



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:18 AM UTC

PDB ID : 1N8F / pdb_00001n8f
Title : Crystal structure of E24Q mutant of phenylalanine-regulated 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase (DAHP synthase) from Escherichia Coli in complex with Mn²⁺ and PEP
Authors : Shumilin, I.A.; Bauerle, R.; Kretsinger, R.H.
Deposited on : 2002-11-20
Resolution : 1.75 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

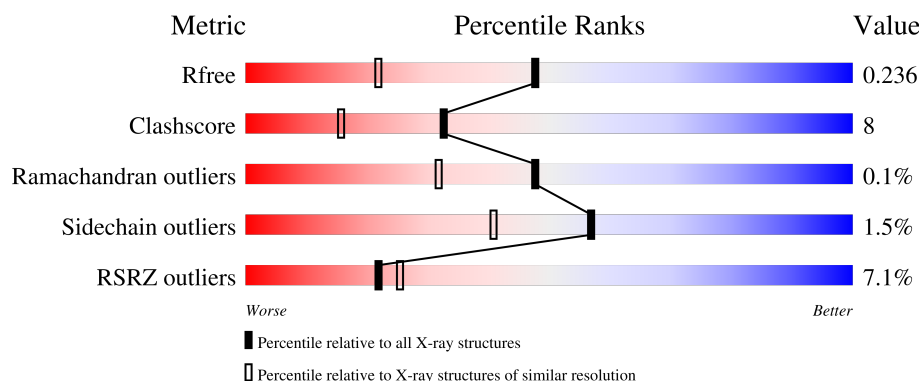
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	350	3% 81% 15% ..
1	B	350	2% 86% 11% ..
1	C	350	12% 76% 20% ..
1	D	350	11% 82% 15% ..

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
4	PEP	D	1399	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11934 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 DAHP Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	3	0
			2621	1646	466	495	14			
1	B	343	Total	C	N	O	S	0	3	0
			2618	1644	465	495	14			
1	C	343	Total	C	N	O	S	0	0	0
			2606	1637	465	490	14			
1	D	343	Total	C	N	O	S	0	1	0
			2610	1639	465	492	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLN	GLU	engineered mutation	UNP P0AB91
B	24	GLN	GLU	engineered mutation	UNP P0AB91
C	24	GLN	GLU	engineered mutation	UNP P0AB91
D	24	GLN	GLU	engineered mutation	UNP P0AB91

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

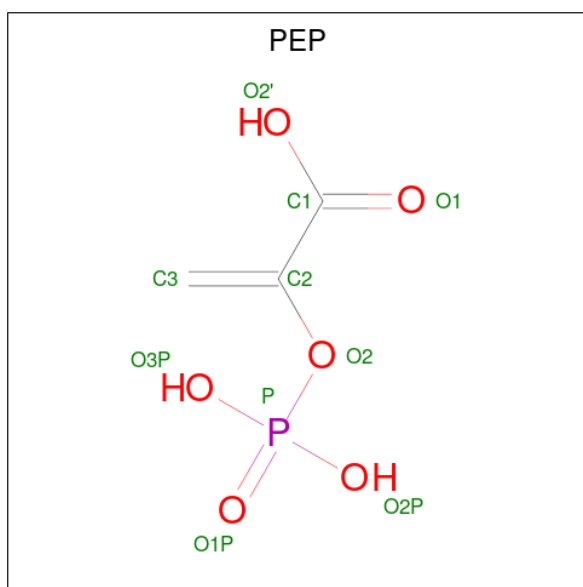
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- 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	A	1	Total	O	S	0	0
			5	4	1		
3	B	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	C	1	Total	O	S	0	0
			5	4	1		
3	D	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: C₃H₅O₆P).



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		

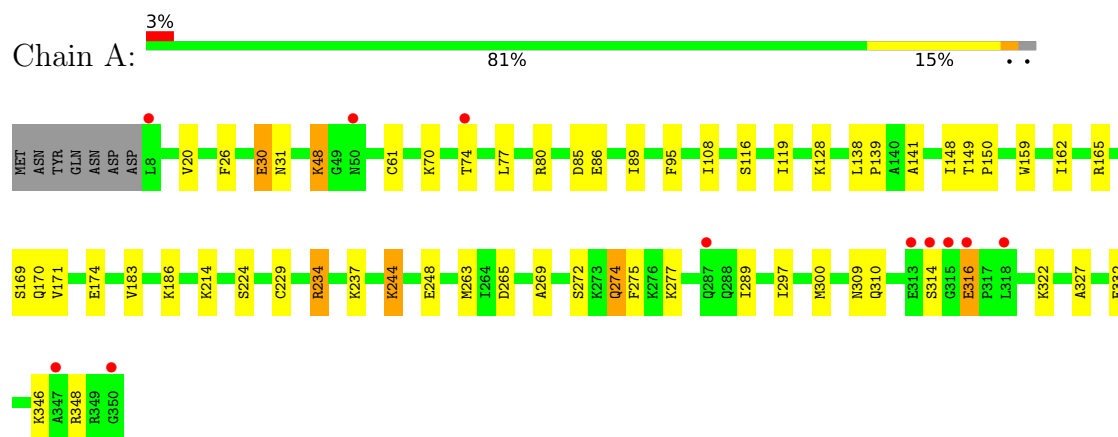
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total	O	0	0
			369	369		
5	B	394	Total	O	0	0
			394	394		
5	C	318	Total	O	0	0
			318	318		
5	D	314	Total	O	0	0
			314	314		

