



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:28 PM UTC

PDB ID : 1QR7 / pdb_00001qr7
Title : CRYSTAL STRUCTURE OF PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM ESCHERICHIA COLI COMPLEXED WITH PB2+ AND PEP
Authors : Shumilin, I.A.; Kretsinger, R.H.; Bauerle, R.H.
Deposited on : 1999-06-18
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

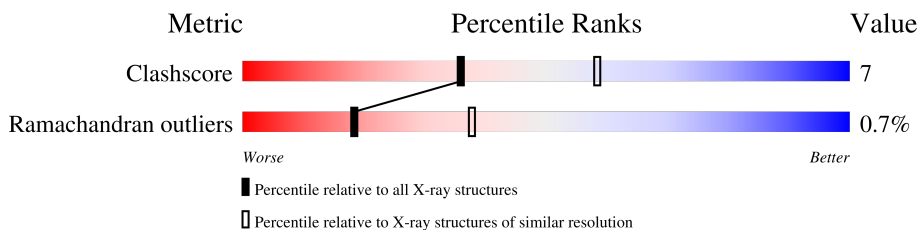
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	
1	B	350	
1	C	350	
1	D	350	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10359 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 PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2571	1617	459	481	14			
1	B	338	Total	C	N	O	S	0	0	0
			2571	1617	459	481	14			
1	C	338	Total	C	N	O	S	0	0	0
			2571	1617	459	481	14			
1	D	339	Total	C	N	O	S	0	0	0
			2578	1622	460	482	14			

- Molecule 2 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

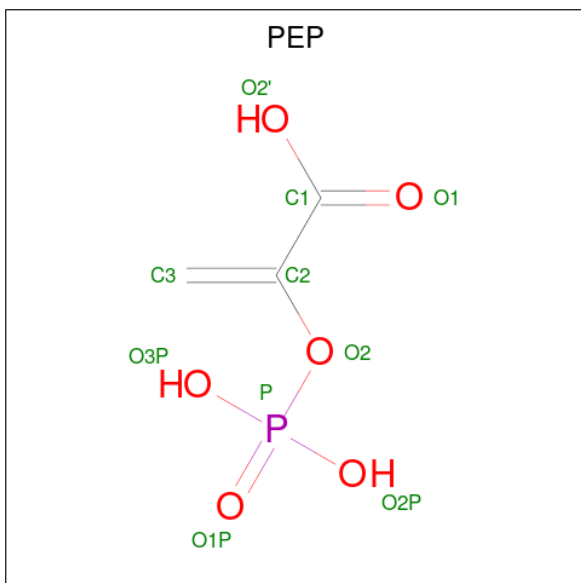
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Pb	0	0
			1	1		
2	B	1	Total	Pb	0	0
			1	1		
2	C	1	Total	Pb	0	0
			1	1		
2	D	1	Total	Pb	0	0
			1	1		

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



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

- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

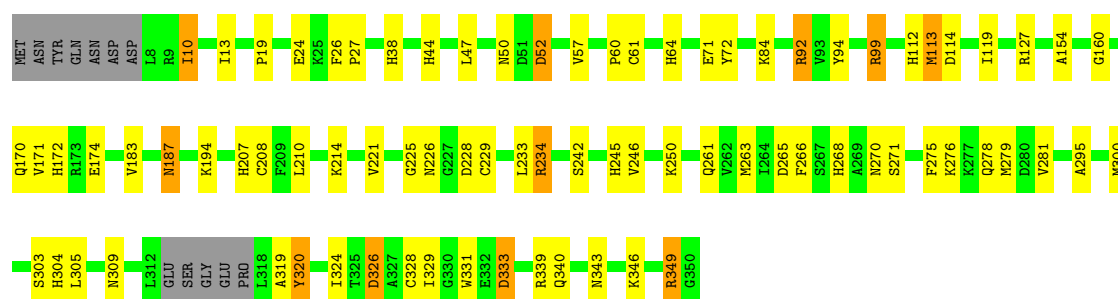
3 Residue-property plots

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

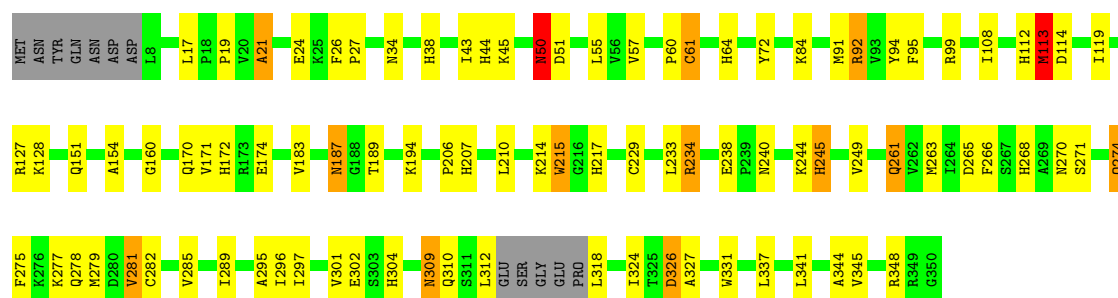
• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

