



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:12 PM UTC

PDB ID : 6A6E / pdb_00006a6e
Title : Crystal structure of thermostable Cysteine desulfurase (FiSufS) from thermophilic *Fervidobacterium Islandicum* AW-1
Authors : Dhanasingh, I.; Jin, H.S.; Lee, D.W.; Lee, S.H.
Deposited on : 2018-06-27
Resolution : 2.09 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

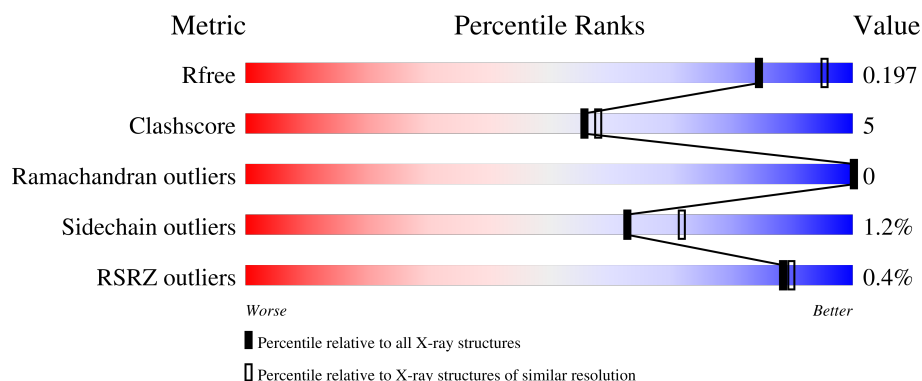
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	425	87% 12% ..
1	B	425	91% 8% .
1	C	425	90% 9% .
1	D	425	89% 10% .

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	CIT	A	503	-	X	-	-
4	CIT	C	505	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14912 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.

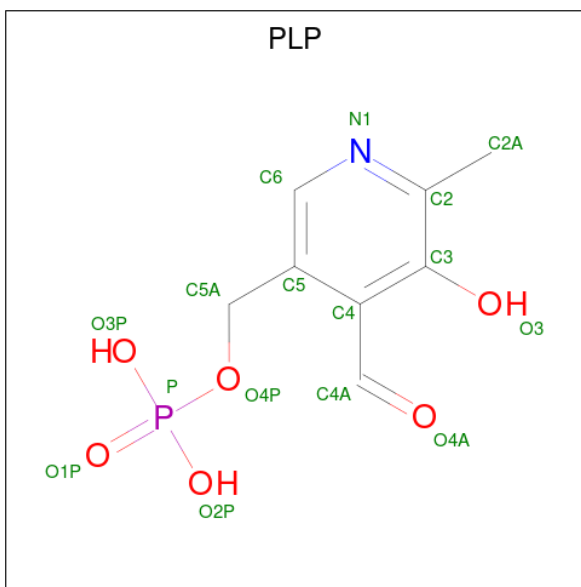
- Molecule 1 is a protein called Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	1	0
			3346	2150	554	631	11			
1	B	422	Total	C	N	O	S	0	0	0
			3340	2146	553	630	11			
1	C	422	Total	C	N	O	S	0	0	0
			3340	2146	553	630	11			
1	D	422	Total	C	N	O	S	0	1	0
			3346	2150	553	632	11			

There are 16 discrepancies between the modelled and reference sequences:

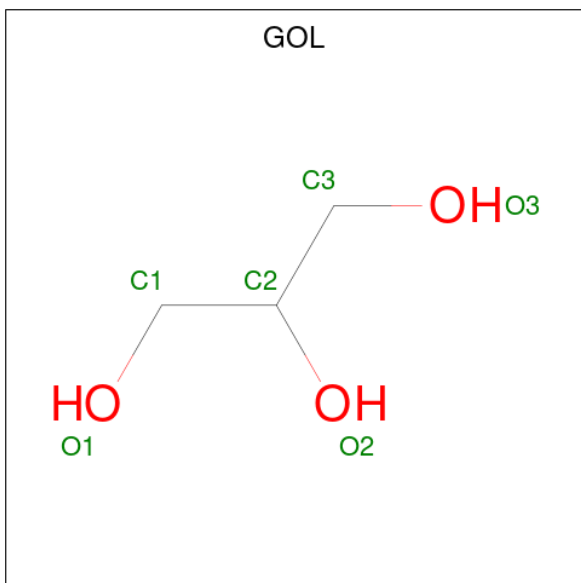
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP A0A1B0VPZ3
A	-2	SER	-	expression tag	UNP A0A1B0VPZ3
A	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
A	0	HIS	-	expression tag	UNP A0A1B0VPZ3
B	-3	SER	-	expression tag	UNP A0A1B0VPZ3
B	-2	SER	-	expression tag	UNP A0A1B0VPZ3
B	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
B	0	HIS	-	expression tag	UNP A0A1B0VPZ3
C	-3	SER	-	expression tag	UNP A0A1B0VPZ3
C	-2	SER	-	expression tag	UNP A0A1B0VPZ3
C	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
C	0	HIS	-	expression tag	UNP A0A1B0VPZ3
D	-3	SER	-	expression tag	UNP A0A1B0VPZ3
D	-2	SER	-	expression tag	UNP A0A1B0VPZ3
D	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
D	0	HIS	-	expression tag	UNP A0A1B0VPZ3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



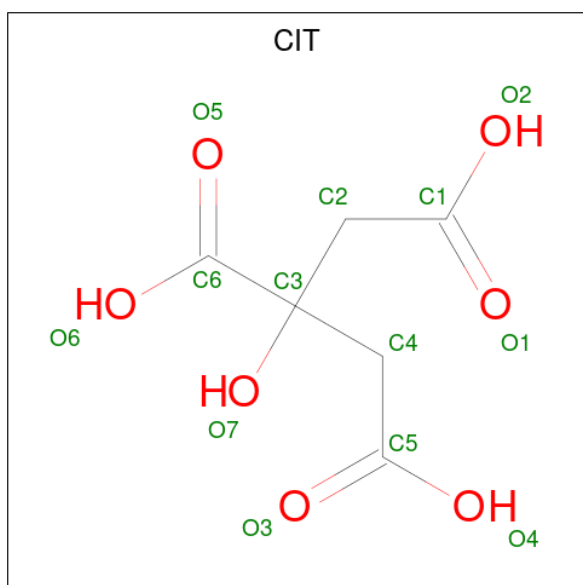
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



