Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:56 am BST

PDB ID	:	1AAM
Title	:	THE STRUCTURAL BASIS FOR THE ALTERED SUBSTRATE SPECIFICITY OF THE R292D ACTIVE SITE MUTANT OF ASPARTATE AMINOTRANSFERASE FROM E. COLI
Authors	:	Almo, S.C.; Smith, D.L.; Danishefsky, A.T.; Ringe, D.
Deposited on	:	1993-07-13
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

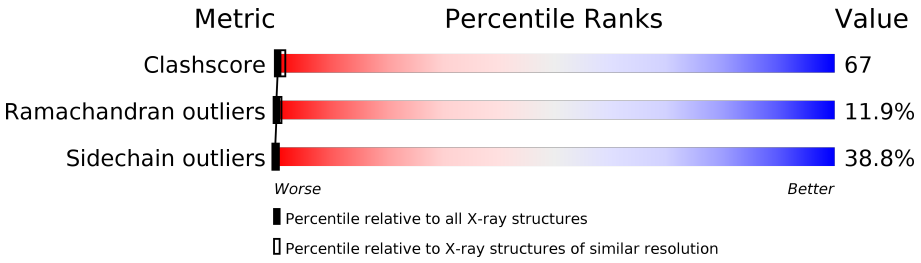
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 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	396	15% 39% 32% 14%

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	PLP	A	409	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3086 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.

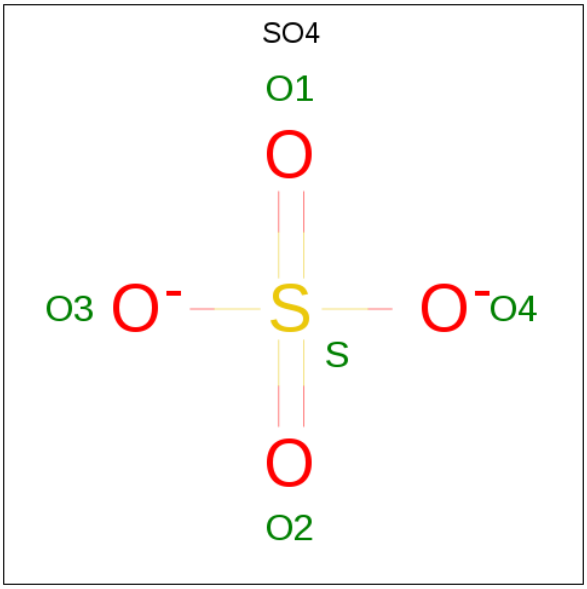
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3066	1934	533	586	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

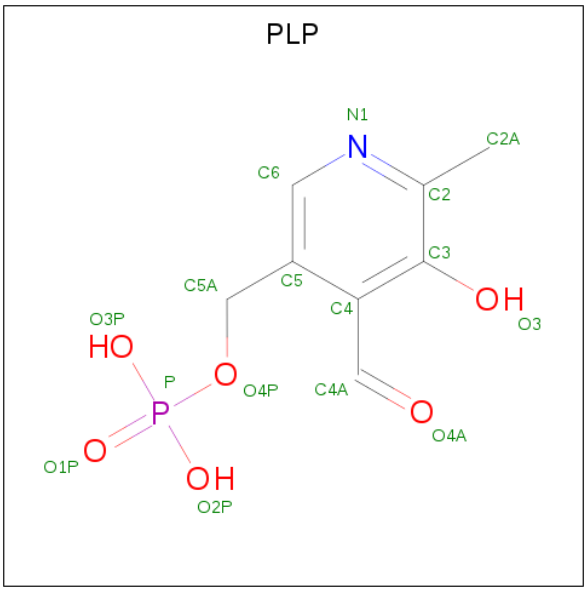
Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ASP	ARG	ENGINEERED MUTATION	UNP P00509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0

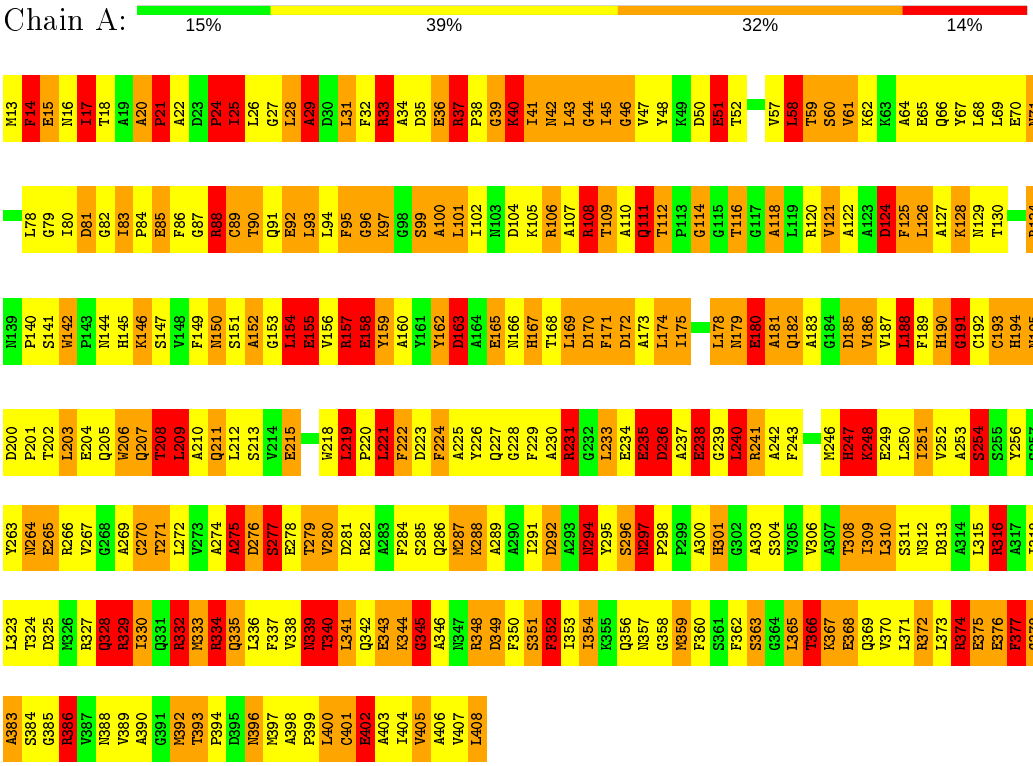
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	155.40Å 87.00Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: SO4, PLP

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	0.89	27/3127 (0.9%)	2.32	171/4237 (4.0%)

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	6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLU	CD-OE2	6.62	1.32	1.25
1	A	65	GLU	CD-OE2	6.29	1.32	1.25
1	A	92	GLU	CD-OE1	6.01	1.32	1.25
1	A	368	GLU	CD-OE1	6.01	1.32	1.25
1	A	215	GLU	CD-OE2	6.00	1.32	1.25
1	A	235	GLU	CD-OE1	5.99	1.32	1.25
1	A	265	GLU	CD-OE1	5.98	1.32	1.25
1	A	36	GLU	CD-OE2	5.96	1.32	1.25
1	A	155	GLU	CD-OE2	5.93	1.32	1.25
1	A	320	GLU	CD-OE1	5.93	1.32	1.25
1	A	51	GLU	CD-OE2	5.92	1.32	1.25
1	A	165	GLU	CD-OE1	5.86	1.32	1.25
1	A	234	GLU	CD-OE2	5.83	1.32	1.25
1	A	180	GLU	CD-OE1	5.82	1.32	1.25
1	A	249	GLU	CD-OE2	5.81	1.32	1.25
1	A	343	GLU	CD-OE1	5.72	1.31	1.25
1	A	72	GLU	CD-OE1	5.70	1.31	1.25
1	A	375	GLU	CD-OE2	5.66	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	GLU	CD-OE1	5.58	1.31	1.25
1	A	70	GLU	CD-OE2	5.58	1.31	1.25
1	A	376	GLU	CD-OE2	5.57	1.31	1.25
1	A	85	GLU	CD-OE2	5.54	1.31	1.25
1	A	158	GLU	CD-OE1	5.44	1.31	1.25
1	A	238	GLU	CD-OE1	5.37	1.31	1.25
1	A	278	GLU	CD-OE1	5.30	1.31	1.25
1	A	322	GLU	CD-OE1	5.24	1.31	1.25
1	A	402	GLU	CD-OE1	5.08	1.31	1.25