Chain A: 



• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

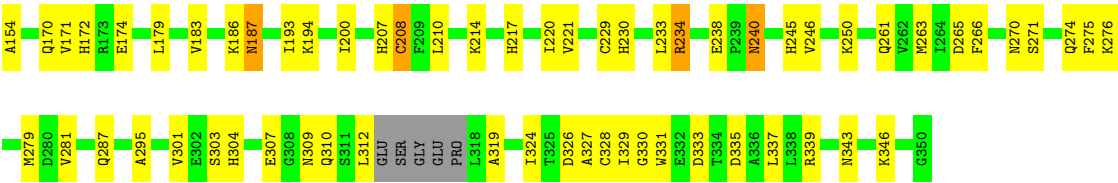
Chain B: 



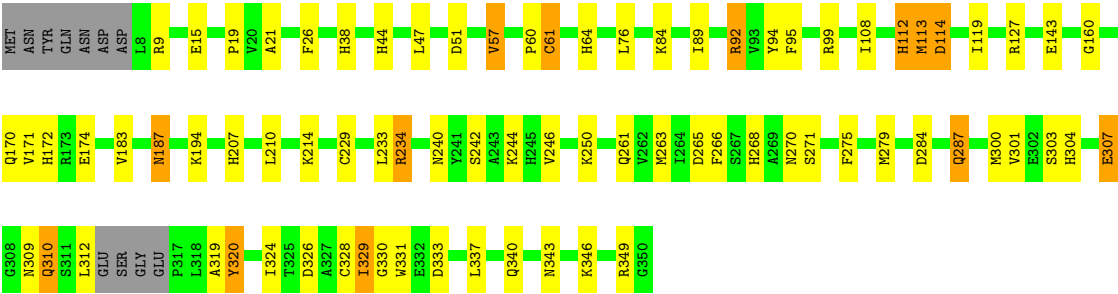
• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

Chain C: 





● Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.73Å 51.33Å 148.10Å 90.00° 116.43° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10359	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: PB, SO4, PEP

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	1.04	12/2614 (0.5%)	1.74	44/3532 (1.2%)
1	B	1.04	12/2614 (0.5%)	1.77	54/3532 (1.5%)
1	C	1.06	12/2614 (0.5%)	1.72	39/3532 (1.1%)
1	D	1.03	10/2622 (0.4%)	1.71	38/3543 (1.1%)
All	All	1.04	46/10464 (0.4%)	1.73	175/14139 (1.2%)

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	1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	HIS	CD2-NE2	-7.38	1.29	1.37
1	C	207	HIS	CD2-NE2	-6.93	1.30	1.37
1	D	172	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	207	HIS	CD2-NE2	-6.79	1.30	1.37
1	B	172	HIS	CD2-NE2	-6.68	1.30	1.37
1	C	230	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	207	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	44	HIS	CD2-NE2	-6.39	1.30	1.37
1	D	64	HIS	CD2-NE2	-6.36	1.30	1.37
1	D	38	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	44	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	112	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	112	HIS	CD2-NE2	-6.24	1.30	1.37
1	D	207	HIS	CD2-NE2	-6.19	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	245	HIS	CD2-NE2	-6.17	1.31	1.37
1	D	112	HIS	CG-ND1	-6.15	1.31	1.38
1	B	38	HIS	CD2-NE2	-6.14	1.31	1.37
1	D	112	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	304	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	268	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	268	HIS	CD2-NE2	-5.96	1.31	1.37
1	D	268	HIS	CG-ND1	-5.88	1.31	1.38
1	A	64	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	112	HIS	CG-ND1	-5.80	1.31	1.38
1	D	44	HIS	CD2-NE2	-5.79	1.31	1.37
1	B	217	HIS	CD2-NE2	-5.76	1.31	1.37
1	C	172	HIS	CG-ND1	-5.75	1.31	1.38
1	C	64	HIS	CD2-NE2	-5.69	1.31	1.37
1	B	44	HIS	CD2-NE2	-5.68	1.31	1.37
1	B	304	HIS	CD2-NE2	-5.67	1.31	1.37
1	D	304	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	38	HIS	CD2-NE2	-5.59	1.31	1.37
1	C	304	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	245	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	268	HIS	CG-ND1	-5.50	1.32	1.38
1	A	44	HIS	CG-ND1	-5.44	1.32	1.38
1	D	268	HIS	CD2-NE2	-5.28	1.32	1.37
1	C	172	HIS	CD2-NE2	-5.26	1.32	1.37
1	B	112	HIS	CG-ND1	-5.18	1.32	1.38
1	C	207	HIS	CG-ND1	-5.18	1.32	1.38
1	C	217	HIS	CD2-NE2	-5.17	1.32	1.37
1	C	245	HIS	CD2-NE2	-5.09	1.32	1.37
1	B	268	HIS	CG-ND1	-5.06	1.32	1.38
1	B	64	HIS	CD2-NE2	-5.03	1.32	1.37
1	C	44	HIS	CG-ND1	-5.01	1.32	1.38