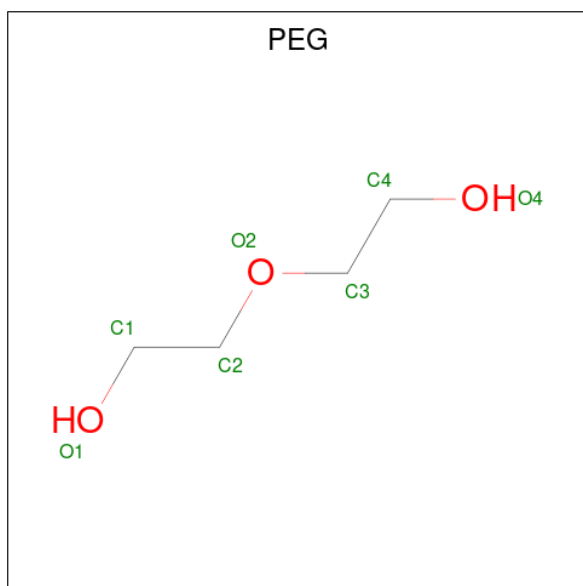
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

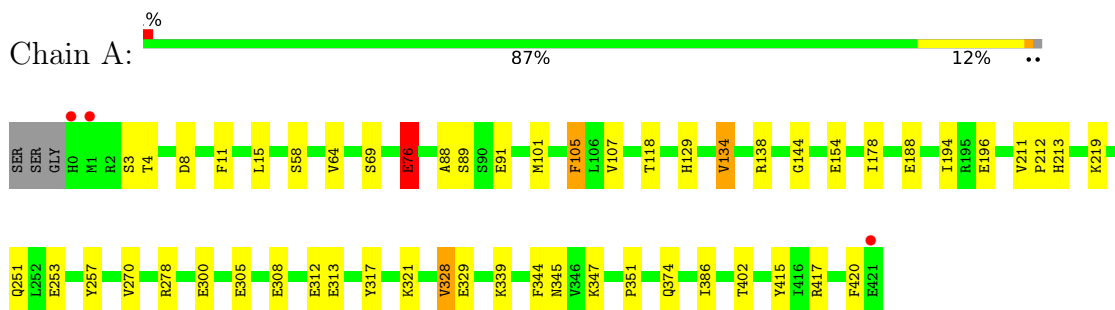
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	311	Total O 311 311	0	0
6	B	331	Total O 331 331	0	0
6	C	307	Total O 307 307	0	0
6	D	277	Total O 277 277	0	0

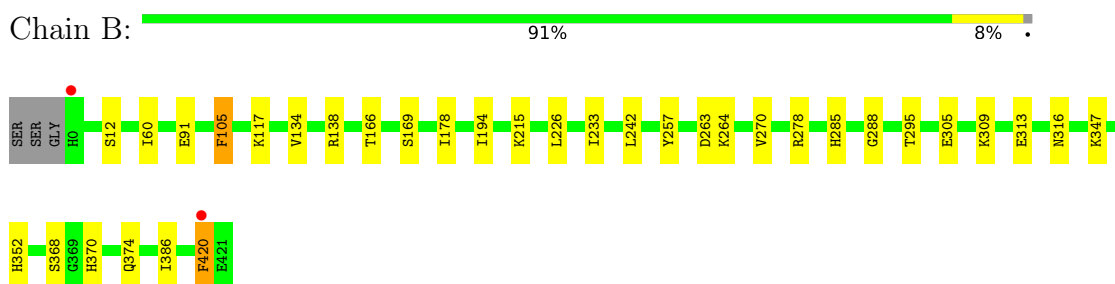
3 Residue-property plots [i](#)

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

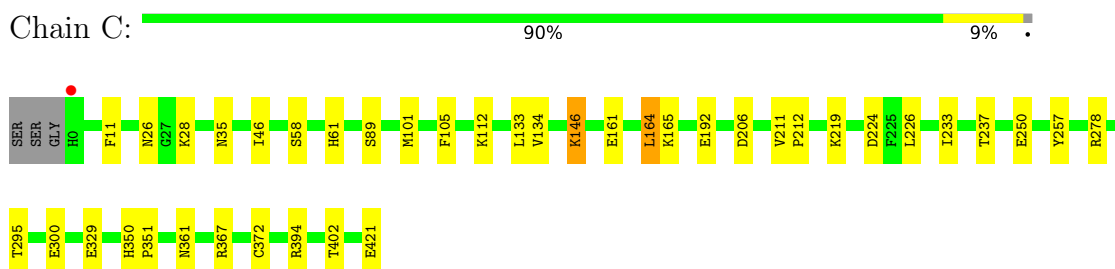
- Molecule 1: Cysteine desulfurase



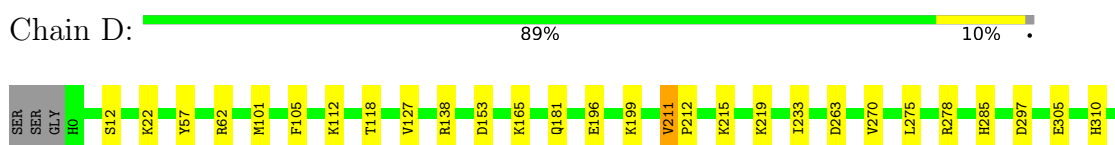
- Molecule 1: Cysteine desulfurase



- Molecule 1: Cysteine desulfurase



- Molecule 1: Cysteine desulfurase



E313	L314	I334	H352	H386	I397	L358	V364	H370	H371	C372	A373	Q374	P375	L376	Y398	R417	R418	E421
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.30Å 218.72Å 89.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.75 – 2.09 26.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.75-2.09) 98.7 (26.75-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.142 , 0.187 0.155 , 0.197	Depositor DCC
R_{free} test set	6103 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14912	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, CIT, GOL, CSS, PEG