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	TRP	CA-CB-CG	14.60	141.44	113.70
1	A	25	ILE	C-N-CA	13.09	154.41	121.70
1	A	241	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	A	39	GLY	N-CA-C	11.31	141.38	113.10
1	A	334	ARG	CD-NE-CZ	11.12	139.17	123.60
1	A	166	ASN	N-CA-CB	10.51	129.52	110.60
1	A	157	ARG	CD-NE-CZ	10.29	138.01	123.60
1	A	137	VAL	N-CA-C	9.89	137.70	111.00
1	A	193	CYS	C-N-CA	9.86	146.36	121.70
1	A	14	PHE	CA-CB-CG	9.72	137.22	113.90
1	A	114	GLY	N-CA-C	9.67	137.28	113.10
1	A	181	ALA	C-N-CA	9.56	145.60	121.70
1	A	17	ILE	N-CA-CB	9.19	131.94	110.80
1	A	334	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	152	ALA	N-CA-CB	9.01	122.71	110.10
1	A	197	THR	N-CA-CB	8.96	127.33	110.30
1	A	88	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	A	241	ARG	CA-CB-CG	8.59	132.29	113.40
1	A	381	ALA	N-CA-CB	8.46	121.94	110.10
1	A	329	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	106	ARG	CA-CB-CG	8.15	131.34	113.40
1	A	366	THR	C-N-CA	8.04	141.80	121.70
1	A	374	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	A	296	SER	N-CA-CB	7.90	122.36	110.50
1	A	400	LEU	CA-CB-CG	7.89	133.44	115.30
1	A	163	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	126	LEU	CA-CB-CG	7.75	133.13	115.30
1	A	182	GLN	N-CA-C	7.73	131.86	111.00
1	A	25	ILE	CA-C-O	7.72	136.31	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	380	TYR	CB-CG-CD1	7.71	125.63	121.00
1	A	380	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	A	109	THR	N-CA-CB	-7.57	95.91	110.30
1	A	154	LEU	CA-CB-CG	7.55	132.67	115.30
1	A	332	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	270	CYS	N-CA-CB	7.50	124.10	110.60
1	A	235	GLU	N-CA-CB	7.43	123.97	110.60
1	A	166	ASN	N-CA-C	-7.24	91.45	111.00
1	A	316	ARG	CD-NE-CZ	7.24	133.74	123.60
1	A	376	GLU	N-CA-CB	7.22	123.59	110.60
1	A	171	PHE	CA-CB-CG	7.18	131.13	113.90
1	A	124	ASP	CA-CB-CG	7.11	129.04	113.40
1	A	17	ILE	CA-C-O	7.10	135.00	120.10
1	A	41	ILE	C-N-CA	7.08	139.41	121.70
1	A	106	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	106	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	372	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	345	GLY	N-CA-C	6.94	130.44	113.10
1	A	292	ASP	CA-CB-CG	6.91	128.61	113.40
1	A	254	SER	O-C-N	6.91	133.75	122.70
1	A	142	TRP	N-CA-C	-6.85	92.50	111.00
1	A	158	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	A	248	LYS	N-CA-CB	6.78	122.81	110.60
1	A	386	ARG	NE-CZ-NH2	6.77	123.69	120.30
1	A	236	ASP	CB-CA-C	6.75	123.90	110.40
1	A	368	GLU	CB-CA-C	6.75	123.90	110.40
1	A	386	ARG	CD-NE-CZ	6.74	133.04	123.60
1	A	108	ARG	CD-NE-CZ	6.73	133.02	123.60
1	A	348	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	50	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	59	THR	N-CA-CB	6.56	122.77	110.30
1	A	50	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	120	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	106	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	A	108	ARG	C-N-CA	6.39	137.68	121.70
1	A	322	GLU	CG-CD-OE2	6.37	131.04	118.30
1	A	328	GLN	CA-CB-CG	6.29	127.25	113.40
1	A	376	GLU	N-CA-C	-6.25	94.11	111.00
1	A	329	ARG	CD-NE-CZ	6.22	132.30	123.60
1	A	37	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	106	ARG	CB-CA-C	6.20	122.80	110.40
1	A	44	GLY	N-CA-C	-6.17	97.68	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	PRO	N-CA-C	6.13	128.05	112.10
1	A	89	CYS	O-C-N	6.13	132.50	122.70
1	A	193	CYS	CA-C-O	6.13	132.97	120.10
1	A	179	ASN	N-CA-CB	-6.12	99.59	110.60
1	A	37	ARG	CB-CA-C	-6.11	98.18	110.40
1	A	170	ASP	N-CA-CB	6.09	121.56	110.60
1	A	118	ALA	N-CA-CB	6.08	118.61	110.10
1	A	264	ASN	N-CA-CB	-6.06	99.70	110.60
1	A	190	HIS	N-CA-C	6.04	127.31	111.00
1	A	158	GLU	CG-CD-OE2	6.04	130.37	118.30
1	A	225	ALA	CB-CA-C	6.02	119.13	110.10
1	A	191	GLY	N-CA-C	5.98	128.04	113.10
1	A	60	SER	CA-C-O	5.94	132.57	120.10
1	A	138	SER	N-CA-CB	5.92	119.39	110.50
1	A	330	ILE	CB-CA-C	-5.92	99.76	111.60
1	A	106	ARG	CD-NE-CZ	5.91	131.87	123.60
1	A	349	ASP	CB-CA-C	5.90	122.21	110.40
1	A	109	THR	N-CA-C	5.90	126.94	111.00
1	A	296	SER	O-C-N	5.90	132.14	122.70
1	A	276	ASP	CB-CG-OD1	-5.88	113.00	118.30
1	A	241	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	A	17	ILE	CA-C-N	-5.86	104.30	117.20
1	A	41	ILE	CA-C-O	5.86	132.41	120.10
1	A	193	CYS	CA-CB-SG	-5.85	103.47	114.00
1	A	159	TYR	CB-CG-CD1	5.84	124.51	121.00
1	A	193	CYS	CA-C-N	-5.84	104.35	117.20
1	A	332	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	226	TYR	N-CA-C	5.81	126.69	111.00
1	A	101	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	332	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	A	186	VAL	CA-C-O	5.75	132.18	120.10
1	A	155	GLU	N-CA-CB	5.74	120.94	110.60
1	A	27	GLY	N-CA-C	-5.74	98.76	113.10
1	A	316	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	28	LEU	C-N-CA	5.71	135.98	121.70
1	A	172	ASP	CB-CG-OD1	5.70	123.42	118.30
1	A	24	PRO	N-CA-C	5.68	126.86	112.10
1	A	207	GLN	CA-CB-CG	5.67	125.88	113.40
1	A	339	ASN	N-CA-CB	5.66	120.80	110.60
1	A	159	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	368	GLU	CA-CB-CG	5.62	125.78	113.40
1	A	235	GLU	OE1-CD-OE2	-5.62	116.55	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	105	LYS	O-C-N	5.62	131.69	122.70
1	A	265	GLU	C-N-CA	5.61	135.72	121.70
1	A	126	LEU	CB-CA-C	5.60	120.85	110.20
1	A	221	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	182	GLN	C-N-CA	5.60	135.70	121.70
1	A	111	GLN	CA-CB-CG	5.59	125.70	113.40
1	A	37	ARG	N-CA-C	5.59	126.09	111.00
1	A	285	SER	N-CA-CB	5.58	118.88	110.50
1	A	172	ASP	CB-CA-C	5.57	121.55	110.40
1	A	359	MET	CA-CB-CG	5.57	122.77	113.30
1	A	341	LEU	CB-CA-C	5.55	120.74	110.20
1	A	188	LEU	O-C-N	5.53	131.54	122.70
1	A	335	GLN	CB-CG-CD	5.51	125.93	111.60
1	A	377	PHE	CA-CB-CG	5.46	127.00	113.90
1	A	22	ALA	N-CA-C	5.46	125.73	111.00
1	A	85	GLU	O-C-N	5.45	131.42	122.70
1	A	29	ALA	N-CA-C	5.44	125.70	111.00
1	A	100	ALA	CA-C-O	-5.44	108.67	120.10
1	A	195	ASN	N-CA-CB	5.44	120.40	110.60
1	A	85	GLU	CG-CD-OE2	-5.42	107.45	118.30
1	A	294	ASN	N-CA-CB	5.42	120.36	110.60
1	A	162	TYR	CA-CB-CG	5.42	123.69	113.40
1	A	165	GLU	CG-CD-OE2	5.42	129.13	118.30
1	A	330	ILE	N-CA-CB	5.41	123.24	110.80
1	A	136	TRP	CB-CA-C	5.39	121.18	110.40
1	A	208	THR	CA-CB-CG2	5.39	119.95	112.40
1	A	127	ALA	N-CA-CB	5.38	117.63	110.10
1	A	179	ASN	CB-CA-C	5.35	121.09	110.40
1	A	209	LEU	CB-CA-C	5.34	120.35	110.20
1	A	318	ILE	CB-CA-C	5.34	122.28	111.60
1	A	170	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	A	155	GLU	O-C-N	5.33	131.23	122.70
1	A	93	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	A	366	THR	CA-C-O	5.33	131.29	120.10
1	A	204	GLU	CB-CG-CD	5.31	128.53	114.20
1	A	165	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	A	275	ALA	N-CA-C	5.25	125.18	111.00
1	A	32	PHE	CB-CA-C	5.25	120.90	110.40
1	A	186	VAL	C-N-CA	5.25	134.82	121.70
1	A	58	LEU	C-N-CA	5.22	134.75	121.70
1	A	21	PRO	C-N-CA	5.21	134.73	121.70
1	A	406	ALA	N-CA-CB	5.20	117.37	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	SER	C-N-CA	5.19	134.68	121.70
1	A	316	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	400	LEU	N-CA-CB	-5.16	100.08	110.40
1	A	241	ARG	CG-CD-NE	5.15	122.61	111.80
1	A	204	GLU	CG-CD-OE1	5.14	128.59	118.30
1	A	239	GLY	N-CA-C	-5.14	100.25	113.10
1	A	332	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	70	GLU	CG-CD-OE1	5.12	128.55	118.30
1	A	180	GLU	CG-CD-OE2	5.11	128.53	118.30
1	A	253	ALA	N-CA-C	-5.08	97.28	111.00
1	A	247	HIS	N-CA-C	5.08	124.71	111.00
1	A	33	ARG	CA-C-N	-5.06	106.08	117.20
1	A	185	ASP	O-C-N	5.05	130.79	122.70
1	A	352	PHE	N-CA-C	5.04	124.59	111.00
1	A	386	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	342	GLN	N-CA-CB	5.02	119.64	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	134	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	374	ARG	Sidechain
1	A	88	ARG	Sidechain