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ASN	CA-CB-CG	12.24	124.84	112.60
1	D	172	HIS	CA-CB-CG	-8.90	104.89	113.80
1	A	331	TRP	N-CA-C	8.86	120.94	111.28
1	A	333	ASP	CA-CB-CG	8.73	121.33	112.60
1	D	114	ASP	N-CA-C	-8.70	96.16	110.17
1	D	114	ASP	O-C-N	-8.61	113.20	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	PHE	N-CA-C	8.56	121.68	111.33
1	A	52	ASP	CA-CB-CG	8.22	120.83	112.60
1	D	275	PHE	N-CA-C	8.12	121.15	111.33
1	D	265	ASP	CA-CB-CG	8.09	120.69	112.60
1	C	114	ASP	N-CA-C	-8.08	97.10	109.95
1	A	319	ALA	N-CA-C	7.99	121.05	108.67
1	A	172	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	114	ASP	N-CA-C	-7.74	97.64	109.95
1	C	234	ARG	N-CA-CB	-7.73	98.23	110.98
1	C	265	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	71	GLU	CA-CB-CG	-7.63	98.84	114.10
1	A	234	ARG	N-CA-CB	-7.55	98.52	110.98
1	D	207	HIS	CB-CG-CD2	-7.53	121.41	131.20
1	C	172	HIS	CA-CB-CG	-7.53	106.27	113.80
1	B	114	ASP	N-CA-C	-7.47	98.07	109.95
1	C	187	ASN	CA-CB-CG	7.33	119.93	112.60
1	A	278	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	D	331	TRP	N-CA-C	7.26	119.20	111.28
1	A	225	GLY	N-CA-C	-7.25	102.46	112.18
1	A	265	ASP	CA-CB-CG	7.21	119.81	112.60
1	D	234	ARG	N-CA-CB	-7.15	99.41	111.27
1	B	234	ARG	N-CA-CB	-7.14	99.20	110.98
1	C	51	ASP	CA-CB-CG	7.04	119.64	112.60
1	B	44	HIS	CB-CG-CD2	-7.02	122.07	131.20
1	D	114	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	265	ASP	CA-CB-CG	6.99	119.59	112.60
1	D	92	ARG	CB-CG-CD	-6.97	95.28	111.30
1	B	172	HIS	CA-CB-CG	-6.90	106.90	113.80
1	D	309	ASN	OD1-CG-ND2	-6.86	115.74	122.60
1	A	92	ARG	CB-CG-CD	-6.83	95.58	111.30
1	B	171	VAL	N-CA-CB	-6.80	101.29	110.54
1	B	295	ALA	N-CA-C	6.80	121.18	112.34
1	C	171	VAL	N-CA-CB	-6.75	102.03	110.47
1	B	281	VAL	N-CA-C	-6.73	103.96	110.42
1	D	309	ASN	CB-CG-ND2	6.68	126.42	116.40
1	C	92	ARG	CB-CG-CD	-6.65	96.00	111.30
1	D	171	VAL	N-CA-CB	-6.65	101.50	110.54
1	B	92	ARG	CB-CG-CD	-6.58	96.16	111.30
1	B	34	ASN	N-CA-CB	-6.58	100.17	110.30
1	D	310	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	172	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	B	61	CYS	N-CA-C	-6.54	104.07	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	C	187	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	B	331	TRP	N-CA-C	6.50	119.19	111.33
1	A	320	TYR	N-CA-C	6.48	124.59	110.80
1	B	189	THR	N-CA-C	6.47	120.03	111.75
1	A	207	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	B	309	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	B	172	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	A	226	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	B	128	LYS	CA-CB-CG	-6.38	101.34	114.10
1	A	275	PHE	N-CA-C	6.36	121.87	111.37
1	B	274	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	349	ARG	N-CA-C	6.33	121.94	113.72
1	B	270	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	B	154	ALA	N-CA-C	6.26	118.91	111.71
1	D	263	MET	N-CA-C	-6.26	99.52	109.59
1	A	187	ASN	CA-CB-CG	6.25	118.85	112.60
1	D	84	LYS	CA-CB-CG	6.22	126.54	114.10
1	D	61	CYS	N-CA-C	-6.20	104.44	111.14