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	1.20	9/3412 (0.3%)	1.09	4/4617 (0.1%)
1	B	1.24	4/3403 (0.1%)	1.09	4/4605 (0.1%)
1	C	1.20	3/3403 (0.1%)	1.07	3/4605 (0.1%)
1	D	1.23	8/3412 (0.2%)	1.09	3/4617 (0.1%)
All	All	1.22	24/13630 (0.2%)	1.09	14/18444 (0.1%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	VAL	CA-CB	6.54	1.58	1.53
1	D	270	VAL	C-O	-6.51	1.17	1.24
1	C	26	ASN	CA-C	-6.28	1.44	1.53
1	C	134	VAL	CA-CB	6.14	1.58	1.53
1	A	374	GLN	C-O	-5.94	1.18	1.24
1	D	297	ASP	CA-C	5.81	1.60	1.52
1	A	328	VAL	N-CA	5.59	1.52	1.46
1	A	270	VAL	C-O	-5.44	1.18	1.23
1	D	418	ARG	C-O	-5.37	1.17	1.24
1	A	308	GLU	N-CA	-5.36	1.40	1.46
1	B	374	GLN	C-O	-5.34	1.19	1.24
1	D	398	TYR	C-O	5.33	1.28	1.24
1	A	253	GLU	CA-C	5.32	1.59	1.53
1	B	368	SER	C-O	-5.26	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	GLU	CD-OE1	5.22	1.35	1.25
1	B	263	ASP	C-O	-5.22	1.17	1.23
1	D	275	LEU	CA-C	-5.12	1.48	1.53
1	A	88	ALA	CA-C	-5.11	1.46	1.52
1	A	196	GLU	N-CA	5.10	1.52	1.46
1	C	46	ILE	CA-C	5.10	1.59	1.52
1	B	313	GLU	CD-OE2	5.09	1.35	1.25
1	A	329	GLU	CA-C	5.07	1.59	1.52
1	D	22	LYS	C-O	-5.05	1.17	1.24
1	D	181	GLN	N-CA	5.04	1.52	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	PHE	N-CA-C	10.22	123.38	110.61
1	A	76	GLU	CB-CG-CD	5.86	122.56	112.60
1	D	12	SER	N-CA-C	5.65	117.44	111.28
1	B	420	PHE	N-CA-CB	-5.50	103.94	111.65
1	B	60	ILE	N-CA-C	5.35	116.56	108.96
1	A	107	VAL	CB-CA-C	-5.29	105.20	111.97
1	D	263	ASP	N-CA-C	-5.22	103.56	111.34
1	B	134	VAL	N-CA-CB	5.16	113.75	110.50
1	A	134	VAL	CA-C-N	-5.14	113.34	119.05
1	A	134	VAL	C-N-CA	-5.14	113.34	119.05
1	D	418	ARG	N-CA-C	5.11	116.86	111.28
1	C	35	ASN	N-CA-C	5.08	117.56	111.71
1	C	421	GLU	CA-C-O	-5.04	112.23	120.80
1	C	300	GLU	CA-CB-CG	-5.01	104.07	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	PHE	Peptide

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	3346	0	3353	40	0
1	B	3340	0	3345	24	0
1	C	3340	0	3345	29	0
1	D	3346	0	3351	30	0
2	A	15	0	6	1	0
2	B	15	0	6	0	0
2	C	15	0	6	1	0
2	D	15	0	6	0	0
3	A	24	0	32	0	0
3	B	6	0	8	3	0
3	C	18	0	24	1	0
3	D	12	0	16	0	0
4	A	26	0	10	5	0
4	B	13	0	5	2	0
4	C	39	0	15	2	0
4	D	39	0	15	2	0
5	A	35	0	50	6	0
5	B	21	0	30	0	0
5	C	21	0	30	0	0
6	A	311	0	0	17	0
6	B	331	0	0	15	0
6	C	307	0	0	12	0
6	D	277	0	0	13	0
All	All	14912	0	13653	128	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 5.