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	3066	0	3006	403	1
2	A	5	0	0	0	0
3	A	15	0	6	8	0
All	All	3086	0	3012	404	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 67.

All (404) 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:258:LYS:HZ1	3:A:409:PLP:C4A	1.50	1.18
1:A:252:VAL:HG13	1:A:271:THR:HG23	1.26	1.14
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.27	1.09
1:A:231:ARG:HG2	1:A:357:ASN:HD22	1.10	1.09
1:A:193:CYS:SG	1:A:200:ASP:HB3	1.94	1.07
1:A:28:LEU:HB2	1:A:382:VAL:HG13	1.35	1.06
1:A:230:ALA:HB3	1:A:358:GLY:H	1.26	0.99
1:A:258:LYS:HZ2	3:A:409:PLP:C4A	1.73	0.96
1:A:218:TRP:O	1:A:219:LEU:HB2	1.65	0.95
1:A:83:ILE:HG22	1:A:84:PRO:HD2	1.46	0.94
1:A:345:GLY:HA2	1:A:405:VAL:HG11	1.48	0.94
1:A:112:THR:HG21	1:A:118:ALA:CB	1.97	0.94
1:A:146:LYS:HG2	1:A:156:VAL:HG21	1.50	0.92
1:A:231:ARG:HG2	1:A:357:ASN:ND2	1.86	0.90
1:A:112:THR:CG2	1:A:118:ALA:HB2	2.01	0.90
1:A:231:ARG:CG	1:A:357:ASN:HD22	1.85	0.89
1:A:134:ARG:HH11	1:A:157:ARG:HG2	1.37	0.89
1:A:195:ASN:OD1	1:A:196:PRO:HA	1.72	0.88
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.55	0.87
1:A:231:ARG:HH11	1:A:231:ARG:HG3	1.38	0.86
1:A:194:HIS:HB3	1:A:197:THR:O	1.76	0.86
1:A:140:PRO:HB2	1:A:196:PRO:HD2	1.60	0.83
1:A:220:PRO:HD3	1:A:247:HIS:CE1	2.15	0.81
1:A:238:GLU:HB2	1:A:241:ARG:HD3	1.61	0.81
1:A:137:VAL:HG21	1:A:156:VAL:HB	1.62	0.81
1:A:137:VAL:HG11	1:A:158:GLU:HG2	1.62	0.81
1:A:208:THR:HG22	1:A:209:LEU:HD13	1.63	0.81
1:A:399:PRO:O	1:A:402:GLU:HG3	1.83	0.79
1:A:300:ALA:O	1:A:303:ALA:HB3	1.83	0.78
1:A:142:TRP:O	1:A:145:HIS:HB2	1.84	0.78
1:A:324:THR:HA	1:A:327:ARG:HD3	1.64	0.78
1:A:108:ARG:HB2	1:A:280:VAL:HG23	1.64	0.77
1:A:333:MET:HG3	1:A:392:MET:HB3	1.66	0.77
1:A:292:ASP:HA	1:A:296:SER:HA	1.68	0.76
1:A:203:LEU:HD13	1:A:207:GLN:HG3	1.68	0.76
1:A:87:GLY:O	1:A:91:GLN:HB2	1.87	0.75
1:A:393:THR:HB	1:A:396:ASN:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HB	3:A:409:PLP:O2P	1.85	0.74
1:A:85:GLU:HG3	1:A:88:ARG:HH21	1.52	0.74
1:A:67:TYR:O	1:A:71:ASN:HB2	1.87	0.74
1:A:333:MET:CE	1:A:336:LEU:HD23	2.18	0.74
1:A:47:VAL:HG22	1:A:263:TYR:CE1	2.23	0.74
1:A:79:GLY:O	1:A:298:PRO:HD2	1.88	0.73
1:A:40:LYS:HZ3	1:A:43:LEU:HD22	1.54	0.73
1:A:174:LEU:O	1:A:178:LEU:HB3	1.87	0.72
1:A:169:LEU:HB2	1:A:199:ILE:CG2	2.19	0.72
1:A:160:ALA:O	1:A:174:LEU:HB2	1.89	0.72
1:A:231:ARG:HB2	1:A:236:ASP:HB2	1.72	0.71
1:A:252:VAL:HG13	1:A:271:THR:CG2	2.14	0.71
1:A:373:LEU:HD13	1:A:407:VAL:HG11	1.72	0.71
1:A:134:ARG:HD2	1:A:157:ARG:HG2	1.72	0.71
1:A:82:GLY:CA	1:A:298:PRO:HG3	2.20	0.71
1:A:213:SER:HG	1:A:218:TRP:HE3	1.39	0.70
1:A:46:GLY:HA2	1:A:360:PHE:HZ	1.56	0.70
1:A:371:LEU:C	1:A:373:LEU:H	1.92	0.70
1:A:373:LEU:HG	1:A:379:VAL:HG13	1.73	0.70
1:A:116:THR:HG22	3:A:409:PLP:O2P	1.90	0.70
1:A:111:GLN:HE21	1:A:298:PRO:HB2	1.54	0.70
1:A:146:LYS:HG2	1:A:156:VAL:CG2	2.22	0.70
1:A:252:VAL:CG1	1:A:271:THR:HG23	2.15	0.69
1:A:359:MET:HG3	1:A:388:ASN:OD1	1.93	0.69
1:A:40:LYS:HE2	1:A:400:LEU:HD13	1.74	0.69
1:A:128:LYS:HD2	1:A:129:ASN:N	2.07	0.69
1:A:333:MET:HE3	1:A:336:LEU:HD23	1.74	0.69
1:A:80:ILE:HD12	1:A:297:ASN:H	1.57	0.69
1:A:171:PHE:HA	1:A:174:LEU:HD23	1.75	0.69
1:A:348:ARG:HH22	1:A:365:LEU:CD2	2.05	0.69
1:A:110:ALA:O	1:A:269:ALA:HA	1.92	0.68
1:A:116:THR:CB	3:A:409:PLP:O2P	2.40	0.68
1:A:208:THR:HA	1:A:211:GLN:NE2	2.08	0.68
1:A:369:GLN:O	1:A:373:LEU:HB2	1.94	0.68
1:A:193:CYS:HG	1:A:200:ASP:HB3	1.58	0.68
1:A:243:PHE:O	1:A:246:MET:HB2	1.93	0.68
1:A:377:PHE:HB3	1:A:379:VAL:HG12	1.75	0.68
1:A:28:LEU:HG	1:A:380:TYR:HD2	1.57	0.68
