



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QR7
Title : CRYSTAL STRUCTURE OF PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM ESCHERICHIA COLI COMPLEXED WITH PB2+ AND PEP
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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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

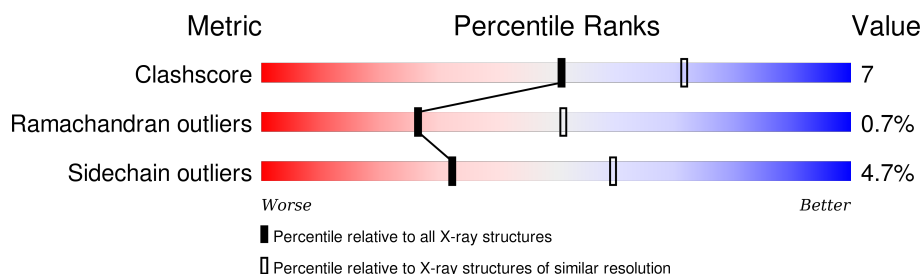
1 Overall quality at a glance

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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.

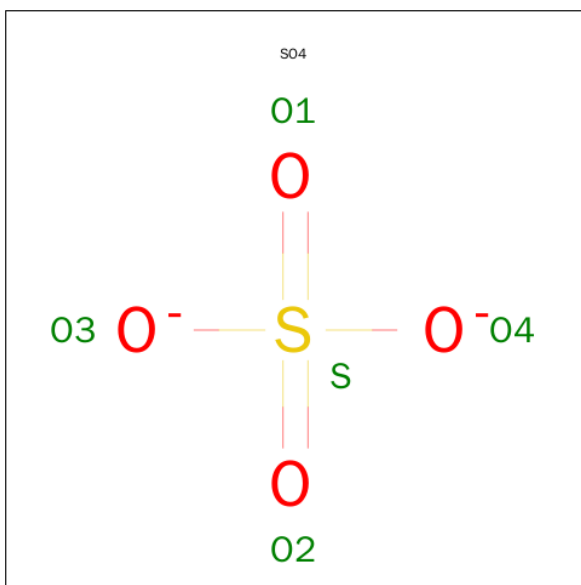
- Molecule 1 is a protein called PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE.

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 (three-letter code: PB) (formula: Pb).

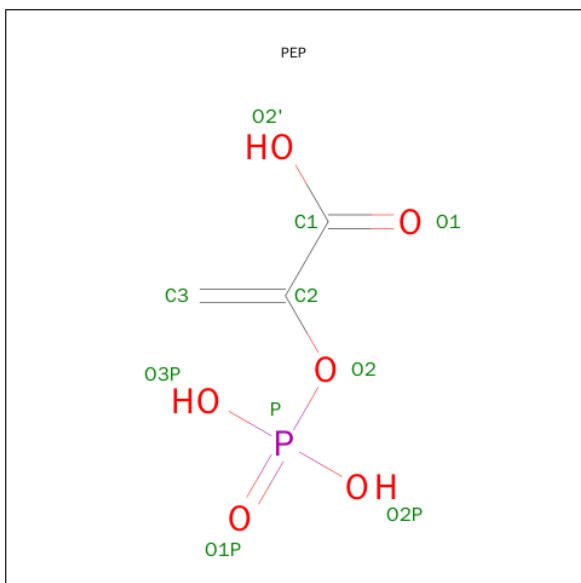
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Pb	0	0
			1	1		
2	A	1	Total	Pb	0	0
			1	1		
2	D	1	Total	Pb	0	0
			1	1		
2	C	1	Total	Pb	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: 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 (three-letter code: 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		

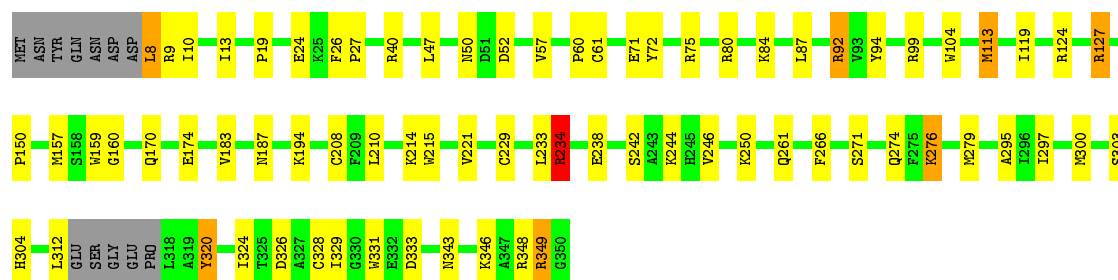
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