All (128) 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:101:MET:HG3	6:A:1481:HOH:O	1.40	1.21
1:D:101:MET:HG3	6:D:860:HOH:O	1.38	1.19
1:C:101:MET:HG3	6:C:894:HOH:O	1.41	1.18
1:A:129:HIS:HE2	4:A:503:CIT:H42	1.28	0.97
1:A:305:GLU:HB3	5:A:511:PEG:H42	1.48	0.92
1:C:58:SER:HB3	6:D:689:HOH:O	1.77	0.83
1:B:316:ASN:HB3	6:B:892:HOH:O	1.82	0.79
1:A:312:GLU:HG3	1:A:339:LYS:HE3	1.65	0.76
1:B:420:PHE:HB3	6:B:703:HOH:O	1.85	0.75
1:C:224:ASP:OD1	3:C:504:GOL:H2	1.87	0.74
1:A:64:VAL:HB	6:B:834:HOH:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:HG22	1:A:313:GLU:OE1	1.88	0.74
4:B:502:CIT:C5	6:B:619:HOH:O	2.35	0.74
1:C:278:ARG:HD3	6:C:801:HOH:O	1.88	0.73
1:B:305:GLU:HG2	6:B:606:HOH:O	1.89	0.72
1:C:219:LYS:HE3	6:C:814:HOH:O	1.88	0.72
1:B:370:HIS:CD2	6:B:613:HOH:O	2.44	0.70
1:A:76:GLU:OE1	6:A:1201:HOH:O	2.08	0.70
4:A:503:CIT:O3	6:A:1202:HOH:O	2.10	0.69
1:A:305:GLU:HB3	5:A:511:PEG:C4	2.22	0.69
1:A:305:GLU:CB	5:A:511:PEG:H42	2.23	0.68
1:C:146:LYS:HD2	6:C:620:HOH:O	1.94	0.67
4:A:503:CIT:O4	4:A:503:CIT:O7	2.12	0.67
1:B:178:ILE:HD13	1:B:194:ILE:HD13	1.78	0.66
1:B:347:LYS:HG2	1:B:386:ILE:HG21	1.79	0.64
1:D:278:ARG:HD2	6:D:695:HOH:O	1.97	0.63
1:D:352:HIS:HB2	6:D:846:HOH:O	1.99	0.62
1:B:278:ARG:HD2	6:B:664:HOH:O	2.00	0.61
1:D:199:LYS:HE2	1:D:199:LYS:HA	1.83	0.60
1:A:251[B]:GLN:HG3	6:A:1210:HOH:O	2.01	0.59
2:A:501:PLP:O2P	4:A:503:CIT:O3	2.20	0.59
1:C:164:LEU:HD12	1:C:164:LEU:O	2.01	0.59
1:A:339:LYS:HE2	6:A:1367:HOH:O	2.02	0.58
1:B:105:PHE:C	1:B:105:PHE:CD1	2.81	0.58
1:C:192:GLU:HG3	6:C:803:HOH:O	2.03	0.57
1:C:237:THR:OG1	1:D:285:HIS:HD2	1.86	0.57
1:C:329:GLU:OE2	6:C:602:HOH:O	2.17	0.57
1:A:219:LYS:HA	1:A:219:LYS:HE2	1.87	0.57
1:D:101:MET:CG	6:D:860:HOH:O	2.17	0.56
1:A:58:SER:HB3	6:B:632:HOH:O	2.04	0.56
5:A:504:PEG:H42	6:A:1241:HOH:O	2.05	0.55
1:A:178:ILE:HD13	1:A:194:ILE:HD13	1.89	0.55
1:A:101:MET:CG	6:A:1481:HOH:O	2.21	0.54
1:B:242:LEU:HD23	1:B:242:LEU:C	2.32	0.54
1:C:219:LYS:CE	6:C:814:HOH:O	2.53	0.54
1:B:105:PHE:C	1:B:105:PHE:HD1	2.16	0.54
1:C:28:LYS:HE3	1:C:361:ASN:O	2.08	0.53
1:A:129:HIS:NE2	4:A:503:CIT:H42	2.11	0.53
1:D:356:HIS:HB2	6:D:855:HOH:O	2.08	0.53
1:A:417:ARG:HG3	6:A:1362:HOH:O	2.09	0.53
1:C:250:GLU:HG2	6:C:839:HOH:O	2.08	0.52
1:D:372:CSS:SG	4:D:505:CIT:H41	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:CG	6:A:1205:HOH:O	2.58	0.51
1:A:11:PHE:CE2	1:A:402:THR:HG22	2.45	0.50
3:B:506:GOL:H32	6:B:836:HOH:O	2.11	0.50
1:D:219:LYS:CE	6:D:764:HOH:O	2.58	0.50
1:B:117:LYS:HB3	6:B:797:HOH:O	2.12	0.50
1:A:134:VAL:HG13	1:B:270:VAL:HG11	1.93	0.50
5:A:509:PEG:C1	6:A:1207:HOH:O	2.59	0.50
1:D:313:GLU:OE1	6:D:601:HOH:O	2.20	0.50
1:D:118:THR:HG23	6:D:669:HOH:O	2.12	0.49
1:A:11:PHE:HE2	1:A:402:THR:HG22	1.77	0.49
1:D:370:HIS:HB2	6:D:666:HOH:O	2.13	0.49
1:C:192:GLU:HB3	6:C:670:HOH:O	2.13	0.49
1:C:105:PHE:CD1	1:C:105:PHE:C	2.90	0.48
1:A:211:VAL:N	1:A:212:PRO:CD	2.77	0.48
1:D:127:VAL:HG12	1:D:376:LEU:HD13	1.95	0.48
1:D:212:PRO:HA	1:D:233:ILE:HD12	1.96	0.48
1:B:178:ILE:HD13	1:B:194:ILE:CD1	2.42	0.48
1:A:105:PHE:C	1:A:105:PHE:CD1	2.92	0.48
1:B:352:HIS:HD2	3:B:506:GOL:O3	1.97	0.47
1:D:219:LYS:HE2	6:D:764:HOH:O	2.14	0.47
1:A:188:GLU:OE2	1:A:213:HIS:HE1	1.98	0.47
1:C:101:MET:CG	6:C:894:HOH:O	2.21	0.47
1:B:347:LYS:HG2	1:B:386:ILE:CG2	2.44	0.47
1:A:8:ASP:HB3	6:A:1269:HOH:O	2.15	0.46
1:D:196:GLU:HA	1:D:199:LYS:HE3	1.96	0.46
1:A:257:TYR:CE1	1:B:138:ARG:HG2	2.50	0.46
1:C:233:ILE:O	1:C:295:THR:HG21	2.16	0.46
1:B:233:ILE:O	1:B:295:THR:HG21	2.16	0.46
1:A:138:ARG:HG2	1:B:257:TYR:CE1	2.50	0.46
1:A:317:TYR:CZ	1:A:321:LYS:HE2	2.51	0.45
1:A:118:THR:HG22	1:A:144:GLY:HA3	1.97	0.45
1:D:417:ARG:HD2	1:D:421:GLU:HG3	1.97	0.45
4:B:502:CIT:H41	6:B:619:HOH:O	2.16	0.45
1:B:166:THR:HG23	6:B:620:HOH:O	2.16	0.45
1:D:305:GLU:H	1:D:305:GLU:CD	2.24	0.45
1:D:334:ILE:HG22	1:D:334:ILE:O	2.17	0.45
1:C:367:ARG:NH1	6:C:601:HOH:O	2.03	0.44
1:D:211:VAL:N	1:D:212:PRO:CD	2.79	0.44
1:A:3:SER:HB2	6:A:1472:HOH:O	2.18	0.44
1:B:309:LYS:HG3	6:B:606:HOH:O	2.17	0.44
1:A:154:GLU:HG2	6:A:1411:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:HIS:NE2	1:D:314:LEU:HD11	2.33	0.44
4:D:504:CIT:O6	4:D:504:CIT:C1	2.62	0.44
1:B:285:HIS:CD2	1:B:288:GLY:H	2.36	0.44
1:C:112:LYS:HD3	6:D:837:HOH:O	2.17	0.44
1:D:215:LYS:HA	1:D:215:LYS:HD2	1.84	0.43
1:B:352:HIS:HD2	3:B:506:GOL:C3	2.31	0.43
1:D:153:ASP:OD1	1:D:153:ASP:C	2.62	0.43
1:A:278:ARG:HD3	6:A:1404:HOH:O	2.18	0.43
1:A:76:GLU:CG	6:A:1201:HOH:O	2.67	0.42
1:A:415:TYR:CD1	1:A:415:TYR:C	2.97	0.42
1:C:161:GLU:OE1	1:C:161:GLU:N	2.43	0.42
1:A:178:ILE:HD13	1:A:194:ILE:CD1	2.49	0.42
1:D:105:PHE:C	1:D:105:PHE:CD1	2.97	0.42
1:D:57:TYR:CD2	1:D:57:TYR:C	2.98	0.42
1:D:358:LEU:HB3	1:D:364:VAL:HB	2.01	0.42
1:B:215:LYS:HG2	6:B:604:HOH:O	2.20	0.42
1:C:394:ARG:HH12	4:C:506:CIT:C5	2.32	0.42
1:D:199:LYS:HE2	1:D:199:LYS:CA	2.50	0.42
1:A:347:LYS:HG2	1:A:386:ILE:HG21	2.02	0.41
1:B:215:LYS:NZ	6:B:622:HOH:O	2.53	0.41
1:D:374:GLN:O	1:D:375:PRO:C	2.60	0.41
1:C:165:LYS:HD3	6:C:875:HOH:O	2.19	0.41
1:C:206:ASP:OD2	2:C:501:PLP:N1	2.53	0.41
1:C:133:LEU:C	1:C:133:LEU:HD23	2.46	0.41
1:C:257:TYR:CE1	1:D:138:ARG:HG2	2.56	0.41
1:A:105:PHE:C	1:A:105:PHE:HD1	2.28	0.41
1:C:61:HIS:ND1	4:C:509:CIT:H22	2.36	0.41
5:A:504:PEG:C4	6:A:1241:HOH:O	2.65	0.41
1:D:112:LYS:HD3	6:D:612:HOH:O	2.20	0.41
1:A:328:VAL:CG1	1:A:344:PHE:HB2	2.51	0.40
1:C:211:VAL:N	1:C:212:PRO:CD	2.84	0.40
1:A:219:LYS:CE	6:A:1293:HOH:O	2.69	0.40
1:A:345:ASN:OD1	1:A:351:PRO:HG3	2.22	0.40
1:C:350:HIS:CG	1:C:351:PRO:HD2	2.57	0.40
1:C:11:PHE:HE2	1:C:402:THR:HG22	1.87	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	420/425 (99%)	404 (96%)	16 (4%)	0	100	100
1	B	419/425 (99%)	405 (97%)	14 (3%)	0	100	100
1	C	419/425 (99%)	403 (96%)	16 (4%)	0	100	100
1	D	420/425 (99%)	405 (96%)	15 (4%)	0	100	100
All	All	1678/1700 (99%)	1617 (96%)	61 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	371/372 (100%)	365 (98%)	6 (2%)	55	64
1	B	370/372 (100%)	364 (98%)	6 (2%)	55	64
1	C	370/372 (100%)	366 (99%)	4 (1%)	65	74
1	D	371/372 (100%)	369 (100%)	2 (0%)	81	88
All	All	1482/1488 (100%)	1464 (99%)	18 (1%)	63	72