1:A:134:ARG:HG3	1:A:135:VAL:N	2.09	0.67
1:A:309:ILE:HG23	1:A:316:ARG:CA	2.24	0.67
1:A:345:GLY:HA2	1:A:405:VAL:CG1	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TRP:HE3	1:A:159:TYR:HD2	1.40	0.67
1:A:193:CYS:SG	1:A:357:ASN:HB3	2.34	0.67
1:A:231:ARG:NH1	1:A:231:ARG:HG3	2.04	0.66
1:A:365:LEU:HD13	1:A:369:GLN:HB3	1.78	0.66
1:A:334:ARG:O	1:A:338:VAL:HG23	1.96	0.65
1:A:135:VAL:O	1:A:156:VAL:HA	1.96	0.65
1:A:146:LYS:HA	1:A:156:VAL:HG21	1.79	0.65
1:A:393:THR:O	1:A:397:MET:N	2.30	0.65
1:A:128:LYS:NZ	1:A:129:ASN:HB2	2.11	0.65
1:A:294:ASN:HD22	1:A:295:TYR:HD1	1.44	0.65
1:A:116:THR:CG2	3:A:409:PLP:O2P	2.44	0.64
1:A:134:ARG:HD2	1:A:157:ARG:CG	2.27	0.64
1:A:348:ARG:HH22	1:A:365:LEU:HD23	1.59	0.64
1:A:309:ILE:HG23	1:A:316:ARG:HA	1.78	0.64
1:A:393:THR:HG23	1:A:394:PRO:HD2	1.80	0.64
1:A:86:PHE:O	1:A:90:THR:HB	1.98	0.64
1:A:333:MET:HG3	1:A:392:MET:CB	2.27	0.64
1:A:28:LEU:HD21	1:A:380:TYR:HB3	1.80	0.64
1:A:35:ASP:HB2	1:A:37:ARG:HH21	1.63	0.63
1:A:142:TRP:CZ2	1:A:144:ASN:HB3	2.34	0.63
1:A:96:GLY:HA3	1:A:102:ILE:HD11	1.81	0.63
1:A:333:MET:CE	1:A:333:MET:HA	2.30	0.62
1:A:31:LEU:H	1:A:31:LEU:HD12	1.63	0.62
1:A:334:ARG:CG	1:A:353:ILE:HG12	2.29	0.62
1:A:91:GLN:HA	1:A:94:LEU:HD12	1.82	0.62
1:A:122:ALA:O	1:A:126:LEU:HB3	2.00	0.62
1:A:13:MET:HG3	1:A:14:PHE:N	2.12	0.62
1:A:247:HIS:O	1:A:248:LYS:HG3	1.99	0.62
1:A:330:ILE:HG21	1:A:358:GLY:O	2.00	0.62
1:A:359:MET:SD	1:A:390:ALA:HB2	2.39	0.62
1:A:40:LYS:O	1:A:41:ILE:HG13	1.99	0.62
1:A:83:ILE:CG2	1:A:84:PRO:HD2	2.26	0.62
1:A:140:PRO:HB2	1:A:196:PRO:CD	2.29	0.61
1:A:20:ALA:HB3	1:A:21:PRO:HD3	1.82	0.61
1:A:40:LYS:NZ	1:A:43:LEU:HD22	2.14	0.61
1:A:137:VAL:CG2	1:A:156:VAL:HB	2.29	0.61
1:A:189:PHE:O	1:A:222:PHE:HA	2.00	0.61
1:A:48:TYR:OH	1:A:329:ARG:HB3	1.99	0.61
1:A:221:LEU:HD12	1:A:222:PHE:N	2.16	0.61
1:A:159:TYR:HB3	1:A:178:LEU:HA	1.83	0.61
1:A:40:LYS:CE	1:A:400:LEU:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HG2	1:A:353:ILE:HG12	1.83	0.60
1:A:188:LEU:HB2	1:A:221:LEU:HG	1.82	0.60
1:A:155:GLU:OE1	1:A:155:GLU:HA	2.01	0.60
1:A:41:ILE:HG23	1:A:42:ASN:H	1.65	0.60
1:A:284:PHE:HA	1:A:287:MET:HB3	1.82	0.60
1:A:99:SER:O	1:A:102:ILE:HB	2.02	0.60
1:A:353:ILE:HG23	1:A:354:ILE:H	1.65	0.60
1:A:276:ASP:HB3	1:A:279:THR:OG1	2.02	0.59
1:A:13:MET:HG3	1:A:14:PHE:HB3	1.84	0.59
1:A:41:ILE:CG2	1:A:42:ASN:N	2.65	0.59
1:A:248:LYS:HB3	1:A:275:ALA:HB2	1.85	0.59
1:A:323:LEU:O	1:A:327:ARG:HG3	2.02	0.59
1:A:89:CYS:HA	1:A:92:GLU:HG2	1.84	0.59
1:A:82:GLY:HA2	1:A:298:PRO:HG3	1.85	0.59
1:A:231:ARG:HB2	1:A:236:ASP:CB	2.32	0.59
1:A:64:ALA:O	1:A:67:TYR:HB3	2.03	0.59
1:A:336:LEU:O	1:A:340:THR:OG1	2.20	0.59
1:A:402:GLU:OE2	1:A:403:ALA:HB2	2.03	0.58
1:A:95:PHE:HD2	1:A:240:LEU:HD21	1.66	0.58
1:A:238:GLU:HA	1:A:241:ARG:CB	2.34	0.58
1:A:91:GLN:HE22	1:A:107:ALA:HB3	1.69	0.58
1:A:170:ASP:O	1:A:174:LEU:HB3	2.04	0.57
1:A:339:ASN:C	1:A:341:LEU:H	2.07	0.57
1:A:368:GLU:HA	1:A:371:LEU:HB3	1.85	0.57
1:A:47:VAL:HG22	1:A:263:TYR:CD1	2.40	0.57
1:A:286:GLN:O	1:A:289:ALA:HB3	2.03	0.57
1:A:353:ILE:HG23	1:A:354:ILE:HD12	1.85	0.57
1:A:61:VAL:HG12	1:A:62:LYS:N	2.19	0.57
1:A:134:ARG:HD2	1:A:157:ARG:HB2	1.85	0.57
1:A:208:THR:HA	1:A:211:GLN:HE22	1.68	0.57
1:A:169:LEU:HB2	1:A:199:ILE:HG21	1.86	0.57
1:A:398:ALA:N	1:A:399:PRO:HD2	2.20	0.56
1:A:309:ILE:HG23	1:A:316:ARG:HB3	1.87	0.56
1:A:58:LEU:HB2	1:A:61:VAL:HG21	1.87	0.56
1:A:46:GLY:HA2	1:A:360:PHE:CZ	2.40	0.56
1:A:180:GLU:HG2	1:A:181:ALA:N	2.20	0.56
1:A:258:LYS:HZ3	3:A:409:PLP:C4A	2.08	0.56
1:A:231:ARG:CB	1:A:357:ASN:HD22	2.19	0.56
1:A:371:LEU:C	1:A:373:LEU:N	2.60	0.56