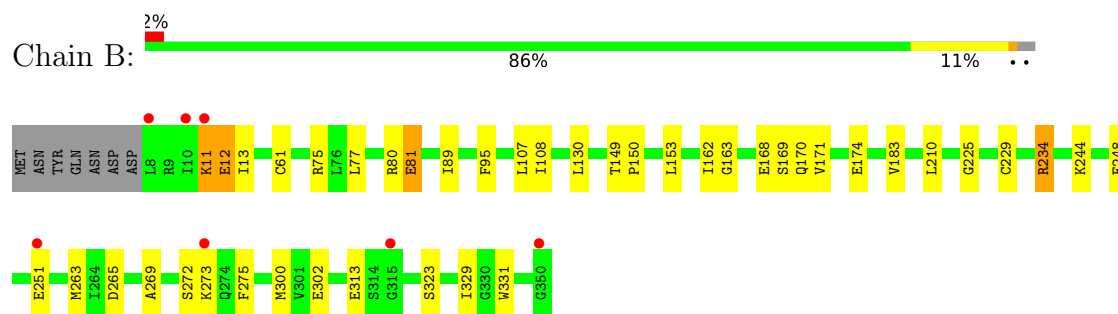
3 Residue-property plots [i](#)

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

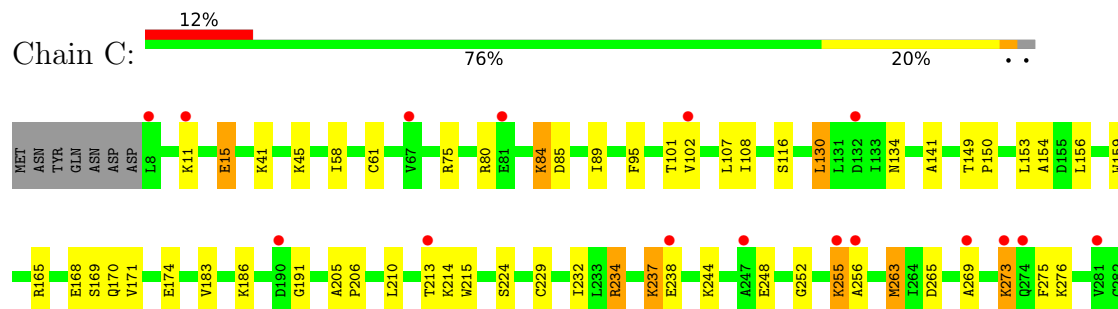
• Molecule 1: DAHP Synthetase

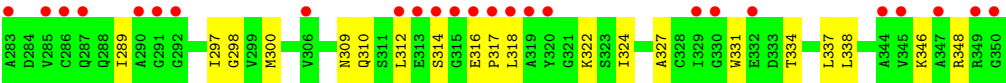


• Molecule 1: DAHP Synthetase

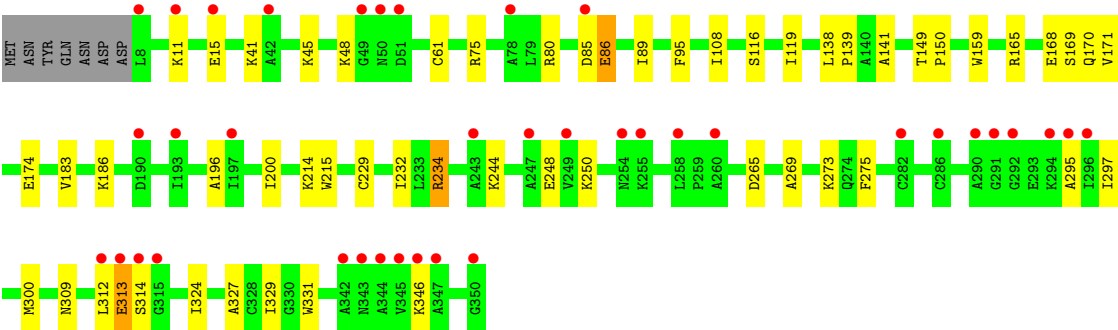
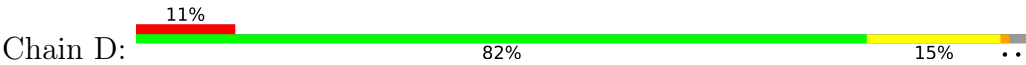