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	69	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	GLU
1	A	89	SER
1	A	105	PHE
1	A	300	GLU
1	B	12	SER
1	B	91	GLU
1	B	105	PHE
1	B	169	SER
1	B	226	LEU
1	B	264	LYS
1	C	89	SER
1	C	146	LYS
1	C	164	LEU
1	C	226	LEU
1	D	62	ARG
1	D	165	LYS

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

Mol	Chain	Res	Type
1	A	361	ASN
1	B	77	GLN
1	B	108	ASN
1	B	285	HIS
1	B	316	ASN
1	B	352	HIS
1	B	356	HIS
1	C	16	ASN
1	C	24	ASN
1	C	160	ASN
1	D	209	GLN
1	D	285	HIS
1	D	350	HIS
1	D	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSS	A	372	1	4,6,7	1.17	0	2,6,8	0.57	0
1	CSS	B	372	1	4,6,7	0.89	0	2,6,8	0.98	0
1	CSS	D	372	1	4,6,7	1.10	0	2,6,8	1.07	0
1	CSS	C	372	1	4,6,7	0.82	0	2,6,8	1.47	1 (50%)

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
1	CSS	A	372	1	-	0/1/5/7	-
1	CSS	B	372	1	-	0/1/5/7	-
1	CSS	D	372	1	-	0/1/5/7	-
1	CSS	C	372	1	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	CSS	CB-CA-C	2.07	116.43	110.80

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
1	D	372	CSS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
4	CIT	C	509	-	12,12,12	1.49	2 (16%)	17,17,17	2.40	8 (47%)
3	GOL	A	505	-	5,5,5	0.22	0	5,5,5	0.53	0
2	PLP	C	501	1	15,15,16	2.73	3 (20%)	21,22,23	2.14	6 (28%)
4	CIT	D	505	-	12,12,12	1.16	0	17,17,17	1.66	5 (29%)
2	PLP	B	501	1	15,15,16	3.37	4 (26%)	21,22,23	1.83	4 (19%)
3	GOL	C	503	-	5,5,5	0.72	0	5,5,5	0.95	0
3	GOL	A	502	-	5,5,5	0.57	0	5,5,5	0.83	0
3	GOL	D	502	-	5,5,5	0.40	0	5,5,5	0.51	0
3	GOL	A	510	-	5,5,5	0.49	0	5,5,5	0.63	0
4	CIT	D	506	-	12,12,12	1.37	1 (8%)	17,17,17	2.12	4 (23%)
5	PEG	B	503	-	6,6,6	0.35	0	5,5,5	0.47	0
5	PEG	A	511	-	6,6,6	0.61	0	5,5,5	0.30	0
5	PEG	C	507	-	6,6,6	0.72	0	5,5,5	0.62	0
2	PLP	A	501	1	15,15,16	2.57	4 (26%)	21,22,23	2.03	5 (23%)
3	GOL	C	502	-	5,5,5	0.70	0	5,5,5	1.20	0
5	PEG	A	504	-	6,6,6	0.75	0	5,5,5	0.86	0
3	GOL	C	504	-	5,5,5	0.77	0	5,5,5	0.60	0
4	CIT	B	502	-	12,12,12	1.82	2 (16%)	17,17,17	1.29	2 (11%)
4	CIT	D	504	-	12,12,12	1.22	0	17,17,17	1.60	4 (23%)
5	PEG	C	508	-	6,6,6	0.47	0	5,5,5	0.30	0
3	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.58	0
5	PEG	A	509	-	6,6,6	0.69	0	5,5,5	0.51	0
3	GOL	B	506	-	5,5,5	0.28	0	5,5,5	0.82	0
4	CIT	A	506	-	12,12,12	1.37	1 (8%)	17,17,17	1.64	6 (35%)
5	PEG	A	512	-	6,6,6	0.62	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	C	506	-	12,12,12	2.04	4 (33%)	17,17,17	2.05	5 (29%)
4	CIT	A	503	-	12,12,12	1.09	1 (8%)	17,17,17	2.70	9 (52%)
4	CIT	C	505	-	12,12,12	1.95	3 (25%)	17,17,17	2.29	7 (41%)
3	GOL	D	503	-	5,5,5	0.46	0	5,5,5	0.69	0
5	PEG	B	505	-	6,6,6	0.45	0	5,5,5	0.27	0
5	PEG	B	504	-	6,6,6	0.62	0	5,5,5	0.60	0
5	PEG	C	510	-	6,6,6	0.74	0	5,5,5	0.48	0
5	PEG	A	508	-	6,6,6	0.58	0	5,5,5	0.52	0
2	PLP	D	501	1	15,15,16	2.26	4 (26%)	21,22,23	1.73	5 (23%)