1:A:339:ASN:O	1:A:341:LEU:N	2.39	0.56
1:A:112:THR:CB	1:A:118:ALA:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HA	1:A:288:LYS:CE	2.37	0.55
1:A:196:PRO:HB2	1:A:386:ARG:HG3	1.88	0.55
1:A:333:MET:HE1	1:A:336:LEU:HD23	1.89	0.55
1:A:203:LEU:HD13	1:A:207:GLN:CG	2.36	0.55
1:A:288:LYS:NZ	1:A:288:LYS:HA	2.21	0.55
1:A:325:ASP:O	1:A:329:ARG:HB2	2.06	0.55
1:A:41:ILE:CG2	1:A:42:ASN:H	2.20	0.55
1:A:386:ARG:CZ	1:A:386:ARG:HB3	2.36	0.55
1:A:100:ALA:O	1:A:104:ASP:N	2.40	0.54
1:A:180:GLU:HG2	1:A:181:ALA:H	1.71	0.54
1:A:188:LEU:HA	1:A:221:LEU:O	2.06	0.54
1:A:367:LYS:N	1:A:367:LYS:HD3	2.22	0.54
1:A:167:HIS:O	1:A:199:ILE:HD11	2.08	0.54
1:A:111:GLN:OE1	1:A:267:VAL:HG23	2.07	0.54
1:A:228:GLY:O	1:A:327:ARG:HD2	2.08	0.54
1:A:260:PHE:HE1	1:A:309:ILE:HD13	1.72	0.54
1:A:31:LEU:HD12	1:A:31:LEU:N	2.20	0.54
1:A:386:ARG:NH1	1:A:386:ARG:HB3	2.22	0.54
1:A:230:ALA:HB3	1:A:358:GLY:N	2.09	0.54
1:A:91:GLN:HE22	1:A:107:ALA:CB	2.21	0.54
1:A:282:ARG:HH11	1:A:282:ARG:HG3	1.73	0.54
1:A:128:LYS:HZ3	1:A:286:GLN:HB3	1.73	0.54
1:A:114:GLY:C	1:A:116:THR:H	2.11	0.54
1:A:163:ASP:HB2	1:A:170:ASP:HB2	1.90	0.54
1:A:404:ILE:O	1:A:408:LEU:OXT	2.25	0.54
1:A:124:ASP:OD1	1:A:152:ALA:HB3	2.08	0.53
1:A:153:GLY:O	1:A:154:LEU:O	2.26	0.53
1:A:137:VAL:CG1	1:A:158:GLU:HG2	2.33	0.53
1:A:229:PHE:HA	1:A:327:ARG:HG2	1.90	0.53
1:A:294:ASN:ND2	1:A:295:TYR:HD1	2.06	0.53
1:A:386:ARG:C	1:A:386:ARG:HH11	2.12	0.53
1:A:64:ALA:O	1:A:68:LEU:HD13	2.08	0.53
1:A:137:VAL:HG12	1:A:158:GLU:HA	1.91	0.53
1:A:397:MET:HE1	1:A:400:LEU:HD23	1.91	0.53
1:A:80:ILE:HD12	1:A:297:ASN:N	2.24	0.53
1:A:40:LYS:HG3	1:A:399:PRO:HG2	1.91	0.53
1:A:202:THR:H	1:A:205:GLN:HE21	1.56	0.53
1:A:341:LEU:HB3	1:A:350:PHE:CD2	2.44	0.53
1:A:230:ALA:CB	1:A:358:GLY:H	2.11	0.53
1:A:135:VAL:HG13	1:A:156:VAL:HG12	1.91	0.53
1:A:256:TYR:O	1:A:260:PHE:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:HA3	1:A:111:GLN:CB	2.39	0.52
1:A:197:THR:HG21	1:A:199:ILE:HD12	1.91	0.52
1:A:42:ASN:OD1	1:A:45:ILE:HG21	2.09	0.52
1:A:338:VAL:HG21	1:A:353:ILE:CG2	2.39	0.52
1:A:339:ASN:O	1:A:343:GLU:N	2.36	0.52
1:A:145:HIS:O	1:A:149:PHE:CD2	2.62	0.52
1:A:401:CYS:O	1:A:405:VAL:HG22	2.10	0.52
1:A:41:ILE:HG22	1:A:43:LEU:H	1.74	0.52
1:A:220:PRO:HD3	1:A:247:HIS:NE2	2.25	0.52
1:A:96:GLY:HA3	1:A:102:ILE:CD1	2.39	0.52
1:A:162:TYR:CD1	1:A:197:THR:HG21	2.45	0.51
1:A:60:SER:OG	1:A:319:TRP:HB2	2.10	0.51
1:A:397:MET:CE	1:A:400:LEU:HD23	2.40	0.51
1:A:309:ILE:HG22	1:A:310:LEU:HD13	1.91	0.51
1:A:136:TRP:CE3	1:A:159:TYR:HD2	2.26	0.51
1:A:179:ASN:HA	1:A:218:TRP:HZ2	1.75	0.51
1:A:128:LYS:HZ3	1:A:129:ASN:HB2	1.74	0.51
1:A:128:LYS:NZ	1:A:286:GLN:HB3	2.26	0.51
1:A:167:HIS:H	1:A:167:HIS:CD2	2.22	0.51
1:A:187:VAL:O	1:A:221:LEU:HB3	2.11	0.51
1:A:135:VAL:HG13	1:A:156:VAL:CG1	2.41	0.51
1:A:188:LEU:HD12	1:A:221:LEU:HD12	1.92	0.51
1:A:349:ASP:O	1:A:352:PHE:HE1	1.93	0.51
1:A:227:GLN:HE21	1:A:237:ALA:HB2	1.76	0.50
1:A:80:ILE:HD11	1:A:292:ASP:N	2.26	0.50
1:A:171:PHE:HA	1:A:174:LEU:CD2	2.41	0.50
1:A:238:GLU:HA	1:A:241:ARG:HB3	1.93	0.50
1:A:203:LEU:HD21	1:A:242:ALA:HB2	1.92	0.50
1:A:330:ILE:HG21	1:A:359:MET:HA	1.93	0.50
1:A:340:THR:O	1:A:344:LYS:CB	2.60	0.50
1:A:140:PRO:CB	1:A:196:PRO:HD2	2.38	0.50
1:A:42:ASN:H	1:A:42:ASN:ND2	2.10	0.50
1:A:363:SER:N	1:A:385:GLY:O	2.45	0.50
1:A:142:TRP:CE2	1:A:144:ASN:HB3	2.47	0.50
1:A:233:LEU:CD1	1:A:323:LEU:HD21	2.42	0.50
1:A:84:PRO:HG2	1:A:85:GLU:OE2	2.12	0.50
1:A:312:ASN:HB3	1:A:315:LEU:HB2	1.93	0.49
1:A:309:ILE:CG2	1:A:316:ARG:HB3	2.42	0.49
1:A:238:GLU:HA	1:A:241:ARG:HB2	1.95	0.49
1:A:309:ILE:HG13	1:A:315:LEU:HG	1.94	0.49