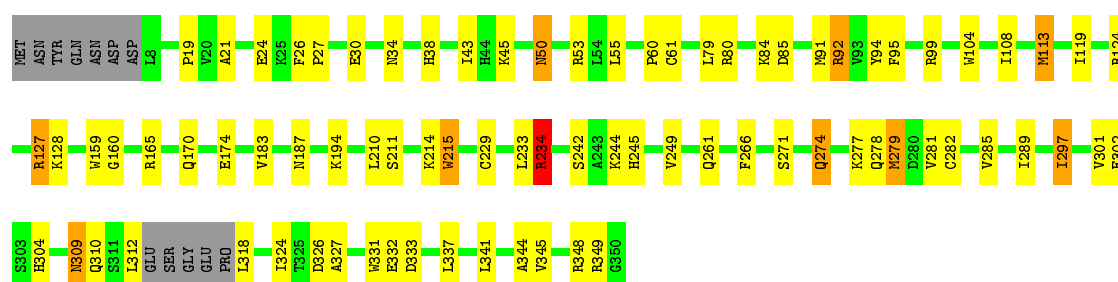
• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

Chain A: 



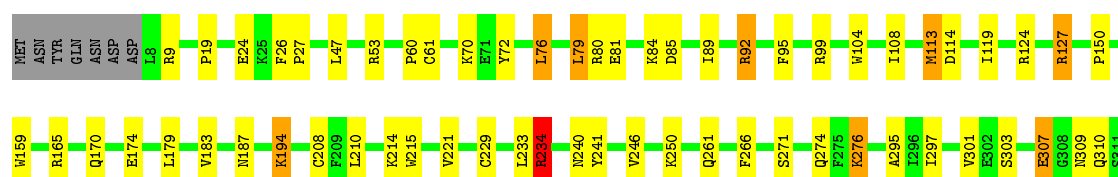
• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

Chain B: 



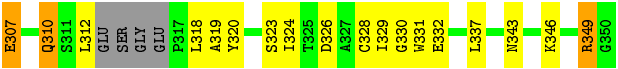
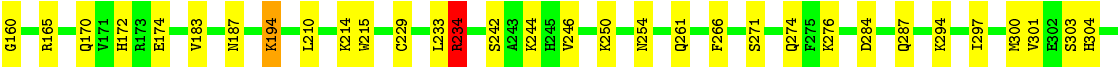
• Molecule 1: PHENYLALANINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONAT E-7-PHOSPHATE SYNTHASE

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 will therefore be 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, PEP, SO4

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	0.80	0/2614	1.44	32/3532 (0.9%)
1	B	0.80	0/2614	1.45	26/3532 (0.7%)
1	C	0.82	0/2614	1.39	23/3532 (0.7%)
1	D	0.81	0/2622	1.40	32/3543 (0.9%)
All	All	0.81	0/10464	1.42	113/14139 (0.8%)

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	1

There are no bond length outliers.