1	C	270	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	D	172	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	D	187	ASN	CA-CB-CG	6.12	118.72	112.60
1	D	320	TYR	N-CA-C	6.08	123.75	110.80
1	C	304	HIS	CB-CG-CD2	-6.05	123.34	131.20
1	A	228	ASP	N-CA-C	6.02	118.65	109.62
1	C	263	MET	N-CA-C	-6.00	99.93	109.59
1	D	307	GLU	CA-CB-CG	5.99	126.09	114.10
1	D	329	ILE	N-CA-C	-5.96	103.55	110.05
1	D	240	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	50	ASN	N-CA-C	5.90	123.36	110.80
1	B	206	PRO	O-C-N	-5.89	115.90	123.03
1	B	207	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	B	274	GLN	CA-CB-CG	5.81	125.72	114.10
1	C	207	HIS	CB-CG-CD2	-5.80	123.65	131.20
1	C	71	GLU	CA-CB-CG	-5.80	102.50	114.10
1	C	114	ASP	O-C-N	-5.79	115.86	123.16
1	C	287	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	B	240	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	154	ALA	N-CA-C	5.74	118.31	111.71
1	B	263	MET	N-CA-C	-5.73	100.36	109.59
1	B	187	ASN	CA-CB-CG	5.68	118.28	112.60
1	A	304	HIS	CB-CG-CD2	-5.67	123.83	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	TYR	CA-C-O	5.66	126.64	120.58
1	C	281	VAL	N-CA-C	-5.61	104.89	110.62
1	D	94	TYR	CA-C-O	5.61	126.58	120.58
1	C	172	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	339	ARG	CA-CB-CG	-5.59	102.91	114.10
1	D	207	HIS	CB-CG-ND1	5.58	131.07	122.70
1	B	245	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	331	TRP	O-C-N	-5.57	116.22	122.12
1	C	99	ARG	CA-C-O	-5.57	114.68	121.36
1	B	94	TYR	CA-C-O	5.56	126.53	120.58
1	A	171	VAL	N-CA-CB	-5.55	102.99	110.54
1	A	309	ASN	CA-CB-CG	5.55	118.15	112.60
1	C	38	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	261	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	D	99	ARG	CA-C-O	-5.49	114.77	121.36
1	B	151	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	D	304	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	C	220	ILE	N-CA-C	-5.46	100.58	108.71
1	C	333	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	10	ILE	O-C-N	-5.42	116.77	122.68
1	B	92	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	D	143	GLU	CB-CG-CD	5.41	121.80	112.60
1	D	349	ARG	CA-CB-CG	5.38	124.87	114.10
1	C	65	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	51	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	172	HIS	CB-CG-ND1	5.35	130.72	122.70
1	D	270	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	207	HIS	CB-CG-ND1	5.34	130.71	122.70
1	C	200	ILE	N-CA-C	-5.32	105.53	110.53
1	B	304	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	A	339	ARG	CA-C-O	-5.32	114.86	120.55
1	B	187	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	C	127	ARG	CB-CG-CD	5.29	123.47	111.30
1	B	331	TRP	CG-CD2-CE3	5.28	139.18	133.90
1	C	154	ALA	N-CA-C	5.27	117.77	111.71
1	D	51	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	17	LEU	CA-C-N	5.26	123.45	119.66
1	B	17	LEU	C-N-CA	5.26	123.45	119.66
1	B	21	ALA	N-CA-C	-5.25	105.46	111.14
1	C	240	ASN	CA-CB-CG	5.24	117.84	112.60
1	B	238	GLU	CA-C-N	5.24	125.25	119.90