1:A:365:LEU:HD22	1:A:369:GLN:CD	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:ND2	1:A:295:TYR:CD1	2.81	0.49
1:A:229:PHE:HD1	1:A:330:ILE:HD11	1.77	0.49
1:A:295:TYR:O	1:A:295:TYR:CG	2.65	0.49
1:A:106:ARG:HG3	1:A:275:ALA:HA	1.94	0.48
1:A:312:ASN:HB3	1:A:315:LEU:CB	2.43	0.48
1:A:188:LEU:HD12	1:A:221:LEU:CD1	2.44	0.48
1:A:194:HIS:HB2	1:A:199:ILE:O	2.13	0.48
1:A:219:LEU:HA	1:A:247:HIS:CE1	2.48	0.48
1:A:309:ILE:HG22	1:A:310:LEU:N	2.27	0.48
1:A:230:ALA:HB3	1:A:357:ASN:HA	1.95	0.48
1:A:372:ARG:NH2	1:A:407:VAL:HA	2.28	0.48
1:A:309:ILE:HG23	1:A:316:ARG:CB	2.43	0.48
1:A:340:THR:O	1:A:344:LYS:HB2	2.13	0.48
1:A:389:VAL:HA	1:A:392:MET:HG3	1.95	0.48
1:A:75:LYS:HE2	1:A:75:LYS:HB2	1.58	0.48
1:A:28:LEU:CD2	1:A:380:TYR:HB3	2.44	0.48
1:A:136:TRP:HB2	1:A:186:VAL:O	2.14	0.48
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.48	0.48
1:A:397:MET:HE2	1:A:401:CYS:SG	2.54	0.48
1:A:274:ALA:HB3	1:A:280:VAL:HA	1.96	0.47
1:A:354:ILE:HD12	1:A:354:ILE:H	1.79	0.47
1:A:159:TYR:CG	1:A:178:LEU:HB2	2.49	0.47
1:A:256:TYR:HA	1:A:259:ASN:OD1	2.13	0.47
1:A:47:VAL:HG22	1:A:263:TYR:CZ	2.48	0.47
1:A:28:LEU:HD21	1:A:380:TYR:C	2.35	0.47
1:A:339:ASN:OD1	1:A:343:GLU:HB2	2.13	0.47
1:A:58:LEU:HB2	1:A:61:VAL:CG2	2.44	0.47
1:A:284:PHE:CE2	1:A:287:MET:HG2	2.50	0.47
1:A:40:LYS:HE3	1:A:40:LYS:HB3	1.56	0.47
1:A:17:ILE:O	1:A:17:ILE:HG23	2.15	0.47
1:A:185:ASP:O	1:A:218:TRP:HA	2.15	0.47
1:A:277:SER:N	1:A:280:VAL:HG13	2.29	0.47
1:A:163:ASP:CG	1:A:170:ASP:HB2	2.36	0.47
1:A:20:ALA:HB3	1:A:21:PRO:CD	2.45	0.47
1:A:26:LEU:C	1:A:28:LEU:N	2.64	0.47
1:A:272:LEU:HB2	1:A:287:MET:CE	2.44	0.47
1:A:324:THR:CA	1:A:327:ARG:HD3	2.41	0.47
1:A:82:GLY:HA3	1:A:111:GLN:HB2	1.98	0.46
1:A:51:GLU:HG3	1:A:329:ARG:HE	1.80	0.46
1:A:189:PHE:HB2	1:A:222:PHE:CD2	2.51	0.46
1:A:228:GLY:N	1:A:233:LEU:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:CB	1:A:241:ARG:HD3	2.39	0.46
1:A:321:GLN:HA	1:A:324:THR:OG1	2.16	0.46
1:A:224:PHE:HB3	1:A:254:SER:OG	2.14	0.46
1:A:339:ASN:C	1:A:341:LEU:N	2.67	0.46
1:A:353:ILE:HG23	1:A:354:ILE:CD1	2.45	0.46
1:A:43:LEU:HD23	1:A:380:TYR:O	2.16	0.46
1:A:191:GLY:HA2	1:A:222:PHE:HE1	1.81	0.46
1:A:301:HIS:O	1:A:304:SER:HB2	2.16	0.46
1:A:24:PRO:C	1:A:26:LEU:N	2.67	0.46
1:A:28:LEU:CG	1:A:29:ALA:H	2.26	0.46
1:A:351:SER:O	1:A:354:ILE:HD12	2.15	0.46
1:A:62:LYS:HA	1:A:62:LYS:HD3	1.58	0.46
1:A:202:THR:H	1:A:205:GLN:HB2	1.80	0.46
1:A:196:PRO:CB	1:A:386:ARG:HG3	2.45	0.46
1:A:112:THR:O	1:A:112:THR:HG22	2.16	0.46
1:A:128:LYS:O	1:A:129:ASN:HB3	2.14	0.46
1:A:134:ARG:HD2	1:A:157:ARG:CB	2.44	0.46
1:A:162:TYR:HD1	1:A:199:ILE:CD1	2.29	0.46
1:A:20:ALA:H	1:A:21:PRO:HD2	1.80	0.46
1:A:80:ILE:HA	1:A:297:ASN:HA	1.97	0.46
1:A:150:ASN:HA	1:A:153:GLY:O	2.16	0.46
1:A:201:PRO:HA	1:A:205:GLN:NE2	2.31	0.46
1:A:142:TRP:HE3	1:A:145:HIS:CE1	2.33	0.46
1:A:337:PHE:CD2	1:A:392:MET:CE	2.99	0.46
1:A:341:LEU:O	1:A:344:LYS:C	2.54	0.46
1:A:371:LEU:HD12	1:A:374:ARG:HD2	1.97	0.46
1:A:64:ALA:HB1	1:A:308:THR:HG21	1.98	0.45
1:A:196:PRO:HB2	1:A:362:PHE:CE1	2.51	0.45
1:A:145:HIS:O	1:A:149:PHE:HD2	2.00	0.45
1:A:106:ARG:HA	1:A:280:VAL:HG11	1.97	0.45
1:A:341:LEU:HA	1:A:345:GLY:N	2.31	0.45
1:A:112:THR:HG21	1:A:118:ALA:CA	2.44	0.45
1:A:35:ASP:HB2	1:A:37:ARG:NH2	2.29	0.45
1:A:25:ILE:HG22	1:A:26:LEU:N	2.32	0.45
1:A:85:GLU:HG3	1:A:88:ARG:NH2	2.26	0.45
1:A:82:GLY:HA2	1:A:298:PRO:CG	2.46	0.45
1:A:134:ARG:NH1	1:A:157:ARG:HG2	2.18	0.45
1:A:196:PRO:HB2	1:A:362:PHE:CD1	2.52	0.45
1:A:40:LYS:HG2	1:A:396:ASN:CG	2.36	0.45
1:A:210:ALA:HB1	1:A:246:MET:SD	2.57	0.45