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	127	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	B	92	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	C	92	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	C	127	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	D	92	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	C	92	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	104	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	D	215	TRP	CD1-CG-CD2	8.42	113.04	106.30
1	A	92	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	104	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	A	127	ARG	NE-CZ-NH1	8.28	124.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	A	215	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	B	159	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	92	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	C	9	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	D	159	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	C	104	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	C	159	TRP	CD1-CG-CD2	7.84	112.58	106.30
1	B	215	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	C	53	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	8	LEU	CA-CB-CG	7.72	133.05	115.30
1	C	215	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	D	92	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	B	215	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	D	104	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	B	331	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	D	215	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	B	104	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	A	215	TRP	CE2-CD2-CG	-7.34	101.42	107.30
1	C	159	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	331	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	C	104	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	B	159	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	104	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	D	331	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	D	165	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	331	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	A	331	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	D	159	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	D	331	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	159	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	C	234	ARG	N-CA-CB	-6.87	98.23	110.60
1	A	75	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	D	104	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	C	215	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	C	331	TRP	CE2-CD2-CG	-6.77	101.88	107.30
1	A	159	TRP	CD1-CG-CD2	6.73	111.68	106.30
1	A	234	ARG	N-CA-CB	-6.71	98.52	110.60
1	A	9	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	80	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	71	GLU	CA-CB-CG	-6.62	98.84	113.40
1	B	91	MET	CG-SD-CE	6.46	110.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	80	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	124	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	348	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	80	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	234	ARG	N-CA-CB	-6.33	99.20	110.60
1	D	92	ARG	CB-CG-CD	-6.28	95.28	111.60
1	D	234	ARG	N-CA-CB	-6.22	99.41	110.60
1	D	53	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	92	ARG	CB-CG-CD	-6.16	95.58	111.60
1	C	9	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	D	318	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	92	ARG	CB-CG-CD	-6.00	96.00	111.60
1	D	84	LYS	CA-CB-CG	5.97	126.54	113.40
1	B	92	ARG	CB-CG-CD	-5.94	96.16	111.60
1	D	114	ASP	O-C-N	-5.94	113.20	122.70
1	C	72	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	D	94	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	D	165	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	331	TRP	CG-CD2-CE3	5.86	139.18	133.90
1	A	75	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	34	ASN	N-CA-CB	-5.80	100.17	110.60
1	D	307	GLU	CA-CB-CG	5.77	126.09	113.40
1	C	165	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	234	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	194	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	D	114	ASP	CA-C-N	5.62	129.57	117.20
1	B	274	GLN	CA-CB-CG	5.60	125.72	113.40
1	B	94	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	C	331	TRP	CD1-CG-CD2	5.56	110.75	106.30
1	D	114	ASP	N-CA-C	-5.50	96.16	111.00
1	B	128	LYS	CA-CB-CG	-5.48	101.34	113.40
1	A	349	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	124	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	D	127	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	165	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	157	MET	CG-SD-CE	5.34	108.74	100.20
1	D	215	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	A	320	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	348	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	80	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	87	LEU	CA-CB-CG	5.28	127.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	349	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	349	ARG	CA-CB-CG	5.21	124.87	113.40
1	D	194	LYS	CD-CE-NZ	-5.20	99.74	111.70
1	A	50	ASN	CA-CB-CG	5.20	124.84	113.40
1	A	94	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	C	114	ASP	N-CA-C	-5.15	97.10	111.00
1	A	40	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	172	HIS	CA-CB-CG	-5.12	104.89	113.60
1	A	8	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	B	53	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	D	234	ARG	CA-CB-CG	5.06	124.54	113.40
1	B	124	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	331	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	A	320	TYR	N-CA-C	5.04	124.59	111.00
1	D	83	LEU	CA-CB-CG	5.03	126.87	115.30
1	C	241	TYR	CB-CG-CD2	-5.03	117.98	121.00