1	B	238	GLU	C-N-CA	5.24	125.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	38	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	207	HIS	CB-CG-ND1	5.23	130.55	122.70
1	D	310	GLN	N-CA-C	5.22	117.19	108.99
1	D	234	ARG	CA-CB-CG	5.22	124.54	114.10
1	C	61	CYS	N-CA-C	-5.21	105.51	111.14
1	A	114	ASP	O-C-N	-5.21	116.60	123.16
1	A	278	GLN	CG-CD-NE2	5.21	124.21	116.40
1	B	326	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	57	VAL	N-CA-C	-5.20	100.26	107.80
1	D	340	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	C	75	ARG	N-CA-C	5.16	116.90	111.28
1	C	208	CYS	N-CA-C	-5.15	100.06	108.76
1	A	270	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	C	270	ASN	CB-CG-ND2	5.14	124.11	116.40
1	B	244	LYS	CA-CB-CG	5.14	124.38	114.10
1	C	234	ARG	CA-CB-CG	5.14	124.37	114.10
1	B	114	ASP	O-C-N	-5.13	116.69	123.16
1	D	333	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	57	VAL	N-CA-C	-5.12	100.52	107.99
1	C	319	ALA	N-CA-C	5.12	117.31	110.35
1	A	94	TYR	N-CA-C	5.12	116.65	108.41
1	B	113	MET	N-CA-C	5.11	121.69	110.80
1	A	326	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	38	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	D	287	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	349	ARG	CB-CG-CD	-5.07	99.64	111.30
1	A	305	LEU	N-CA-C	-5.07	105.67	111.14
1	A	340	GLN	CA-CB-CG	5.07	124.23	114.10
1	C	193	ILE	CA-C-O	5.04	125.69	120.25
1	C	274	GLN	CA-C-O	5.04	125.75	120.36
1	A	263	MET	N-CA-C	-5.03	101.49	109.59
1	B	215	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	B	44	HIS	CB-CG-ND1	5.02	130.23	122.70
1	A	50	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	A	99	ARG	CA-C-O	-5.02	115.70	121.47
1	A	281	VAL	N-CA-C	-5.02	105.50	110.62
1	B	296	ILE	CA-C-N	5.01	128.59	121.02
1	B	296	ILE	C-N-CA	5.01	128.59	121.02
1	B	275	PHE	N-CA-C	5.01	116.43	111.07
1	C	238	GLU	CA-C-N	5.01	125.01	119.90
1	C	238	GLU	C-N-CA	5.01	125.01	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	TYR	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	2571	0	2608	34	0
1	B	2571	0	2608	46	0
1	C	2571	0	2608	42	0
1	D	2578	0	2616	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	0	0
4	C	10	0	2	1	0
4	D	10	0	2	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	10359	0	10448	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (152) 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:C:113:MET:HE3	1:C:324:ILE:HD13	1.64	0.80
1:B:113:MET:HE3	1:B:324:ILE:HD13	1.64	0.78
1:A:113:MET:HE3	1:A:324:ILE:HD13	1.65	0.78
1:C:276:LYS:HD3	1:C:276:LYS:H	1.56	0.71
1:D:113:MET:HE3	1:D:324:ILE:HD13	1.74	0.69
1:B:278:GLN:HE22	1:B:302:GLU:H	1.40	0.68
1:D:113:MET:HE2	1:D:312:LEU:HD21	1.76	0.68
1:A:194:LYS:HD2	1:A:194:LYS:H	1.60	0.67
1:A:276:LYS:HD3	1:A:276:LYS:H	1.60	0.67
1:B:312:LEU:HD11	1:B:324:ILE:HD12	1.76	0.66
1:B:289:ILE:HG23	1:B:348:ARG:NH1	2.11	0.65
1:D:187:ASN:HD21	1:D:234:ARG:H	1.42	0.65
1:D:194:LYS:H	1:D:194:LYS:HD2	1.66	0.61
1:A:210:LEU:HD21	1:B:119:ILE:HG21	1.83	0.60
1:B:261:GLN:HB2	1:B:297:ILE:HD13	1.83	0.60
1:C:119:ILE:HG21	1:D:210:LEU:HD21	1.83	0.60
1:C:194:LYS:H	1:C:194:LYS:HD2	1.66	0.60
1:D:187:ASN:ND2	1:D:234:ARG:H	2.00	0.60