• Molecule 1: DAHP Synthetase





● Molecule 1: DAHP Synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.22Å 53.28Å 150.25Å 90.00° 116.90° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 20.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.75) 99.3 (20.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.237 0.208 , 0.236	Depositor DCC
R_{free} test set	3033 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11934	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEP, MN, 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	0.35	0/2678	0.87	10/3620 (0.3%)
1	B	0.42	0/2675	0.92	14/3616 (0.4%)
1	C	0.31	0/2651	0.81	4/3584 (0.1%)
1	D	0.34	0/2659	0.86	4/3595 (0.1%)
All	All	0.36	0/10663	0.86	32/14415 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ILE	N-CA-C	-6.87	102.56	110.05
1	B	263	MET	N-CA-C	-6.64	98.90	109.59
1	B	61	CYS	N-CA-C	-6.44	104.26	111.28
1	B	275	PHE	N-CA-C	6.42	119.09	111.33
1	B	81[A]	GLU	N-CA-CB	-6.19	100.99	110.16
1	B	81[B]	GLU	N-CA-CB	-6.19	100.99	110.16
1	D	61	CYS	N-CA-C	-6.09	104.64	111.28
1	B	313	GLU	N-CA-C	6.02	118.63	111.71
1	B	107	LEU	N-CA-C	5.76	117.56	111.28
1	A	61	CYS	N-CA-C	-5.75	105.09	111.36
1	B	163	GLY	N-CA-C	5.75	118.65	112.33
1	B	162	ILE	N-CA-C	-5.72	99.51	107.80
1	C	116	SER	N-CA-C	-5.70	106.16	113.23
1	D	275	PHE	N-CA-C	5.55	118.05	111.33
1	A	237	LYS	N-CA-C	-5.54	105.39	111.82
1	C	263	MET	N-CA-C	-5.51	100.71	109.59
1	A	30[A]	GLU	CB-CA-C	5.49	119.91	110.79
1	A	30[B]	GLU	CB-CA-C	5.49	119.91	110.79
1	D	116	SER	N-CA-C	-5.49	106.63	113.38
1	C	61	CYS	N-CA-C	-5.46	105.41	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274[A]	GLN	N-CA-CB	5.40	119.58	110.46
1	A	274[B]	GLN	N-CA-CB	5.40	119.58	110.46
1	B	323	SER	N-CA-C	5.39	117.85	110.24
1	C	154	ALA	N-CA-C	5.35	117.81	111.33
1	B	12[A]	GLU	N-CA-CB	5.32	120.95	111.69
1	B	12[B]	GLU	N-CA-CB	5.32	120.95	111.69
1	A	263	MET	N-CA-C	-5.32	100.73	109.40
1	B	225	GLY	N-CA-C	-5.31	104.76	111.72
1	A	116	SER	N-CA-C	-5.15	107.00	113.28
1	B	329	ILE	N-CA-C	-5.08	104.51	110.05
1	A	275	PHE	N-CA-C	5.05	117.44	111.33
1	A	162	ILE	N-CA-C	-5.04	100.49	107.80

There are no chirality outliers.

There are no planarity outliers.

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	2621	0	2645	39	0
1	B	2618	0	2642	27	0
1	C	2606	0	2637	72	0
1	D	2610	0	2637	37	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	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	10	0	2	1	0
4	B	10	0	2	0	0
4	C	10	0	2	0	0
4	D	10	0	2	0	0
5	A	369	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	394	0	0	2	0
5	C	318	0	0	4	0
5	D	314	0	0	4	0
All	All	11934	0	10569	167	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 8.