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

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	44	0
1	C	2571	0	2608	39	0
1	D	2578	0	2616	36	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	144	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 (144) 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:276:LYS:HD3	1:C:276:LYS:H	1.56	0.71
1:B:278:GLN:HE22	1:B:302:GLU:H	1.40	0.68
1:A:194:LYS:H	1:A:194:LYS:HD2	1.60	0.67
1:A:276:LYS:H	1:A:276:LYS:HD3	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:C:113:MET:HE3	1:C:324:ILE:HD13	1.80	0.62
1:D:113:MET:HE2	1:D:312:LEU:HD21	1.83	0.61
1:D:194:LYS:H	1:D:194:LYS:HD2	1.66	0.61
1:B:261:GLN:HB2	1:B:297:ILE:HD13	1.83	0.60
1:A:210:LEU:HD21	1:B:119:ILE:HG21	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:113:MET:HE3	1:B:324:ILE:HD13	1.82	0.59
1:B:194:LYS:H	1:B:194:LYS:HD2	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:D:113:MET:HE2	1:D:324:ILE:HD13	1.87	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:160:GLY:O	1:B:183:VAL:HA	2.09	0.53
1:A:119:ILE:HG21	1:B:210:LEU:HD21	1.91	0.53
1:B:113:MET:CE	1:B:324:ILE:HD13	2.39	0.52
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:A:113:MET:CE	1:A:324:ILE:HD13	2.40	0.51
1:C:113:MET:CE	1:C:324:ILE:HD13	2.39	0.51
1:C:76:LEU:HD22	1:C:89:ILE:HG21	1.93	0.51
1:C:301:VAL:HG21	1:C:337:LEU:HD21	1.92	0.51
1:C:210:LEU:HD21	1:D:119:ILE:HG21	1.93	0.51
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:D:170:GLN:O	1:D:174:GLU:HG3	2.12	0.50
1:A:160:GLY:O	1:A:183:VAL:HA	2.12	0.50
1:D:113:MET:CE	1:D:324:ILE:HD13	2.42	0.49
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:C:183:VAL:O	1:C:229:CYS:HA	2.12	0.48
1:A:279:MET:SD	1:A:333:ASP:HB3	2.53	0.48
1:A:26:PHE:HB2	1:A:127:ARG:HD3	1.94	0.48
1:C:95:PHE:HB3	1:C:108:ILE:HG13	1.96	0.47
1:B:95:PHE:HB3	1:B:108:ILE:HG13	1.96	0.47
1:C:113:MET:HB3	1:C:312:LEU:HD21	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:A:303:SER:HB3	1:A:329:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:310:GLN:HE22	1:D:319:ALA:H	1.64	0.46
1:B:274:GLN:O	1:B:277:LYS:HB2	2.16	0.46
1:B:274:GLN:HB2	1:B:277:LYS:HG3	1.96	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:B:309:ASN:OD1	1:B:327:ALA:HB2	2.16	0.45
1:A:242:SER:O	1:A:246:VAL:HG23	2.17	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:D:187:ASN:HD22	1:D:233:LEU:HA	1.82	0.44
1:B:187:ASN:ND2	1:B:233:LEU:HA	2.33	0.44
1:D:57:VAL:O	1:D:300:MET:HA	2.18	0.44
1:A:24:GLU:O	1:A:27:PRO:HD3	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:61:CYS:SG	1:C:326:ASP:HB2	2.58	0.43
1:C:24:GLU:O	1:C:27:PRO:HD3	2.18	0.43
1:B:187:ASN:HD22	1:B:233:LEU:HA	1.83	0.43
1:C:309:ASN:HB3	1:C:327:ALA:HA	2.00	0.43
1:A:47:LEU:O	1:A:261:GLN:NE2	2.51	0.43
1:D:187:ASN:ND2	1:D:233:LEU:HA	2.33	0.43
1:C:310:GLN:HG3	1:C:324:ILE:HG22	1.99	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: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:C:343:ASN:HA	1:C:346:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:HG12	1:B:55:LEU:HD13	2.01	0.43
1:A:303:SER:HA	1:A:328:CYS:HB3	2.00	0.42
1:A:246:VAL:O	1:A:250:LYS:HG3	2.18	0.42
1:D:284:ASP:O	1:D:287:GLN:HB3	2.18	0.42
1:A:57:VAL:O	1:A:300:MET:HA	2.20	0.42
1:D:61:CYS:SG	1:D:326:ASP:HB2	2.59	0.42
1:D:303:SER:HB3	1:D:329:ILE:HG13	2.01	0.42
1:B:24:GLU:O	1:B:27:PRO:HD3	2.20	0.42
1:C:124:ARG:HD2	1:C:124:ARG:HH11	1.71	0.42
1:D:303:SER:HA	1:D:328:CYS:HB3	2.01	0.42
1:A:60:PRO:O	1:A:92:ARG:HD3	2.20	0.42
1:C:246:VAL:O	1:C:250:LYS:HG3	2.20	0.42
1:D:19:PRO:HB2	1:D:214:LYS:HA	2.02	0.42
1:C:335:ASP:O	1:C:339:ARG:HG3	2.19	0.42
1:C:47:LEU:O	1:C:261:GLN:NE2	2.53	0.42
1:A:99:ARG:HD3	1:A:99:ARG:HA	1.71	0.42
1:B:279:MET:HE1	1:B:333:ASP:HB3	2.02	0.41
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:303:SER:HA	1:C:328:CYS:HB3	2.01	0.41
1:C:208:CYS:HA	1:C:221:VAL:O	2.20	0.41
1:D:160:GLY:O	1:D:183:VAL:HA	2.21	0.41
1:A:10:ILE:HG21	1:A:13:ILE:HD11	2.02	0.41
1:D:307:GLU:HB3	1:D:330:GLY:N	2.36	0.41
1:B:19:PRO:HB2	1:B:214:LYS:HA	2.02	0.41
1:D:60:PRO:O	1:D:92:ARG:HD3	2.20	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: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:B:99:ARG:HA	1:B:99:ARG:HD3	1.75	0.41
1:A:113:MET:HE3	1:A:324:ILE:HD13	2.00	0.41
1:A:113:MET:HE2	1:A:324:ILE:HD13	2.02	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: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%)	21	42
1	B	334/350 (95%)	314 (94%)	17 (5%)	3 (1%)	21	42
1	C	334/350 (95%)	315 (94%)	17 (5%)	2 (1%)	30	56
1	D	335/350 (96%)	315 (94%)	18 (5%)	2 (1%)	30	56
All	All	1337/1400 (96%)	1258 (94%)	69 (5%)	10 (1%)	26	51