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	CIT	C	509	-	-	5/16/16/16	-
3	GOL	A	505	-	-	2/4/4/4	-
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
4	CIT	D	505	-	-	8/16/16/16	-
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	D	502	-	-	4/4/4/4	-
3	GOL	A	510	-	-	0/4/4/4	-
4	CIT	D	506	-	-	9/16/16/16	-
5	PEG	B	503	-	-	2/4/4/4	-
5	PEG	A	511	-	-	3/4/4/4	-
5	PEG	C	507	-	-	2/4/4/4	-
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
3	GOL	C	502	-	-	4/4/4/4	-
5	PEG	A	504	-	-	3/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
4	CIT	B	502	-	-	6/16/16/16	-
4	CIT	D	504	-	-	7/16/16/16	-
5	PEG	C	508	-	-	3/4/4/4	-
3	GOL	A	507	-	-	2/4/4/4	-
5	PEG	A	509	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	506	-	-	2/4/4/4	-
4	CIT	A	506	-	-	2/16/16/16	-
5	PEG	A	512	-	-	2/4/4/4	-
4	CIT	C	506	-	-	2/16/16/16	-
4	CIT	A	503	-	-	13/16/16/16	-
4	CIT	C	505	-	-	9/16/16/16	-
3	GOL	D	503	-	-	2/4/4/4	-
5	PEG	B	505	-	-	2/4/4/4	-
5	PEG	B	504	-	-	2/4/4/4	-
5	PEG	C	510	-	-	3/4/4/4	-
5	PEG	A	508	-	-	1/4/4/4	-
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLP	C3-C2	9.40	1.50	1.41
2	B	501	PLP	C5-C4	8.49	1.50	1.40
2	B	501	PLP	C3-C2	8.09	1.49	1.41
2	D	501	PLP	C3-C2	6.26	1.47	1.41
2	A	501	PLP	C5-C4	5.83	1.47	1.40
2	A	501	PLP	C3-C2	5.55	1.46	1.41
4	C	506	CIT	C3-C6	4.58	1.58	1.53
4	C	505	CIT	C3-C6	-4.34	1.49	1.53
2	B	501	PLP	C3-C4	3.89	1.47	1.40
4	B	502	CIT	C3-C6	3.77	1.57	1.53
2	D	501	PLP	C3-C4	3.60	1.47	1.40
4	B	502	CIT	O5-C6	3.52	1.33	1.22
2	D	501	PLP	C5-C4	3.50	1.44	1.40
2	A	501	PLP	C3-C4	3.41	1.46	1.40
2	B	501	PLP	C4A-C4	-3.29	1.45	1.51
4	C	509	CIT	C4-C3	3.25	1.58	1.54
4	C	505	CIT	C4-C3	3.11	1.57	1.54
2	A	501	PLP	C4A-C4	-3.06	1.45	1.51
4	D	506	CIT	O7-C3	2.91	1.48	1.43
4	C	506	CIT	O3-C5	2.82	1.31	1.22
2	C	501	PLP	C2-N1	-2.47	1.29	1.33
4	C	506	CIT	C2-C3	2.41	1.56	1.54
2	D	501	PLP	C4A-C4	-2.30	1.47	1.51
4	A	506	CIT	O4-C5	-2.25	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	506	CIT	O5-C6	2.20	1.29	1.22
4	A	503	CIT	C4-C3	-2.19	1.51	1.54
4	C	505	CIT	O7-C3	2.14	1.47	1.43
4	C	509	CIT	C2-C3	2.12	1.56	1.54
2	C	501	PLP	C4A-C4	-2.01	1.47	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLP	O4P-C5A-C5	5.86	120.35	109.36
2	A	501	PLP	O4P-C5A-C5	5.33	119.34	109.36
4	D	506	CIT	O7-C3-C6	5.12	116.22	108.96
4	C	509	CIT	C4-C3-C2	4.64	121.21	109.31
4	C	505	CIT	O2-C1-C2	4.18	127.58	114.35
4	D	504	CIT	O4-C5-C4	4.13	127.44	114.35
2	B	501	PLP	O4P-C5A-C5	4.11	117.06	109.36
4	C	506	CIT	C3-C2-C1	4.05	124.98	113.92
4	A	503	CIT	O3-C5-C4	-4.02	111.56	122.95
4	A	503	CIT	O4-C5-C4	4.00	127.03	114.35
4	A	503	CIT	O7-C3-C6	3.95	114.56	108.96
4	C	509	CIT	O6-C6-C3	3.86	120.54	113.14
4	A	503	CIT	O5-C6-C3	-3.83	114.67	122.09
4	D	506	CIT	C4-C3-C6	-3.83	101.57	110.03
4	A	503	CIT	O6-C6-C3	3.79	120.41	113.14
4	D	506	CIT	O6-C6-C3	3.75	120.34	113.14
4	C	509	CIT	O7-C3-C6	-3.71	103.70	108.96
4	C	505	CIT	C3-C4-C5	3.65	123.89	113.92
4	C	505	CIT	O5-C6-C3	-3.63	115.05	122.09
2	B	501	PLP	C6-N1-C2	3.44	125.43	119.20
4	A	503	CIT	O1-C1-C2	-3.43	113.23	122.95
2	D	501	PLP	O4P-C5A-C5	3.41	115.75	109.36
2	C	501	PLP	C3-C4-C5	-3.38	114.53	118.59
4	A	503	CIT	C3-C2-C1	-3.35	104.77	113.92
4	C	506	CIT	O7-C3-C6	3.19	113.48	108.96
4	A	503	CIT	O7-C3-C4	-3.12	102.26	109.38
4	C	506	CIT	O6-C6-C3	3.09	119.08	113.14
4	C	505	CIT	O7-C3-C4	3.09	116.42	109.38
2	A	501	PLP	C6-C5-C4	-3.00	115.64	118.10
4	C	509	CIT	O4-C5-C4	2.96	123.73	114.35
2	D	501	PLP	C3-C2-N1	-2.93	117.27	120.96
2	A	501	PLP	C3-C2-N1	-2.91	117.29	120.96
4	C	505	CIT	O1-C1-C2	-2.91	114.71	122.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	506	CIT	O7-C3-C2	2.91	116.01	109.38
4	A	506	CIT	C3-C4-C5	2.85	121.73	113.92
4	A	506	CIT	O4-C5-O3	-2.85	116.00	123.33
2	C	501	PLP	O2P-P-O4P	-2.85	99.25	106.67
2	D	501	PLP	C6-C5-C4	-2.80	115.80	118.10
4	C	506	CIT	O7-C3-C4	-2.78	103.04	109.38
4	D	505	CIT	C4-C3-C6	-2.78	103.89	110.03
2	D	501	PLP	O3P-P-O2P	2.71	117.95	107.80
4	B	502	CIT	O4-C5-C4	2.70	122.90	114.35
2	C	501	PLP	C2A-C2-C3	-2.69	117.65	120.80
2	C	501	PLP	C2A-C2-N1	2.69	122.70	117.64
2	A	501	PLP	O3P-P-O4P	-2.69	99.67	106.67
4	D	504	CIT	O3-C5-C4	-2.65	115.45	122.95
4	C	505	CIT	O7-C3-C6	-2.65	105.21	108.96
4	A	503	CIT	O2-C1-C2	2.64	122.70	114.35
4	C	509	CIT	O2-C1-O1	-2.51	116.88	123.33
2	B	501	PLP	O3P-P-O2P	2.47	117.08	107.80
2	D	501	PLP	O2P-P-O4P	-2.43	100.32	106.67
4	C	509	CIT	O2-C1-C2	2.43	122.06	114.35
4	D	504	CIT	O4-C5-O3	-2.42	117.11	123.33
4	B	502	CIT	O3-C5-C4	-2.41	116.12	122.95
4	A	506	CIT	O2-C1-C2	2.37	121.85	114.35
4	D	506	CIT	O3-C5-C4	-2.36	116.25	122.95
4	D	504	CIT	O6-C6-C3	2.33	117.60	113.14
4	C	509	CIT	O4-C5-O3	-2.32	117.36	123.33
4	D	505	CIT	O4-C5-C4	2.28	121.56	114.35
4	A	506	CIT	O6-C6-C3	2.27	117.50	113.14
4	C	505	CIT	O2-C1-O1	-2.21	117.66	123.33
4	D	505	CIT	O2-C1-C2	2.19	121.30	114.35
4	D	505	CIT	O1-C1-C2	-2.17	116.81	122.95
2	A	501	PLP	C6-N1-C2	2.17	123.13	119.20
2	B	501	PLP	O2P-P-O4P	-2.14	101.09	106.67
4	C	509	CIT	O7-C3-C4	-2.12	104.54	109.38
2	C	501	PLP	C5A-C5-C4	-2.11	118.48	122.64
4	A	506	CIT	O4-C5-C4	2.10	121.02	114.35
4	A	506	CIT	O1-C1-C2	-2.10	117.01	122.95
4	D	505	CIT	O5-C6-C3	-2.06	118.11	122.09