1:B:194:LYS:HD2	1:B:194:LYS:H	1.67	0.59
1:A:187:ASN:HD21	1:A:234:ARG:H	1.51	0.57
1:C:187:ASN:ND2	1:C:234:ARG:H	2.01	0.57
1:B:187:ASN:HD21	1:B:234:ARG:H	1.53	0.56
1:D:246:VAL:O	1:D:250:LYS:HG3	2.05	0.56
1:C:187:ASN:HD21	1:C:234:ARG:H	1.54	0.56
1:C:113:MET:HB3	1:C:312:LEU:HD11	1.87	0.55
1:C:279:MET:HE1	1:C:337:LEU:HB2	1.88	0.55
1:B:45:LYS:HB2	1:B:45:LYS:NZ	2.22	0.55
1:A:187:ASN:ND2	1:A:234:ARG:H	2.04	0.55
1:B:187:ASN:ND2	1:B:234:ARG:H	2.06	0.54
1:C:99:ARG:H	1:D:170:GLN:NE2	2.06	0.54
1:B:160:GLY:O	1:B:183:VAL:HA	2.09	0.53
1:B:301:VAL:HG21	1:B:337:LEU:HD21	1.91	0.53
1:D:183:VAL:O	1:D:229:CYS:HA	2.09	0.53
1:A:119:ILE:HG21	1:B:210:LEU:HD21	1.91	0.53
1:A:170:GLN:NE2	1:B:99:ARG:H	2.07	0.52
1:B:310:GLN:OE1	1:B:318:LEU:HD12	2.10	0.52
1:B:312:LEU:HD12	1:B:312:LEU:H	1.74	0.52
1:C:76:LEU:HD22	1:C:89:ILE:HG21	1.93	0.51
1:C:113:MET:CE	1:C:324:ILE:HD13	2.39	0.51
1:C:210:LEU:HD21	1:D:119:ILE:HG21	1.93	0.51
1:C:301:VAL:HG21	1:C:337:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:OD1	1:A:349:ARG:HD3	2.11	0.51
1:B:279:MET:O	1:B:282:CYS:HB3	2.11	0.51
1:D:301:VAL:HG21	1:D:337:LEU:HD21	1.93	0.51
1:D:76:LEU:HD22	1:D:89:ILE:HG21	1.93	0.50
1:C:266:PHE:O	1:C:271:SER:HB3	2.11	0.50
1:A:160:GLY:O	1:A:183:VAL:HA	2.12	0.50
1:D:170:GLN:O	1:D:174:GLU:HG3	2.12	0.50
1:D:279:MET:HE1	1:D:337:LEU:HB2	1.94	0.50
1:A:183:VAL:O	1:A:229:CYS:HA	2.12	0.49
1:B:215:TRP:CZ2	1:D:15:GLU:HG3	2.48	0.49
1:B:183:VAL:O	1:B:229:CYS:HA	2.12	0.49
1:D:26:PHE:HB2	1:D:127:ARG:HD3	1.95	0.49
1:C:250:LYS:HD3	1:C:295:ALA:CB	2.43	0.49
1:D:113:MET:CE	1:D:324:ILE:HD13	2.42	0.48
1:C:183:VAL:O	1:C:229:CYS:HA	2.12	0.48
1:B:72:TYR:CD2	1:B:91:MET:HE3	2.48	0.48
1:A:26:PHE:HB2	1:A:127:ARG:HD3	1.94	0.48
1:A:279:MET:SD	1:A:333:ASP:HB3	2.53	0.48
1:C:95:PHE:HB3	1:C:108:ILE:HG13	1.96	0.47
1:B:113:MET:CE	1:B:324:ILE:HD13	2.39	0.47
1:A:113:MET:CE	1:A:324:ILE:HD13	2.40	0.47
1:B:95:PHE:HB3	1:B:108:ILE:HG13	1.96	0.47
1:B:60:PRO:O	1:B:92:ARG:HD3	2.15	0.47
1:C:26:PHE:HB2	1:C:127:ARG:HD3	1.95	0.47
1:C:113:MET:HB3	1:C:312:LEU:HD21	1.96	0.47
1:A:303:SER:HB3	1:A:329:ILE:HG13	1.96	0.47
1:A:266:PHE:O	1:A:271:SER:HB3	2.15	0.46
1:A:170:GLN:O	1:A:174:GLU:HG3	2.14	0.46
1:B:21:ALA:HA	1:D:21:ALA:HA	1.97	0.46
1:D:95:PHE:HB3	1:D:108:ILE:HG13	1.97	0.46
1:B:45:LYS:HB3	1:B:50:ASN:HB2	1.96	0.46
1:A:61:CYS:SG	1:A:326:ASP:HB2	2.56	0.46
1:B:274:GLN:HB2	1:B:277:LYS:HG3	1.96	0.46
1:B:274:GLN:O	1:B:277:LYS:HB2	2.16	0.46
1:D:310:GLN:HE22	1:D:319:ALA:H	1.64	0.46
1:B:61:CYS:SG	1:B:326:ASP:HB2	2.56	0.46
1:C:187:ASN:HD22	1:C:233:LEU:HA	1.81	0.45
1:B:245:HIS:O	1:B:249:VAL:HG23	2.16	0.45
1:C:60:PRO:O	1:C:92:ARG:HD3	2.17	0.45
1:C:170:GLN:O	1:C:174:GLU:HG3	2.16	0.45
1:A:242:SER:O	1:A:246:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASN:OD1	1:B:327:ALA:HB2	2.16	0.45
1:D:266:PHE:O	1:D:271:SER:HB3	2.16	0.45
1:A:19:PRO:HB2	1:A:214:LYS:HA	1.99	0.45
1:B:281:VAL:O	1:B:285:VAL:HG23	2.17	0.44
1:C:307:GLU:HB3	1:C:330:GLY:N	2.33	0.44
1:B:170:GLN:O	1:B:174:GLU:HG3	2.17	0.44
1:B:187:ASN:ND2	1:B:233:LEU:HA	2.33	0.44
1:C:113:MET:HE3	1:C:324:ILE:CD1	2.41	0.44