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

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	272/283 (96%)	262 (96%)	10 (4%)	41	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	272/283 (96%)	259 (95%)	13 (5%)	31	58
1	C	272/283 (96%)	261 (96%)	11 (4%)	38	67
1	D	273/283 (96%)	256 (94%)	17 (6%)	23	45
All	All	1089/1132 (96%)	1038 (95%)	51 (5%)	32	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	150	PRO
1	A	234	ARG
1	A	238	GLU
1	A	244	LYS
1	A	274	GLN
1	A	276	LYS
1	A	297	ILE
1	A	304	HIS
1	A	312	LEU
1	B	30	GLU
1	B	38	HIS
1	B	79	LEU
1	B	85	ASP
1	B	211	SER
1	B	234	ARG
1	B	242	SER
1	B	244	LYS
1	B	279	MET
1	B	297	ILE
1	B	304	HIS
1	B	309	ASN
1	B	332	GLU
1	C	70	LYS
1	C	76	LEU
1	C	79	LEU
1	C	81	GLU
1	C	85	ASP
1	C	150	PRO
1	C	234	ARG
1	C	274	GLN
1	C	276	LYS
1	C	297	ILE

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Mol	Chain	Res	Type
1	C	307	GLU
1	D	47	LEU
1	D	75	ARG
1	D	76	LEU
1	D	83	LEU
1	D	85	ASP
1	D	150	PRO
1	D	234	ARG
1	D	254	ASN
1	D	274	GLN
1	D	276	LYS
1	D	294	LYS
1	D	297	ILE
1	D	304	HIS
1	D	310	GLN
1	D	323	SER
1	D	332	GLU
1	D	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	50	ASN
1	A	170	GLN
1	A	187	ASN
1	A	254	ASN
1	B	170	GLN
1	B	187	ASN
1	B	278	GLN
1	C	170	GLN
1	C	187	ASN
1	C	254	ASN
1	D	38	HIS
1	D	170	GLN
1	D	187	ASN

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 ⓘ

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	$\# Z > 2$
4	PEP	A	1352	-	5,9,9	1.44	0	8,13,13	2.57	4 (50%)
3	SO4	A	1353	-	4,4,4	0.23	0	6,6,6	0.63	0
4	PEP	B	2352	-	5,9,9	1.22	0	8,13,13	2.55	3 (37%)
3	SO4	B	2353	-	4,4,4	0.68	0	6,6,6	0.55	0
4	PEP	C	3352	-	5,9,9	1.38	0	8,13,13	2.58	3 (37%)
3	SO4	C	3353	-	4,4,4	0.34	0	6,6,6	0.76	0
4	PEP	D	4352	-	5,9,9	1.31	0	8,13,13	2.65	4 (50%)
3	SO4	D	4353	-	4,4,4	0.59	0	6,6,6	0.66	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
4	PEP	A	1352	-	-	0/5/9/9	0/0/0/0
3	SO4	A	1353	-	-	0/0/0/0	0/0/0/0
4	PEP	B	2352	-	-	0/5/9/9	0/0/0/0
3	SO4	B	2353	-	-	0/0/0/0	0/0/0/0
4	PEP	C	3352	-	-	0/5/9/9	0/0/0/0
3	SO4	C	3353	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEP	D	4352	-	-	0/5/9/9	0/0/0/0
3	SO4	D	4353	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4352	PEP	O2-C2-C3	-4.51	115.62	124.73
4	B	2352	PEP	O2-C2-C3	-4.38	115.88	124.73
4	C	3352	PEP	O2-C2-C3	-4.36	115.91	124.73
4	A	1352	PEP	O2-C2-C3	-4.27	116.09	124.73
4	A	1352	PEP	P-O2-C2	2.21	127.88	122.96
4	B	2352	PEP	O3P-P-O2P	2.24	115.91	107.38
4	D	4352	PEP	P-O2-C2	2.30	128.07	122.96
4	A	1352	PEP	O3P-P-O2P	2.33	116.25	107.38
4	D	4352	PEP	O3P-P-O2P	2.47	116.78	107.38
4	C	3352	PEP	O3P-P-O2P	2.47	116.79	107.38
4	A	1352	PEP	C1-C2-C3	4.49	128.92	120.97
4	D	4352	PEP	C1-C2-C3	4.63	129.17	120.97
4	C	3352	PEP	C1-C2-C3	4.65	129.20	120.97
4	B	2352	PEP	C1-C2-C3	4.68	129.25	120.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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