1:A:231:ARG:CG	1:A:357:ASN:ND2	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HH22	1:A:365:LEU:HD21	1.79	0.44
1:A:121:VAL:O	1:A:125:PHE:HB3	2.17	0.44
1:A:242:ALA:O	1:A:246:MET:HG3	2.17	0.44
1:A:397:MET:CE	1:A:401:CYS:SG	3.05	0.44
1:A:333:MET:HB3	1:A:389:VAL:CG1	2.47	0.44
1:A:333:MET:HB3	1:A:389:VAL:HG13	1.99	0.44
1:A:203:LEU:O	1:A:207:GLN:HG3	2.17	0.44
1:A:338:VAL:CG2	1:A:353:ILE:HG21	2.48	0.44
1:A:43:LEU:HA	1:A:45:ILE:CD1	2.48	0.44
1:A:87:GLY:O	1:A:91:GLN:CB	2.63	0.44
1:A:136:TRP:CE3	1:A:157:ARG:O	2.70	0.44
1:A:180:GLU:CG	1:A:181:ALA:N	2.76	0.44
1:A:282:ARG:C	1:A:284:PHE:N	2.70	0.44
1:A:135:VAL:O	1:A:157:ARG:N	2.51	0.44
1:A:95:PHE:CD2	1:A:240:LEU:HD21	2.51	0.44
1:A:171:PHE:O	1:A:175:ILE:HB	2.18	0.44
1:A:186:VAL:HG12	1:A:219:LEU:O	2.18	0.44
1:A:316:ARG:HA	1:A:319:TRP:HB3	1.98	0.44
1:A:334:ARG:HB3	1:A:354:ILE:HG13	2.00	0.44
1:A:135:VAL:HG13	1:A:156:VAL:HA	2.00	0.44
1:A:209:LEU:HA	1:A:212:LEU:HB2	2.00	0.44
1:A:201:PRO:HA	1:A:205:GLN:HE21	1.83	0.43
1:A:260:PHE:CE1	1:A:309:ILE:HD13	2.52	0.43
1:A:328:GLN:O	1:A:332:ARG:HB2	2.18	0.43
1:A:316:ARG:HG3	1:A:316:ARG:H	1.58	0.43
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.82	0.43
1:A:274:ALA:HB3	1:A:280:VAL:CA	2.49	0.43
1:A:365:LEU:HD22	1:A:369:GLN:NE2	2.33	0.43
1:A:112:THR:O	1:A:114:GLY:N	2.50	0.43
1:A:260:PHE:CD2	1:A:306:VAL:HG22	2.52	0.43
1:A:337:PHE:CD2	1:A:392:MET:HE3	2.54	0.43
1:A:31:LEU:O	1:A:34:ALA:HB2	2.19	0.43
1:A:83:ILE:HG12	1:A:83:ILE:H	1.76	0.42
1:A:28:LEU:HG	1:A:29:ALA:H	1.84	0.42
1:A:68:LEU:O	1:A:72:GLU:HB2	2.20	0.42
1:A:203:LEU:O	1:A:207:GLN:HB2	2.18	0.42
1:A:288:LYS:HA	1:A:288:LYS:HE3	2.01	0.42
1:A:128:LYS:C	1:A:130:THR:H	2.22	0.42
1:A:168:THR:HA	1:A:199:ILE:CD1	2.50	0.42
1:A:228:GLY:HA3	1:A:233:LEU:HB2	2.01	0.42
1:A:138:SER:O	1:A:141:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:O	1:A:251:ILE:HG22	2.19	0.42
1:A:353:ILE:HA	1:A:356:GLN:OE1	2.19	0.42
1:A:377:PHE:O	1:A:378:GLY:C	2.58	0.42
1:A:86:PHE:CE1	1:A:256:TYR:HE2	2.37	0.42
1:A:206:TRP:CH2	1:A:222:PHE:CZ	3.08	0.42
1:A:272:LEU:HD21	1:A:274:ALA:HB2	2.02	0.42
1:A:369:GLN:HE21	1:A:407:VAL:HG23	1.84	0.42
1:A:90:THR:CG2	1:A:91:GLN:N	2.82	0.42
1:A:359:MET:SD	1:A:390:ALA:CB	3.08	0.42
1:A:163:ASP:CB	1:A:170:ASP:HB2	2.50	0.42
1:A:81:ASP:OD2	1:A:288:LYS:HE2	2.20	0.42
1:A:140:PRO:CB	1:A:196:PRO:CD	2.98	0.41
1:A:213:SER:OG	1:A:218:TRP:HE3	2.00	0.41
1:A:284:PHE:C	1:A:286:GLN:N	2.72	0.41
1:A:277:SER:CA	1:A:280:VAL:HG13	2.49	0.41
1:A:327:ARG:O	1:A:330:ILE:N	2.53	0.41
1:A:334:ARG:HB3	1:A:354:ILE:HA	2.01	0.41
1:A:333:MET:HE2	1:A:333:MET:HA	2.02	0.41
1:A:284:PHE:O	1:A:288:LYS:N	2.49	0.41
1:A:341:LEU:HA	1:A:341:LEU:HD23	1.85	0.41
1:A:344:LYS:HA	1:A:344:LYS:HD2	1.88	0.41
1:A:89:CYS:HA	1:A:92:GLU:CG	2.50	0.41
1:A:146:LYS:O	1:A:150:ASN:OD1	2.37	0.41
1:A:37:ARG:HD3	1:A:37:ARG:HA	1.97	0.41
1:A:227:GLN:NE2	1:A:237:ALA:HB2	2.34	0.41
3:A:409:PLP:O4P	3:A:409:PLP:C4A	2.68	0.41
1:A:188:LEU:HD11	1:A:223:ASP:HB2	2.02	0.41
1:A:327:ARG:C	1:A:329:ARG:N	2.74	0.41
1:A:44:GLY:H	1:A:45:ILE:HG12	1.85	0.41
1:A:85:GLU:C	1:A:87:GLY:N	2.74	0.41
1:A:193:CYS:HB3	1:A:198:GLY:O	2.20	0.41
1:A:393:THR:HG23	1:A:394:PRO:CD	2.49	0.41
1:A:397:MET:O	1:A:400:LEU:HB3	2.21	0.41
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.86	0.40
1:A:235:GLU:HG2	1:A:235:GLU:O	2.21	0.40
1:A:44:GLY:H	1:A:388:ASN:HB2	1.86	0.40
1:A:170:ASP:HB3	1:A:173:ALA:HB3	2.02	0.40
1:A:309:ILE:CG2	1:A:316:ARG:HA	2.49	0.40
1:A:40:LYS:HE3	1:A:41:ILE:H	1.86	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:A:144:ASN:ND2	1:A:292:ASP:OD1[4_566]	2.11	0.09

