	0.45
1:A:73:ALA:CB	1:A:74:PRO:CD	2.90	0.45
1:A:325:THR:O	1:A:349:ILE:CD1	2.52	0.45
1:A:68:VAL:HA	1:A:72:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:O	1:A:281:LEU:HD12	2.17	0.45
1:A:387:VAL:CG2	1:A:392:THR:OG1	2.59	0.45
1:A:43:HIS:ND1	1:A:329:ARG:NH2	2.65	0.45
1:A:26:GLU:OE1	1:A:26:GLU:N	2.44	0.45
1:A:362:SER:HB3	1:A:367:TRP:HB2	1.99	0.45
1:A:4:LYS:CB	4:A:763:HOH:O	2.64	0.45
1:A:131:LYS:HD3	1:A:131:LYS:C	2.38	0.45
1:A:264:ASN:CG	1:A:266:ASN:N	2.61	0.45
1:A:390:LEU:O	1:A:391:ARG:HB3	2.16	0.44
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.52	0.44
1:A:259:ASP:OD1	1:A:272:TRP:CD1	2.71	0.44
1:A:378:THR:O	1:A:408:LYS:NZ	2.50	0.44
1:A:46:LEU:HD22	1:A:103:SER:HA	1.99	0.44
1:A:132:HIS:O	1:A:135:ASP:HB2	2.17	0.44
1:A:46:LEU:CD1	1:A:103:SER:HB2	2.47	0.44
1:A:70:ASP:O	1:A:74:PRO:HG3	2.18	0.44
1:A:233:LYS:CE	1:A:238:ASP:OD2	2.65	0.44
1:A:317:ILE:HG21	4:A:709:HOH:O	2.17	0.44
1:A:67:ASN:O	1:A:71:VAL:HB	2.18	0.44
1:A:167:GLN:HE22	3:A:439:2PG:H31	1.82	0.44
1:A:330:ILE:HG22	1:A:334:ILE:CD1	2.48	0.43
1:A:97:ASP:O	1:A:99:THR:HG23	2.19	0.43
1:A:218:ILE:HD13	1:A:218:ILE:HG21	1.81	0.43
1:A:248:ALA:CB	4:A:654:HOH:O	2.66	0.43
1:A:46:LEU:CD1	1:A:103:SER:CB	2.82	0.43
1:A:41:GLY:O	1:A:44:GLU:CD	2.56	0.43
1:A:42:VAL:CG1	4:A:761:HOH:O	2.62	0.43
1:A:143:PRO:HG3	1:A:424:VAL:HG11	2.00	0.43
3:A:439:2PG:C1	4:A:525:HOH:O	2.67	0.43
1:A:363:PHE:CZ	1:A:392:THR:HG22	2.54	0.42
1:A:204:SER:OG	1:A:205:ALA:N	2.52	0.42
1:A:271:LYS:CB	4:A:622:HOH:O	2.66	0.42
1:A:387:VAL:O	1:A:387:VAL:HG22	2.19	0.42
1:A:133:LEU:HD23	1:A:386:LEU:HA	2.01	0.42
1:A:31:ARG:HH11	1:A:31:ARG:HD2	1.51	0.42
1:A:201:TYR:HB2	1:A:205:ALA:CB	2.49	0.42
1:A:295:GLU:HA	1:A:318:VAL:HB	2.01	0.42
1:A:121:ALA:HB3	1:A:132:HIS:NE2	2.35	0.42
1:A:177:LYS:HD2	1:A:177:LYS:HA	1.85	0.42
1:A:59:LYS:HD2	4:A:555:HOH:O	2.19	0.42
1:A:39:SER:O	1:A:40:THR:CG2	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HG2	1:A:198:LYS:HE3	2.02	0.42
1:A:326:ASN:HD22	1:A:327:PRO:N	2.18	0.42
1:A:381:THR:OG1	4:A:507:HOH:O	2.18	0.41
1:A:401:ALA:O	1:A:402:ARG:HB2	2.19	0.41
1:A:168:GLU:HG3	1:A:246:ASP:HB3	2.02	0.41
1:A:317:ILE:O	1:A:339:ALA:HB1	2.20	0.41
1:A:344:LEU:CD1	1:A:359:ALA:HB2	2.49	0.41
1:A:373:HIS:CE1	1:A:405:ARG:HH11	2.36	0.41
1:A:46:LEU:HD13	1:A:103:SER:CA	2.49	0.41
1:A:267:SER:HB3	1:A:272:TRP:CH2	2.56	0.41
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.84	0.41
1:A:159:HIS:HE2	1:A:210:ASP:CG	2.23	0.41
1:A:143:PRO:CG	1:A:424:VAL:HG13	2.49	0.41
1:A:77:VAL:HB	4:A:673:HOH:O	2.20	0.40
1:A:111:LEU:HD12	1:A:111:LEU:HA	1.90	0.40
1:A:159:HIS:CE1	1:A:210:ASP:H	2.40	0.40
3:A:439:2PG:H2	4:A:525:HOH:O	2.21	0.40
1:A:266:ASN:HD22	1:A:266:ASN:HA	1.37	0.40
1:A:127:VAL:HB	1:A:128:PRO:HD2	2.02	0.40
1:A:390:LEU:HB3	1:A:392:THR:HG23	2.03	0.40
1:A:101:ASN:HD21	1:A:103:SER:HB3	1.86	0.40
1:A:267:SER:HB3	1:A:272:TRP:CZ2	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:O	4:A:643:HOH:O[3_644]	2.14	0.06
1:A:79:ALA:CA	4:A:643:HOH:O[3_644]	2.15	0.05