All (167) 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:101:THR:HG23	1:C:102:VAL:H	1.20	1.05
1:C:213:THR:HG23	1:C:215:TRP:H	1.41	0.85
1:A:30[B]:GLU:HG3	1:A:31:ASN:N	1.91	0.85
1:C:130:LEU:HD12	1:C:156:LEU:HB3	1.60	0.82
1:C:80:ARG:HA	1:C:89:ILE:HD12	1.62	0.81
1:B:77:LEU:O	1:B:81[A]:GLU:HG3	1.86	0.76
1:C:334:THR:O	1:C:338:LEU:HD13	1.85	0.75
1:C:314:SER:HB2	1:C:316:GLU:OE2	1.87	0.75
1:D:48:LYS:HE2	1:D:48:LYS:HA	1.69	0.74
1:A:244:LYS:HE3	1:A:244:LYS:H	1.53	0.74
1:C:101:THR:HG23	1:C:102:VAL:N	1.98	0.74
1:C:237:LYS:HE2	1:C:237:LYS:N	2.06	0.71
1:B:272:SER:C	1:B:273:LYS:HD2	2.17	0.70
1:C:234:ARG:O	1:C:269:ALA:HB3	1.92	0.69
1:C:101:THR:CG2	1:C:102:VAL:H	2.03	0.69
1:A:80:ARG:HA	1:A:89:ILE:HD12	1.73	0.69
1:C:186:LYS:HD3	1:C:234:ARG:HG2	1.76	0.67
1:A:48:LYS:HA	1:A:48:LYS:HE3	1.75	0.66
1:A:272:SER:O	1:A:274[B]:GLN:HG2	1.96	0.66
1:C:11:LYS:HA	1:C:11:LYS:HE2	1.78	0.65
1:A:169:SER:OG	1:A:171:VAL:HG22	1.96	0.65
1:B:273:LYS:HD2	1:B:273:LYS:N	2.11	0.65
1:D:169:SER:OG	1:D:171:VAL:HG22	1.98	0.63
1:B:300:MET:HG2	5:B:2580:HOH:O	1.98	0.62
1:C:273:LYS:O	1:C:273:LYS:HD2	2.00	0.62
1:D:312:LEU:HD11	1:D:324:ILE:HD12	1.82	0.61
1:C:169:SER:OG	1:C:171:VAL:HG22	2.00	0.61
1:B:130:LEU:HD12	1:B:153:LEU:HD22	1.83	0.61
1:D:80:ARG:HA	1:D:89:ILE:HD12	1.82	0.60
1:D:170:GLN:O	1:D:174:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:HG22	5:A:5575:HOH:O	2.01	0.59
1:D:244:LYS:O	1:D:248:GLU:HG3	2.02	0.59
1:C:300:MET:HG2	5:C:3579:HOH:O	2.01	0.59
1:C:108:ILE:HD11	1:C:153:LEU:HD11	1.84	0.59
1:B:170:GLN:O	1:B:174:GLU:HG3	2.02	0.58
1:A:224:SER:HB3	1:B:11:LYS:HD3	1.85	0.58
1:C:237:LYS:HE2	1:C:237:LYS:H	1.67	0.56
1:A:95:PHE:HB3	1:A:108:ILE:HG13	1.87	0.56
1:C:310:GLN:NE2	1:C:322:LYS:HB3	2.21	0.56
1:D:300:MET:HG2	5:D:4575:HOH:O	2.05	0.55
1:C:95:PHE:HE1	1:C:130:LEU:HD23	1.72	0.55
1:A:170:GLN:O	1:A:174:GLU:HG3	2.07	0.55
1:A:244:LYS:H	1:A:244:LYS:CE	2.19	0.54
1:C:58:ILE:HD13	1:C:338:LEU:HD11	1.89	0.54
1:A:274[A]:GLN:HG3	5:A:5543:HOH:O	2.06	0.54
1:B:11:LYS:C	1:B:12[B]:GLU:HG3	2.32	0.54
1:D:41:LYS:HZ3	1:D:45:LYS:HE3	1.73	0.54
1:C:224:SER:HA	1:D:11:LYS:HE3	1.90	0.54
1:B:169:SER:OG	1:B:171:VAL:HG22	2.08	0.53
1:D:85[B]:ASP:HB2	1:D:86:GLU:OE1	2.09	0.53
1:D:234:ARG:O	1:D:269:ALA:HB3	2.08	0.53
1:D:313:GLU:H	1:D:313:GLU:CD	2.17	0.53
1:A:314:SER:HB2	1:A:316:GLU:OE2	2.09	0.52
1:C:289:ILE:HG23	1:C:348:ARG:HD3	1.93	0.51
1:D:149:THR:N	1:D:150:PRO:CD	2.74	0.51
1:A:141:ALA:HB1	1:A:159:TRP:HE3	1.74	0.51
1:C:213:THR:HG23	1:C:215:TRP:N	2.18	0.51
1:C:252:GLY:O	1:C:255:LYS:HE2	2.11	0.51
1:D:312:LEU:C	1:D:314:SER:H	2.19	0.51
1:C:168:GLU:HG2	1:D:165:ARG:HB3	1.92	0.51
1:C:149:THR:N	1:C:150:PRO:CD	2.74	0.51
1:C:191:GLY:HA3	1:C:237:LYS:HZ1	1.76	0.51
1:D:273:LYS:NZ	1:D:273:LYS:HB3	2.26	0.51
1:D:86:GLU:HG2	1:D:346:LYS:HG3	1.93	0.50
1:B:244:LYS:O	1:B:248:GLU:HG3	2.11	0.50
1:C:165:ARG:HB3	1:D:168:GLU:HG2	1.93	0.50
1:D:312:LEU:O	1:D:314:SER:N	2.44	0.50
1:A:149:THR:N	1:A:150:PRO:CD	2.75	0.50
1:B:265:ASP:HA	1:B:300:MET:HB3	1.93	0.50
1:C:171:VAL:HG12	5:D:4441:HOH:O	2.10	0.50
1:A:86:GLU:HG2	1:A:346:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:GLY:HA3	1:C:237:LYS:NZ	2.27	0.50
1:C:41:LYS:HE2	1:C:45:LYS:NZ	2.27	0.50
1:D:196:ALA:O	1:D:200:ILE:HG13	2.12	0.50
1:A:234:ARG:O	1:A:269:ALA:HB3	2.12	0.50
1:A:265:ASP:HA	1:A:300:MET:HB3	1.95	0.49
1:A:289:ILE:O	1:A:348:ARG:HB2	2.11	0.49
1:A:310:GLN:NE2	1:A:322:LYS:HB3	2.27	0.49
1:B:80:ARG:HA	1:B:89:ILE:HD12	1.94	0.49
1:C:265:ASP:HA	1:C:300:MET:HB3	1.94	0.49
1:D:214:LYS:HE3	1:D:215:TRP:CZ2	2.47	0.49
1:A:165:ARG:HB3	1:B:168:GLU:HG2	1.95	0.49
1:D:15:GLU:HG2	5:D:4621:HOH:O	2.12	0.49