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	GOL	O1-C1-C2-C3
3	A	507	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	C	504	GOL	C1-C2-C3-O3
3	D	502	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
4	A	503	CIT	O7-C3-C4-C5
4	A	503	CIT	C6-C3-C4-C5
4	A	503	CIT	C2-C3-C6-O5
4	A	503	CIT	C2-C3-C6-O6
4	A	503	CIT	O7-C3-C6-O5
4	A	503	CIT	O7-C3-C6-O6
4	B	502	CIT	O7-C3-C6-O5
4	B	502	CIT	O7-C3-C6-O6
4	B	502	CIT	C4-C3-C6-O5
4	B	502	CIT	C4-C3-C6-O6
4	D	504	CIT	C2-C3-C6-O5
4	D	504	CIT	C2-C3-C6-O6
4	D	504	CIT	O7-C3-C6-O5
4	D	504	CIT	O7-C3-C6-O6
5	A	511	PEG	O2-C3-C4-O4
5	B	505	PEG	O2-C3-C4-O4
4	A	503	CIT	C2-C3-C4-C5
4	C	505	CIT	C1-C2-C3-C4
4	C	505	CIT	C1-C2-C3-C6
5	C	507	PEG	O2-C3-C4-O4
4	C	505	CIT	C1-C2-C3-O7
4	D	505	CIT	C2-C3-C4-C5
3	B	506	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	D	502	GOL	O1-C1-C2-C3
5	A	508	PEG	O1-C1-C2-O2
5	C	508	PEG	O2-C3-C4-O4
3	A	505	GOL	O1-C1-C2-O2
3	A	507	GOL	O2-C2-C3-O3
3	B	506	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	C	503	GOL	O2-C2-C3-O3
3	C	504	GOL	O2-C2-C3-O3
3	D	502	GOL	O2-C2-C3-O3
3	D	503	GOL	O1-C1-C2-O2
5	A	504	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	503	CIT	C1-C2-C3-C6
4	C	509	CIT	C1-C2-C3-C6
4	D	505	CIT	C1-C2-C3-O7
4	D	505	CIT	C1-C2-C3-C6
5	A	504	PEG	O2-C3-C4-O4
5	B	503	PEG	O2-C3-C4-O4
4	D	504	CIT	C3-C4-C5-O3
5	B	504	PEG	O2-C3-C4-O4
4	D	504	CIT	C3-C4-C5-O4
3	D	502	GOL	O1-C1-C2-O2
4	D	506	CIT	C3-C4-C5-O3
4	D	506	CIT	C3-C4-C5-O4
4	A	503	CIT	C1-C2-C3-C4
4	D	505	CIT	C1-C2-C3-C4
3	C	502	GOL	O2-C2-C3-O3
4	C	506	CIT	C2-C3-C4-C5
5	C	510	PEG	C4-C3-O2-C2
5	A	511	PEG	C4-C3-O2-C2
5	A	504	PEG	C1-C2-O2-C3
5	C	508	PEG	O1-C1-C2-O2
4	C	509	CIT	C4-C3-C6-O6
4	D	506	CIT	C1-C2-C3-C6
5	A	512	PEG	O2-C3-C4-O4
5	A	509	PEG	C1-C2-O2-C3
5	C	508	PEG	C4-C3-O2-C2
4	C	509	CIT	O7-C3-C4-C5
4	D	504	CIT	O7-C3-C4-C5
4	D	505	CIT	O7-C3-C4-C5
4	D	505	CIT	C6-C3-C4-C5
5	A	509	PEG	O1-C1-C2-O2
5	B	503	PEG	C4-C3-O2-C2
4	A	503	CIT	C3-C4-C5-O3
4	A	503	CIT	C3-C4-C5-O4
5	A	512	PEG	O1-C1-C2-O2
4	B	502	CIT	C2-C3-C6-O5
4	B	502	CIT	C2-C3-C6-O6
4	C	505	CIT	C2-C3-C6-O6
4	C	505	CIT	C4-C3-C6-O6
4	C	509	CIT	C4-C3-C6-O5
4	D	506	CIT	C2-C3-C6-O5
4	D	506	CIT	C2-C3-C6-O6
4	D	506	CIT	C4-C3-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	503	CIT	C1-C2-C3-O7
5	C	510	PEG	O1-C1-C2-O2
4	C	505	CIT	C2-C3-C6-O5
4	D	506	CIT	C4-C3-C6-O5
4	A	506	CIT	O2-C1-C2-C3
4	D	505	CIT	O2-C1-C2-C3
5	C	507	PEG	C1-C2-O2-C3
5	B	505	PEG	C1-C2-O2-C3
4	A	506	CIT	O1-C1-C2-C3
4	D	505	CIT	O1-C1-C2-C3
5	B	504	PEG	C4-C3-O2-C2
4	D	506	CIT	O1-C1-C2-C3
4	C	505	CIT	C4-C3-C6-O5
5	A	511	PEG	O1-C1-C2-O2
4	D	506	CIT	O2-C1-C2-C3
5	C	510	PEG	O2-C3-C4-O4
4	C	506	CIT	C1-C2-C3-C4
4	C	509	CIT	C1-C2-C3-C4
4	C	505	CIT	O1-C1-C2-C3
4	C	505	CIT	O2-C1-C2-C3
4	A	503	CIT	O2-C1-C2-C3