1:D:187:ASN:HD22	1:D:233:LEU:HA	1.82	0.44
1:A:24:GLU:O	1:A:27:PRO:HD3	2.18	0.44
1:D:57:VAL:O	1:D:300:MET:HA	2.18	0.44
1:D:47:LEU:O	1:D:261:GLN:NE2	2.51	0.44
1:A:250:LYS:HD3	1:A:295:ALA:CB	2.47	0.43
1:C:19:PRO:HB2	1:C:214:LYS:HA	2.00	0.43
1:C:24:GLU:O	1:C:27:PRO:HD3	2.18	0.43
1:C:61:CYS:SG	1:C:326:ASP:HB2	2.58	0.43
1:B:187:ASN:HD22	1:B:233:LEU:HA	1.83	0.43
1:A:47:LEU:O	1:A:261:GLN:NE2	2.51	0.43
1:C:309:ASN:HB3	1:C:327:ALA:HA	2.00	0.43
1:A:343:ASN:HA	1:A:346:LYS:HE3	1.99	0.43
1:C:179:LEU:O	1:D:9:ARG:HD2	2.19	0.43
1:C:310:GLN:HG3	1:C:324:ILE:HG22	1.99	0.43
1:D:187:ASN:ND2	1:D:233:LEU:HA	2.33	0.43
1:C:79:LEU:HD22	1:C:331:TRP:HZ2	1.83	0.43
1:A:208:CYS:HA	1:A:221:VAL:O	2.18	0.43
1:B:266:PHE:O	1:B:271:SER:HB3	2.19	0.43
1:B:43:ILE:HG12	1:B:55:LEU:HD13	2.01	0.43
1:C:343:ASN:HA	1:C:346:LYS:HE3	2.01	0.43
1:B:113:MET:HE3	1:B:324:ILE:CD1	2.43	0.42
1:A:246:VAL:O	1:A:250:LYS:HG3	2.18	0.42
1:A:303:SER:HA	1:A:328:CYS:HB3	2.00	0.42
1:A:57:VAL:O	1:A:300:MET:HA	2.20	0.42
1:D:284:ASP:O	1:D:287:GLN:HB3	2.18	0.42
1:D:61:CYS:SG	1:D:326:ASP:HB2	2.59	0.42
1:C:186:LYS:NZ	4:C:3352:PEP:O3P	2.48	0.42
1:A:113:MET:HE3	1:A:324:ILE:CD1	2.42	0.42
1:B:24:GLU:O	1:B:27:PRO:HD3	2.20	0.42
1:C:124:ARG:HH11	1:C:124:ARG:HD2	1.71	0.42
1:D:303:SER:HB3	1:D:329:ILE:HG13	2.01	0.42
1:A:60:PRO:O	1:A:92:ARG:HD3	2.20	0.42
1:D:303:SER:HA	1:D:328:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HD3	1:A:99:ARG:HA	1.71	0.42
1:C:47:LEU:O	1:C:261:GLN:NE2	2.53	0.42
1:C:246:VAL:O	1:C:250:LYS:HG3	2.20	0.42
1:C:335:ASP:O	1:C:339:ARG:HG3	2.19	0.42
1:D:19:PRO:HB2	1:D:214:LYS:HA	2.02	0.42
1:B:341:LEU:O	1:B:345:VAL:HG23	2.19	0.41
1:B:285:VAL:O	1:B:289:ILE:HG12	2.20	0.41
1:C:208:CYS:HA	1:C:221:VAL:O	2.20	0.41
1:C:303:SER:HA	1:C:328:CYS:HB3	2.01	0.41
1:A:10:ILE:HG21	1:A:13:ILE:HD11	2.02	0.41
1:B:19:PRO:HB2	1:B:214:LYS:HA	2.02	0.41
1:D:160:GLY:O	1:D:183:VAL:HA	2.21	0.41
1:D:307:GLU:HB3	1:D:330:GLY:N	2.36	0.41
1:D:60:PRO:O	1:D:92:ARG:HD3	2.20	0.41
1:B:279:MET:HE2	1:B:279:MET:HB2	1.92	0.41
1:D:343:ASN:HA	1:D:346:LYS:HD2	2.02	0.41
1:A:187:ASN:ND2	1:A:233:LEU:HA	2.35	0.41
1:A:187:ASN:HD22	1:A:233:LEU:HA	1.85	0.41
1:D:112:HIS:O	1:D:114:ASP:N	2.54	0.41
1:D:113:MET:HE2	1:D:312:LEU:CD2	2.47	0.41
1:B:99:ARG:HD3	1:B:99:ARG:HA	1.75	0.41
1:B:113:MET:HB3	1:B:312:LEU:HD23	2.01	0.41
1:C:187:ASN:ND2	1:C:240:ASN:HD21	2.18	0.41
1:C:187:ASN:ND2	1:C:233:LEU:HA	2.35	0.41
1:C:303:SER:HB3	1:C:329:ILE:HG13	2.03	0.41
1:B:289:ILE:HB	1:B:344:ALA:HB1	2.03	0.40
1:D:113:MET:HE3	1:D:324:ILE:CD1	2.48	0.40
1:B:26:PHE:HB2	1:B:127:ARG:HD3	2.02	0.40
1:D:242:SER:OG	1:D:244:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/350 (95%)	314 (94%)	17 (5%)	3 (1%)	14	30
1	B	334/350 (95%)	314 (94%)	17 (5%)	3 (1%)	14	30
1	C	334/350 (95%)	315 (94%)	17 (5%)	2 (1%)	21	42
1	D	335/350 (96%)	315 (94%)	18 (5%)	2 (1%)	21	42
All	All	1337/1400 (96%)	1258 (94%)	69 (5%)	10 (1%)	18	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	MET
1	A	320	TYR
1	B	50	ASN
1	B	113	MET
1	C	113	MET
1	D	113	MET
1	D	320	TYR
1	A	84	LYS
1	B	84	LYS
1	C	84	LYS