1:B:11:LYS:HB3	1:B:11:LYS:NZ	2.27	0.49
1:C:214:LYS:HE3	1:C:215:TRP:CZ2	2.48	0.49
1:C:237:LYS:HE2	1:C:238:GLU:H	1.78	0.48
1:C:84:LYS:HD3	1:C:84:LYS:C	2.39	0.48
1:C:234:ARG:HD3	1:C:234:ARG:C	2.38	0.48
1:C:11:LYS:HE2	1:C:11:LYS:CA	2.43	0.48
1:D:265:ASP:HA	1:D:300:MET:HB3	1.96	0.48
1:D:250:LYS:HD3	1:D:295:ALA:CB	2.43	0.48
1:D:141:ALA:HB1	1:D:159:TRP:HE3	1.79	0.47
1:A:274[A]:GLN:CD	5:A:5651:HOH:O	2.57	0.47
1:A:70:LYS:O	1:A:74:THR:HG23	2.14	0.47
1:D:214:LYS:HE3	1:D:215:TRP:CE2	2.49	0.47
1:B:11:LYS:HB2	1:B:12[B]:GLU:HG3	1.95	0.47
1:B:234:ARG:O	1:B:269:ALA:HB3	2.15	0.47
1:B:11:LYS:CB	1:B:12[B]:GLU:HG3	2.44	0.47
1:C:130:LEU:CD1	1:C:134:ASN:ND2	2.78	0.47
1:A:244:LYS:O	1:A:248:GLU:HG3	2.15	0.47
1:A:297:ILE:C	1:A:297:ILE:HD12	2.40	0.47
1:D:95:PHE:HB3	1:D:108:ILE:HG13	1.97	0.46
1:B:149:THR:N	1:B:150:PRO:CD	2.79	0.46
1:A:274[A]:GLN:HB3	1:A:277:LYS:CG	2.46	0.46
1:C:255:LYS:HD2	1:C:255:LYS:C	2.41	0.46
1:C:75:ARG:HB3	1:C:331:TRP:CZ2	2.51	0.46
1:C:80:ARG:CA	1:C:89:ILE:HD12	2.40	0.46
1:D:183:VAL:O	1:D:229:CYS:HA	2.16	0.45
1:C:15:GLU:H	1:C:15:GLU:CD	2.17	0.45
1:C:324:ILE:HG12	5:C:3436:HOH:O	2.16	0.45
1:C:316:GLU:OE2	1:C:316:GLU:N	2.49	0.45
1:B:183:VAL:O	1:B:229:CYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:PHE:HB3	1:C:108:ILE:HG13	1.99	0.45
1:C:95:PHE:CE1	1:C:130:LEU:HD23	2.51	0.45
1:A:119:ILE:HG21	1:B:210:LEU:HD21	1.98	0.45
1:C:237:LYS:HG2	1:C:238:GLU:HG2	1.98	0.45
1:B:95:PHE:HB3	1:B:108:ILE:HG13	1.99	0.45
1:C:252:GLY:O	1:C:255:LYS:HG3	2.16	0.45
1:D:186:LYS:HD3	1:D:234:ARG:HG2	1.98	0.44
1:C:130:LEU:CD1	1:C:134:ASN:HD22	2.31	0.44
1:C:275:PHE:CE1	1:C:276:LYS:HG3	2.53	0.44
1:C:170:GLN:O	1:C:174:GLU:HG3	2.18	0.44
1:A:85:ASP:HB2	5:A:5557:HOH:O	2.18	0.44
1:C:244:LYS:O	1:C:248:GLU:HG3	2.18	0.44
1:C:297:ILE:HD12	1:C:297:ILE:C	2.43	0.43
1:C:316:GLU:HG2	1:C:317:PRO:O	2.17	0.43
1:D:75:ARG:HB3	1:D:331:TRP:CZ2	2.53	0.43
1:A:20:VAL:HG13	1:A:214:LYS:O	2.19	0.43
1:A:183:VAL:O	1:A:229:CYS:HA	2.17	0.43
1:C:183:VAL:O	1:C:229:CYS:HA	2.19	0.43
1:C:297:ILE:HA	5:C:3594:HOH:O	2.18	0.43
1:C:312:LEU:HD23	1:C:318:LEU:HD21	2.01	0.43
1:D:312:LEU:C	1:D:314:SER:N	2.77	0.43
1:A:309:ASN:HB3	1:A:327:ALA:HA	2.01	0.42
1:A:332:GLU:HB2	5:A:5657:HOH:O	2.18	0.42
1:D:297:ILE:HA	5:D:4586:HOH:O	2.18	0.42
1:B:12[A]:GLU:HG2	1:B:13:ILE:N	2.34	0.42
1:C:101:THR:HG22	5:C:3480:HOH:O	2.19	0.42
1:C:210:LEU:HD21	1:D:119:ILE:HG21	2.01	0.42
1:C:297:ILE:HD12	1:C:298:GLY:N	2.34	0.42
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.94	0.42
1:D:309:ASN:HB3	1:D:327:ALA:HA	2.01	0.42
1:D:186:LYS:HG2	1:D:232:ILE:HB	2.01	0.42
1:C:337:LEU:HD23	1:C:338:LEU:HD12	2.02	0.42
1:A:169:SER:HG	1:A:171:VAL:HG22	1.83	0.41
1:B:302:GLU:HG3	5:B:2580:HOH:O	2.19	0.41
1:C:224:SER:CB	1:D:11:LYS:HE3	2.51	0.41
1:C:255:LYS:HD2	1:C:256:ALA:N	2.35	0.41
1:D:138:LEU:HA	1:D:139:PRO:HD3	1.89	0.41
1:C:159:TRP:CZ2	1:C:232:ILE:HD11	2.55	0.41
1:C:309:ASN:O	1:C:322:LYS:HE2	2.20	0.41
1:A:26:PHE:CE2	1:A:128:LYS:HD3	2.56	0.41
1:B:234:ARG:HD3	1:B:234:ARG:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:H	1:C:237:LYS:CE	2.31	0.41
1:C:309:ASN:HB3	1:C:327:ALA:HA	2.03	0.41
1:A:148:ILE:C	1:A:150:PRO:HD2	2.46	0.41
1:A:186:LYS:HD3	4:A:1396:PEP:O3P	2.21	0.41
1:A:244:LYS:N	1:A:244:LYS:HD3	2.35	0.41
1:C:107:LEU:C	1:C:107:LEU:HD23	2.46	0.41
1:C:263:MET:HA	1:C:298:GLY:O	2.21	0.41
1:B:251:GLU:CD	1:B:251:GLU:C	2.89	0.40
1:A:244:LYS:N	1:A:244:LYS:CD	2.84	0.40
1:B:11:LYS:C	1:B:12[B]:GLU:CG	2.90	0.40
1:B:75:ARG:HB3	1:B:331:TRP:CZ2	2.57	0.40
1:C:205:ALA:HB1	1:C:206:PRO:HD2	2.03	0.40
1:C:84:LYS:HD3	1:C:85:ASP:N	2.37	0.40
1:C:141:ALA:HB1	1:C:159:TRP:HE3	1.86	0.40