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	434/436 (100%)	392 (90%)	34 (8%)	8 (2%)	8 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LYS
1	A	265	PRO
1	A	267	SER
1	A	270	SER
1	A	164	LEU
1	A	402	ARG
1	A	160	ALA
1	A	324	VAL

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%)	316 (92%)	28 (8%)	11 12

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	13	SER
1	A	23	LEU
1	A	39	SER
1	A	43	HIS
1	A	46	LEU
1	A	50	ASP
1	A	53	LYS
1	A	54	SER
1	A	96	LEU
1	A	101	ASN
1	A	140	LYS
1	A	143	PRO

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Mol	Chain	Res	Type
1	A	147	PRO
1	A	149	PRO
1	A	151	LEU
1	A	155	ASN
1	A	187	SER
1	A	194	LYS
1	A	255	ASP
1	A	266	ASN
1	A	270	SER
1	A	284	SER
1	A	311	LYS
1	A	324	VAL
1	A	325	THR
1	A	326	ASN
1	A	373	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	101	ASN
1	A	167	GLN
1	A	207	ASN
1	A	266	ASN
1	A	283	HIS
1	A	326	ASN
1	A	432	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	2PG	A	439	2	9,10,10	1.51	2 (22%)	11,14,14	1.36	3 (27%)

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
3	2PG	A	439	2	-	8/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	439	2PG	P-O4P	-2.60	1.44	1.54
3	A	439	2PG	O1-C1	2.28	1.29	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	439	2PG	O1-C1-C2	-2.26	117.22	122.57
3	A	439	2PG	O4P-P-O3P	2.12	115.75	107.64
3	A	439	2PG	O3-C3-C2	2.01	116.83	111.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	439	2PG	O2-C1-C2-O1P
3	A	439	2PG	O1P-C2-C3-O3
3	A	439	2PG	C3-C2-O1P-P

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Mol	Chain	Res	Type	Atoms
3	A	439	2PG	C1-C2-C3-O3
3	A	439	2PG	C2-O1P-P-O3P
3	A	439	2PG	O1-C1-C2-C3
3	A	439	2PG	O2-C1-C2-C3
3	A	439	2PG	C2-O1P-P-O4P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	2PG	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.