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	3353	-	4,4,4	0.11	0	6,6,6	0.87	0
3	SO4	B	2353	-	4,4,4	0.20	0	6,6,6	0.49	0
3	SO4	D	4353	-	4,4,4	0.24	0	6,6,6	0.59	0
4	PEP	A	1352	-	9,9,9	2.12	3 (33%)	11,13,13	2.99	5 (45%)
3	SO4	A	1353	-	4,4,4	0.19	0	6,6,6	0.45	0
4	PEP	C	3352	-	9,9,9	1.91	3 (33%)	11,13,13	3.17	5 (45%)
4	PEP	B	2352	-	9,9,9	1.81	2 (22%)	11,13,13	3.22	5 (45%)
4	PEP	D	4352	-	9,9,9	2.09	3 (33%)	11,13,13	3.10	5 (45%)

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	PEP	C	3352	-	-	0/9/9/9	-
4	PEP	B	2352	-	-	0/9/9/9	-
4	PEP	D	4352	-	-	0/9/9/9	-
4	PEP	A	1352	-	-	0/9/9/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3352	PEP	O2'-C1	-3.60	1.20	1.30
4	D	4352	PEP	O2'-C1	-3.45	1.21	1.30
4	A	1352	PEP	O2'-C1	-3.23	1.21	1.30
4	B	2352	PEP	O2'-C1	-3.15	1.22	1.30
4	A	1352	PEP	C2-C1	3.10	1.52	1.49
4	D	4352	PEP	C2-C1	3.03	1.52	1.49
4	A	1352	PEP	O1-C1	3.01	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4352	PEP	O1-C1	2.94	1.29	1.22
4	B	2352	PEP	O1-C1	2.74	1.29	1.22
4	C	3352	PEP	O1-C1	2.26	1.28	1.22
4	C	3352	PEP	C2-C1	2.05	1.51	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3352	PEP	O2'-C1-C2	5.96	124.07	113.91
4	B	2352	PEP	O2'-C1-C2	5.94	124.05	113.91
4	B	2352	PEP	O1-C1-C2	-5.93	112.85	121.79
4	D	4352	PEP	O2'-C1-C2	5.66	123.56	113.91
4	C	3352	PEP	O1-C1-C2	-5.54	113.44	121.79
4	A	1352	PEP	O2'-C1-C2	5.38	123.10	113.91
4	D	4352	PEP	O1-C1-C2	-5.24	113.89	121.79
4	A	1352	PEP	O1-C1-C2	-5.22	113.91	121.79
4	D	4352	PEP	O2-C2-C3	-4.83	115.62	124.85
4	B	2352	PEP	O2-C2-C3	-4.70	115.88	124.85
4	C	3352	PEP	O2-C2-C3	-4.68	115.91	124.85
4	A	1352	PEP	O2-C2-C3	-4.58	116.09	124.85
4	B	2352	PEP	C3-C2-C1	3.53	129.25	122.73
4	C	3352	PEP	C3-C2-C1	3.50	129.20	122.73
4	D	4352	PEP	C3-C2-C1	3.48	129.17	122.73
4	A	1352	PEP	C3-C2-C1	3.35	128.92	122.73
4	C	3352	PEP	O3P-P-O2P	2.40	116.79	107.80
4	D	4352	PEP	O3P-P-O2P	2.39	116.78	107.80
4	A	1352	PEP	O3P-P-O2P	2.25	116.25	107.80
4	B	2352	PEP	O3P-P-O2P	2.16	115.91	107.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3352	PEP	1	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 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.