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	394/396 (100%)	274 (70%)	73 (18%)	47 (12%)	0 1

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	21	PRO
1	A	29	ALA
1	A	39	GLY
1	A	43	LEU
1	A	58	LEU
1	A	59	THR
1	A	97	LYS
1	A	138	SER
1	A	154	LEU
1	A	158	GLU
1	A	165	GLU
1	A	167	HIS
1	A	180	GLU
1	A	183	ALA
1	A	219	LEU
1	A	247	HIS
1	A	248	LYS
1	A	277	SER
1	A	301	HIS
1	A	345	GLY
1	A	352	PHE
1	A	367	LYS

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Mol	Chain	Res	Type
1	A	377	PHE
1	A	383	ALA
1	A	393	THR
1	A	46	GLY
1	A	96	GLY
1	A	182	GLN
1	A	191	GLY
1	A	233	LEU
1	A	240	LEU
1	A	340	THR
1	A	20	ALA
1	A	266	ARG
1	A	275	ALA
1	A	346	ALA
1	A	351	SER
1	A	366	THR
1	A	401	CYS
1	A	40	LYS
1	A	382	VAL
1	A	297	ASN
1	A	24	PRO
1	A	17	ILE
1	A	354	ILE
1	A	378	GLY

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	320/320 (100%)	196 (61%)	124 (39%)	0 0

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	16	ASN

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Mol	Chain	Res	Type
1	A	17	ILE
1	A	18	THR
1	A	21	PRO
1	A	25	ILE
1	A	31	LEU
1	A	33	ARG
1	A	36	GLU
1	A	37	ARG
1	A	38	PRO
1	A	40	LYS
1	A	42	ASN
1	A	45	ILE
1	A	51	GLU
1	A	52	THR
1	A	57	VAL
1	A	58	LEU
1	A	61	VAL
1	A	66	GLN
1	A	69	LEU
1	A	71	ASN
1	A	73	THR
1	A	75	LYS
1	A	78	LEU
1	A	81	ASP
1	A	83	ILE
1	A	88	ARG
1	A	90	THR
1	A	93	LEU
1	A	95	PHE
1	A	97	LYS
1	A	99	SER
1	A	101	LEU
1	A	108	ARG
1	A	109	THR
1	A	111	GLN
1	A	112	THR
1	A	116	THR
1	A	121	VAL
1	A	124	ASP
1	A	125	PHE
1	A	128	LYS
1	A	146	LYS

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Mol	Chain	Res	Type
1	A	147	SER
1	A	150	ASN
1	A	151	SER
1	A	154	LEU
1	A	155	GLU
1	A	157	ARG
1	A	163	ASP
1	A	169	LEU
1	A	172	ASP
1	A	174	LEU
1	A	175	ILE
1	A	178	LEU
1	A	188	LEU
1	A	190	HIS
1	A	192	CYS
1	A	194	HIS
1	A	197	THR
1	A	203	LEU
1	A	208	THR
1	A	209	LEU
1	A	211	GLN
1	A	215	GLU
1	A	219	LEU
1	A	221	LEU
1	A	222	PHE
1	A	224	PHE
1	A	231	ARG
1	A	235	GLU
1	A	236	ASP
1	A	238	GLU
1	A	240	LEU
1	A	247	HIS
1	A	251	ILE
1	A	254	SER
1	A	258	LYS
1	A	260	PHE
1	A	264	ASN
1	A	265	GLU
1	A	270	CYS
1	A	271	THR
1	A	277	SER
1	A	279	THR

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Mol	Chain	Res	Type
1	A	280	VAL
1	A	281	ASP
1	A	287	MET
1	A	288	LYS
1	A	294	ASN
1	A	297	ASN
1	A	308	THR
1	A	309	ILE
1	A	310	LEU
1	A	311	SER
1	A	313	ASP
1	A	316	ARG
1	A	320	GLU
1	A	321	GLN
1	A	328	GLN
1	A	329	ARG
1	A	332	ARG
1	A	333	MET
1	A	334	ARG
1	A	335	GLN
1	A	339	ASN
1	A	340	THR
1	A	344	LYS
1	A	363	SER
1	A	365	LEU
1	A	366	THR
1	A	374	ARG
1	A	375	GLU
1	A	376	GLU
1	A	379	VAL
1	A	382	VAL
1	A	384	SER
1	A	386	ARG
1	A	392	MET
1	A	396	ASN
1	A	402	GLU
1	A	405	VAL
1	A	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	91	GLN
1	A	111	GLN
1	A	167	HIS
1	A	205	GLN
1	A	247	HIS
1	A	294	ASN
1	A	331	GLN
1	A	357	ASN
1	A	369	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PLP	A	409	1	15,15,16	2.15	4 (26%)	20,22,23	2.74	11 (55%)
2	SO4	A	410	-	4,4,4	0.67	0	6,6,6	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	409	1	-	5/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	409	PLP	O3-C3	-6.52	1.21	1.37
3	A	409	PLP	C4A-C4	-2.76	1.45	1.51
3	A	409	PLP	C5-C4	-2.70	1.37	1.40
3	A	409	PLP	C3-C2	2.48	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	409	PLP	C3-C4-C5	4.61	123.72	118.74
3	A	409	PLP	O4P-C5A-C5	4.20	117.35	109.35
3	A	409	PLP	C5-C6-N1	-4.18	116.86	123.82
3	A	409	PLP	C6-N1-C2	4.12	126.80	119.17
3	A	409	PLP	C5A-C5-C6	-3.94	112.89	119.37
3	A	409	PLP	O3-C3-C4	3.43	127.13	118.10
3	A	409	PLP	C4-C3-C2	-3.24	115.28	120.07
3	A	409	PLP	O2P-P-O4P	-2.91	98.99	106.73
3	A	409	PLP	C2A-C2-C3	2.74	124.28	120.89
3	A	409	PLP	C4A-C4-C5	-2.29	118.57	120.94
3	A	409	PLP	O4P-P-O1P	2.14	112.49	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	409	PLP	C4-C5-C5A-O4P
3	A	409	PLP	C6-C5-C5A-O4P
3	A	409	PLP	C5A-O4P-P-O1P
3	A	409	PLP	C5A-O4P-P-O2P
3	A	409	PLP	C5A-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	PLP	8	0

5.7 Other polymers

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.