There are no symmetry-related clashes.

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	344/350 (98%)	334 (97%)	10 (3%)	0	100	100
1	B	344/350 (98%)	336 (98%)	8 (2%)	0	100	100
1	C	341/350 (97%)	329 (96%)	12 (4%)	0	100	100
1	D	342/350 (98%)	335 (98%)	6 (2%)	1 (0%)	36	21
All	All	1371/1400 (98%)	1334 (97%)	36 (3%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	313	GLU

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	279/283 (99%)	274 (98%)	5 (2%)	51	33
1	B	279/283 (99%)	277 (99%)	2 (1%)	76	67
1	C	276/283 (98%)	268 (97%)	8 (3%)	37	17
1	D	277/283 (98%)	275 (99%)	2 (1%)	76	67
All	All	1111/1132 (98%)	1094 (98%)	17 (2%)	57	41

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	77	LEU
1	A	234	ARG
1	A	244	LYS
1	A	316	GLU
1	B	11	LYS
1	B	234	ARG
1	C	15	GLU
1	C	84	LYS
1	C	130	LEU
1	C	234	ARG
1	C	237	LYS
1	C	255	LYS
1	C	273	LYS
1	C	346	LYS
1	D	86	GLU
1	D	234	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	112	HIS
1	A	261	GLN
1	B	34	ASN
1	B	50	ASN
1	B	109	ASN
1	B	115	ASN
1	B	134	ASN
1	B	254	ASN
1	C	34	ASN
1	C	38	HIS
1	C	50	ASN
1	C	109	ASN
1	C	115	ASN
1	C	134	ASN
1	C	261	GLN
1	C	343	ASN
1	D	34	ASN
1	D	50	ASN
1	D	109	ASN
1	D	115	ASN
1	D	151	GLN
1	D	254	ASN
1	D	343	ASN