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	509	CIT	1	0
2	C	501	PLP	1	0
4	D	505	CIT	1	0
5	A	511	PEG	3	0
2	A	501	PLP	1	0
5	A	504	PEG	2	0
3	C	504	GOL	1	0
4	B	502	CIT	2	0
4	D	504	CIT	1	0
5	A	509	PEG	1	0
3	B	506	GOL	3	0
4	C	506	CIT	1	0
4	A	503	CIT	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	421/425 (99%)	-0.39	3 (0%) 84 86	12, 24, 47, 85	1 (0%)
1	B	421/425 (99%)	-0.55	2 (0%) 87 88	12, 21, 40, 82	0
1	C	421/425 (99%)	-0.51	1 (0%) 91 92	15, 23, 41, 82	0
1	D	421/425 (99%)	-0.28	0 100 100	14, 27, 48, 76	1 (0%)
All	All	1684/1700 (99%)	-0.43	6 (0%) 88 90	12, 23, 44, 85	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	HIS	3.8
1	B	420	PHE	3.0
1	A	421	GLU	2.8
1	A	0	HIS	2.6
1	B	0	HIS	2.5
1	A	1	MET	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSS	A	372	7/8	0.96	0.07	21,22,33,36	0
1	CSS	B	372	7/8	0.97	0.06	15,19,26,29	0
1	CSS	C	372	7/8	0.98	0.05	17,20,27,28	0
1	CSS	D	372	7/8	0.98	0.06	22,26,29,34	0

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
5	PEG	A	512	7/7	0.65	0.17	47,62,77,77	0
5	PEG	C	508	7/7	0.65	0.20	86,87,96,96	0
5	PEG	C	507	7/7	0.66	0.20	65,70,82,87	0
5	PEG	A	504	7/7	0.71	0.21	55,68,71,77	0
5	PEG	A	508	7/7	0.72	0.18	68,71,75,77	0
3	GOL	C	504	6/6	0.73	0.17	60,64,67,69	0
5	PEG	A	511	7/7	0.77	0.21	58,71,82,83	0
5	PEG	B	504	7/7	0.77	0.18	49,76,86,88	0
4	CIT	D	506	13/13	0.78	0.14	44,65,83,92	0
4	CIT	C	509	13/13	0.82	0.13	34,60,74,75	0
5	PEG	C	510	7/7	0.82	0.14	48,57,63,64	0
4	CIT	C	506	13/13	0.83	0.15	36,54,61,62	0
5	PEG	A	509	7/7	0.83	0.16	61,67,73,74	0
4	CIT	C	505	13/13	0.84	0.12	35,50,73,82	0
5	PEG	B	505	7/7	0.85	0.15	75,77,89,91	0
3	GOL	C	503	6/6	0.85	0.15	60,60,63,66	0
5	PEG	B	503	7/7	0.85	0.11	55,57,62,68	0
3	GOL	A	507	6/6	0.85	0.13	65,68,69,77	0
3	GOL	A	505	6/6	0.86	0.14	64,65,69,69	0
4	CIT	A	506	13/13	0.87	0.10	40,53,79,86	0
3	GOL	D	502	6/6	0.87	0.11	56,68,70,71	0
3	GOL	A	510	6/6	0.88	0.13	49,57,60,61	0
3	GOL	D	503	6/6	0.88	0.15	27,49,52,59	0
3	GOL	B	506	6/6	0.88	0.11	36,52,54,58	0
4	CIT	D	504	13/13	0.88	0.13	38,65,82,89	0
4	CIT	B	502	13/13	0.89	0.12	29,50,54,54	0
4	CIT	D	505	13/13	0.89	0.14	35,59,72,75	0
4	CIT	A	503	13/13	0.91	0.10	27,49,66,69	0
3	GOL	C	502	6/6	0.92	0.15	29,50,50,55	0
3	GOL	A	502	6/6	0.93	0.15	26,49,56,56	0
2	PLP	C	501	15/16	0.97	0.06	17,20,23,24	0
2	PLP	A	501	15/16	0.98	0.05	17,19,22,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	D	501	15/16	0.98	0.05	19,22,26,30	0
2	PLP	B	501	15/16	0.99	0.04	15,17,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.