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 [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	B	2356	-	4,4,4	0.41	0	6,6,6	0.14	0
3	SO4	B	2353	-	4,4,4	0.36	0	6,6,6	0.07	0
4	PEP	B	1397	-	9,9,9	1.97	3 (33%)	11,13,13	2.65	5 (45%)
3	SO4	A	5353	-	4,4,4	0.37	0	6,6,6	0.07	0
4	PEP	A	1396	-	9,9,9	2.11	3 (33%)	11,13,13	2.74	5 (45%)
3	SO4	C	3356	-	4,4,4	0.42	0	6,6,6	0.11	0
3	SO4	D	4356	-	4,4,4	0.41	0	6,6,6	0.08	0
4	PEP	D	1399	-	9,9,9	1.99	4 (44%)	11,13,13	2.70	5 (45%)
4	PEP	C	1398	-	9,9,9	2.01	3 (33%)	11,13,13	2.78	5 (45%)
3	SO4	A	5356	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	D	4353	-	4,4,4	0.37	0	6,6,6	0.07	0
3	SO4	C	3353	-	4,4,4	0.37	0	6,6,6	0.07	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	D	1399	-	-	4/9/9/9	-
4	PEP	B	1397	-	-	4/9/9/9	-
4	PEP	A	1396	-	-	4/9/9/9	-
4	PEP	C	1398	-	-	4/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1396	PEP	O2'-C1	-3.44	1.21	1.30
4	B	1397	PEP	O2'-C1	-3.42	1.21	1.30
4	A	1396	PEP	C2-C1	3.41	1.52	1.49
4	C	1398	PEP	O2'-C1	-3.39	1.21	1.30
4	D	1399	PEP	O2'-C1	-3.37	1.21	1.30
4	C	1398	PEP	C2-C1	2.77	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1399	PEP	O1-C1	2.75	1.29	1.22
4	C	1398	PEP	O1-C1	2.71	1.29	1.22
4	A	1396	PEP	O1-C1	2.69	1.29	1.22
4	B	1397	PEP	C2-C1	2.66	1.52	1.49
4	B	1397	PEP	O1-C1	2.55	1.28	1.22
4	D	1399	PEP	C2-C1	2.36	1.51	1.49
4	D	1399	PEP	C3-C2	2.03	1.37	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1396	PEP	O2'-C1-C2	5.34	123.03	113.91
4	C	1398	PEP	O2'-C1-C2	5.32	122.99	113.91
4	B	1397	PEP	O2'-C1-C2	5.17	122.74	113.91
4	D	1399	PEP	O2'-C1-C2	5.14	122.69	113.91
4	C	1398	PEP	O1-C1-C2	-5.02	114.21	121.79
4	A	1396	PEP	O1-C1-C2	-4.92	114.37	121.79
4	B	1397	PEP	O1-C1-C2	-4.92	114.37	121.79
4	D	1399	PEP	O1-C1-C2	-4.75	114.63	121.79
4	C	1398	PEP	O2-C2-C3	-3.48	118.21	124.85
4	D	1399	PEP	C3-C2-C1	3.47	129.14	122.73
4	A	1396	PEP	C3-C2-C1	3.41	129.03	122.73
4	C	1398	PEP	C3-C2-C1	3.39	129.00	122.73
4	D	1399	PEP	O2-C2-C3	-3.36	118.43	124.85
4	B	1397	PEP	C3-C2-C1	3.31	128.85	122.73
4	A	1396	PEP	O2-C2-C3	-3.28	118.59	124.85
4	B	1397	PEP	O2-C2-C3	-3.01	119.09	124.85
4	D	1399	PEP	O3P-P-O2P	2.22	116.11	107.80
4	C	1398	PEP	O3P-P-O2P	2.19	116.03	107.80
4	A	1396	PEP	O3P-P-O2P	2.17	115.94	107.80
4	B	1397	PEP	O3P-P-O2P	2.04	115.45	107.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1396	PEP	O1-C1-C2-C3
4	A	1396	PEP	O2'-C1-C2-C3
4	B	1397	PEP	O1-C1-C2-C3
4	B	1397	PEP	O2'-C1-C2-C3
4	C	1398	PEP	O1-C1-C2-C3
4	C	1398	PEP	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	1398	PEP	O2'-C1-C2-C3
4	C	1398	PEP	O2'-C1-C2-O2
4	D	1399	PEP	O1-C1-C2-C3
4	D	1399	PEP	O2'-C1-C2-C3
4	A	1396	PEP	O1-C1-C2-O2
4	B	1397	PEP	O1-C1-C2-O2
4	D	1399	PEP	O1-C1-C2-O2
4	A	1396	PEP	O2'-C1-C2-O2
4	B	1397	PEP	O2'-C1-C2-O2
4	D	1399	PEP	O2'-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1396	PEP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	343/350 (98%)	0.52	11 (3%) 50 57	19, 30, 43, 67	3 (0%)
1	B	343/350 (98%)	-0.03	7 (2%) 65 71	13, 20, 31, 47	3 (0%)
1	C	343/350 (98%)	0.96	41 (11%) 9 10	23, 34, 49, 69	0
1	D	343/350 (98%)	0.74	38 (11%) 10 11	19, 29, 49, 64	1 (0%)
All	All	1372/1400 (98%)	0.55	97 (7%) 22 25	13, 29, 46, 69	7 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	GLY	5.1
1	B	8	LEU	5.1
1	D	313	GLU	4.9
1	A	314	SER	4.7
1	D	315	GLY	4.5
1	C	344	ALA	4.3
1	D	344	ALA	4.1
1	C	317	PRO	3.7
1	D	49	GLY	3.6
1	D	8	LEU	3.6
1	D	312	LEU	3.6
1	C	291	GLY	3.5
1	B	350	GLY	3.3
1	C	81	GLU	3.3
1	D	350	GLY	3.2
1	C	290	ALA	3.2
1	C	350	GLY	3.1
1	A	315	GLY	3.0
1	C	247	ALA	3.0
1	A	347	ALA	3.0
1	D	345	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	243	ALA	3.0
1	A	313	GLU	2.9
1	D	258	LEU	2.9
1	C	320	TYR	2.9
1	A	8	LEU	2.9
1	C	8	LEU	2.9
1	C	314	SER	2.9
1	C	285	VAL	2.8
1	B	315	GLY	2.8
1	D	190	ASP	2.8
1	C	273	LYS	2.8
1	D	314	SER	2.7
1	C	238	GLU	2.7
1	D	255	LYS	2.7
1	C	306	VAL	2.7
1	C	313	GLU	2.6
1	C	287	GLN	2.6
1	D	294	LYS	2.6
1	D	260	ALA	2.6
1	D	347	ALA	2.6
1	D	254	ASN	2.6
1	C	213	THR	2.6
1	C	316	GLU	2.5
1	D	197	ILE	2.5
1	C	292	GLY	2.5
1	C	102	VAL	2.5
1	C	315	GLY	2.5
1	B	11	LYS	2.5
1	D	346	LYS	2.5
1	C	255	LYS	2.5
1	B	251	GLU	2.5
1	D	290	ALA	2.4
1	C	190	ASP	2.4
1	D	85[A]	ASP	2.4
1	D	295	ALA	2.4
1	A	316	GLU	2.4
1	C	332	GLU	2.3
1	D	282	CYS	2.3
1	C	349	ARG	2.3
1	D	342	ALA	2.3
1	A	287	GLN	2.3
1	D	50	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLY	2.3
1	D	247	ALA	2.2
1	A	74	THR	2.2
1	C	256	ALA	2.2
1	C	347	ALA	2.2
1	C	312	LEU	2.2
1	C	329	ILE	2.2
1	C	11	LYS	2.2
1	C	281	VAL	2.2
1	C	319	ALA	2.2
1	C	286	CYS	2.2
1	A	318	LEU	2.2
1	B	273	LYS	2.1
1	D	51	ASP	2.1
1	D	249	VAL	2.1
1	D	296	ILE	2.1
1	D	78	ALA	2.1
1	C	345	VAL	2.1
1	D	343	ASN	2.1
1	D	193	ILE	2.1
1	C	330	GLY	2.0
1	D	291	GLY	2.0
1	C	269	ALA	2.0
1	C	274	GLN	2.0
1	C	67	VAL	2.0
1	C	132	ASP	2.0
1	C	318	LEU	2.0
1	D	11	LYS	2.0
1	D	15	GLU	2.0
1	A	50	ASN	2.0
1	B	10	ILE	2.0
1	C	283	ALA	2.0
1	D	42	ALA	2.0
1	D	286	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	3356	5/5	0.81	0.12	47,48,50,51	0
3	SO4	A	5356	5/5	0.83	0.18	44,45,48,49	0
3	SO4	B	2356	5/5	0.85	0.20	41,41,46,48	0
3	SO4	D	4356	5/5	0.86	0.11	49,49,51,53	0
3	SO4	C	3353	5/5	0.89	0.15	45,47,47,47	0
3	SO4	B	2353	5/5	0.92	0.12	28,30,35,38	0
3	SO4	D	4353	5/5	0.93	0.10	38,39,41,42	0
4	PEP	C	1398	10/10	0.93	0.11	31,36,36,37	0
3	SO4	A	5353	5/5	0.94	0.10	39,40,43,44	0
4	PEP	D	1399	10/10	0.96	0.07	27,29,30,30	0
2	MN	C	351	1/1	0.97	0.05	31,31,31,31	0
4	PEP	A	1396	10/10	0.97	0.07	24,26,29,32	0
4	PEP	B	1397	10/10	0.98	0.06	18,19,21,23	0
2	MN	D	351	1/1	0.98	0.04	23,23,23,23	0
2	MN	B	351	1/1	0.98	0.06	19,19,19,19	0
2	MN	A	351	1/1	0.99	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.