



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:29 PM EDT

PDB ID : 1A2Z  
Title : PYRROLIDONE CARBOXYL PEPTIDASE FROM THERMOCOCCUS LITORALIS  
Authors : Singleton, M.R.; Isupov, M.N.; Littlechild, J.A.  
Deposited on : 1998-01-13  
Resolution : 1.73 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

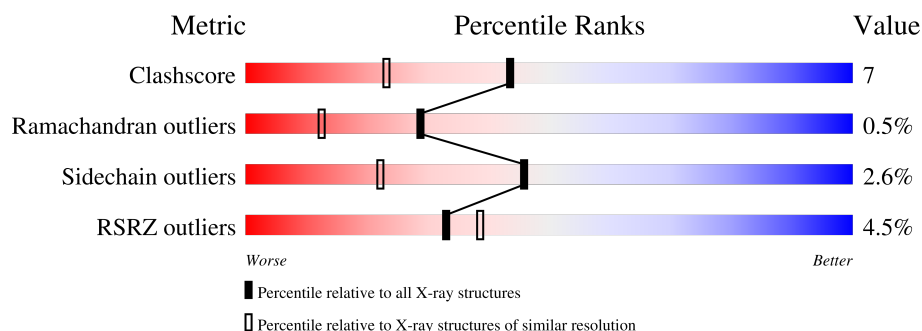
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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  $\geq 3$ , 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	220	
1	B	220	
1	C	220	
1	D	220	

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
2	SO4	C	623	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7666 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 PYRROLIDONE CARBOXYL PEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1746	1130	284	324	8			
1	B	220	Total	C	N	O	S	0	2	0
			1746	1130	284	324	8			
1	C	220	Total	C	N	O	S	0	3	0
			1747	1130	284	325	8			
1	D	220	Total	C	N	O	S	0	3	0
			1747	1130	284	325	8			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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

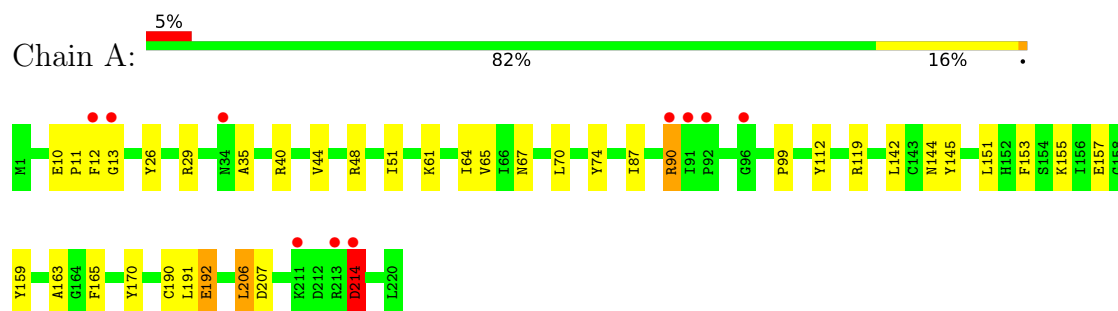
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	152	Total	O	0	0
			152	152		
3	C	172	Total	O	0	0
			172	172		
3	D	165	Total	O	0	0
			165	165		

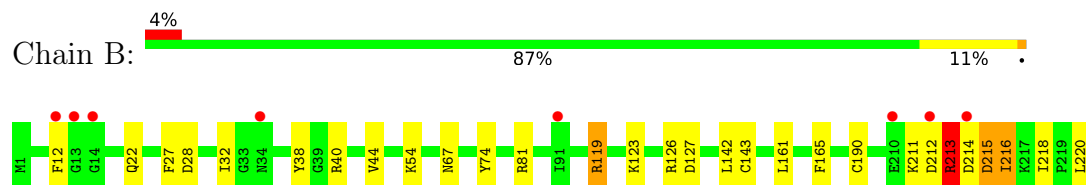
### 3 Residue-property plots [i](#)

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.

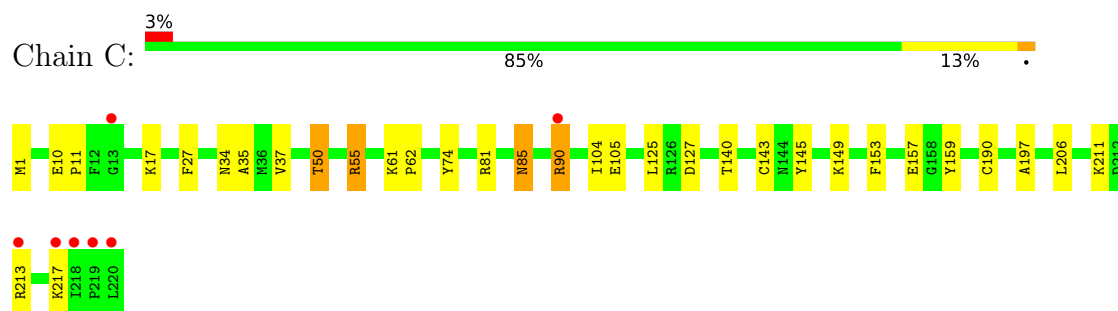
#### • Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE



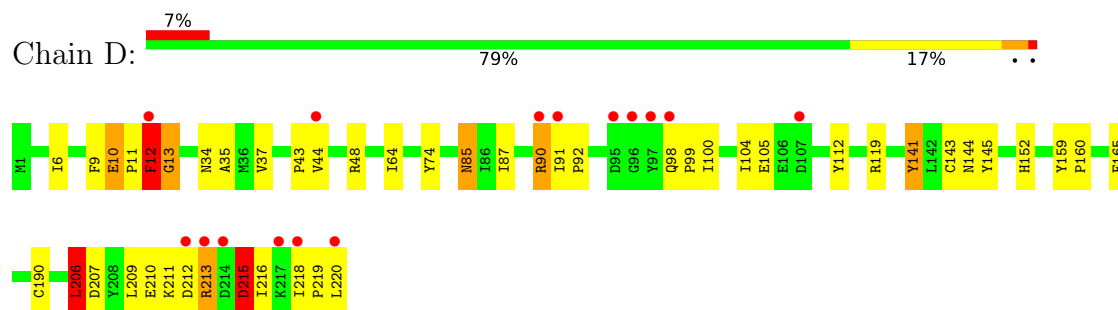
#### • Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.64Å 147.01Å 71.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.73 19.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-1.73) 97.4 (19.74-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.220 0.172 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.67	0/1792	1.43	14/2429 (0.6%)
1	B	0.65	0/1792	1.37	16/2429 (0.7%)
1	C	0.70	0/1798	1.31	7/2437 (0.3%)
1	D	0.68	0/1798	1.34	14/2437 (0.6%)
All	All	0.67	0/7180	1.36	51/9732 (0.5%)

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	D	0	1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	NE-CZ-NH1	12.33	126.46	120.30
1	A	29	ARG	CD-NE-CZ	10.56	138.38	123.60
1	B	38	TYR	CB-CG-CD2	-10.51	114.69	121.00
1	A	119	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	C	90	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	48	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	D	48	ARG	CD-NE-CZ	9.13	136.39	123.60
1	B	213	ARG	CD-NE-CZ	9.05	136.27	123.60
1	D	74	TYR	CB-CG-CD2	-8.86	115.69	121.00
1	A	214	ASP	CB-CG-OD1	8.42	125.88	118.30
1	C	90	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	26	TYR	CB-CG-CD1	-8.01	116.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	145	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	D	206	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	40	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	38	TYR	CB-CG-CD1	7.10	125.26	121.00
1	D	74	TYR	CB-CG-CD1	6.97	125.18	121.00
1	D	141	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	B	119	ARG	CD-NE-CZ	6.80	133.12	123.60
1	A	112	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	A	119	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	D	12	PHE	CB-CA-C	-6.60	97.20	110.40
1	C	90	ARG	CD-NE-CZ	6.60	132.84	123.60
1	B	213	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	190[A]	CYS	CA-CB-SG	6.41	125.54	114.00
1	B	190[B]	CYS	CA-CB-SG	6.41	125.54	114.00
1	A	119	ARG	CG-CD-NE	-6.40	98.36	111.80
1	D	48	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	40	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	10	GLU	OE1-CD-OE2	6.25	130.79	123.30
1	A	192	GLU	CB-CG-CD	6.24	131.04	114.20
1	A	74	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	B	28	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	48	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	145	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	170	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	C	145	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	74	TYR	CB-CG-CD1	5.66	124.39	121.00
1	D	141	TYR	N-CA-CB	-5.63	100.46	110.60
1	B	119	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	81	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	29	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	126	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	D	215	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	C	74	TYR	CB-CG-CD1	5.21	124.12	121.00
1	D	12	PHE	CA-CB-CG	5.16	126.29	113.90
1	C	127	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	81	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	13	GLY	N-CA-C	5.06	125.74	113.10
1	B	74	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	12	PHE	Mainchain

## 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	1746	0	1803	21	0
1	B	1746	0	1803	16	0
1	C	1747	0	1804	25	0
1	D	1747	0	1804	35	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	171	0	0	2	0
3	B	152	0	0	0	0
3	C	172	0	0	2	0
3	D	165	0	0	1	0
All	All	7666	0	7214	94	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 (94) 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:D:10:GLU:HG3	1:D:44:VAL:HG23	1.44	0.96
1:A:64:ILE:HD12	1:A:206:LEU:HD22	1.47	0.95
1:C:85:ASN:HD21	1:C:105:GLU:H	1.13	0.90
1:D:85:ASN:HD21	1:D:105:GLU:H	1.16	0.90
1:A:190[B]:CYS:HG	1:C:190[B]:CYS:HG	0.87	0.82
1:D:211:LYS:HD3	1:D:213:ARG:HH21	1.50	0.76
1:A:214:ASP:HB3	3:A:757:HOH:O	1.88	0.73
1:B:213:ARG:HH22	1:B:216:ILE:HD12	1.60	0.66
1:C:90:ARG:HH12	1:C:140:THR:H	1.43	0.66
1:B:44:VAL:HG13	1:B:142:LEU:HD12	1.76	0.66
1:C:55:ARG:HB3	1:C:55:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ALA:HB2	1:D:206:LEU:HD11	1.78	0.64
1:C:35:ALA:HB2	1:C:206:LEU:HD21	1.81	0.61
1:D:85:ASN:ND2	1:D:105:GLU:H	1.94	0.61
1:D:216:ILE:HB	1:D:218:ILE:HD12	1.83	0.61
1:C:50:THR:HG23	1:C:149:LYS:HD2	1.84	0.60
1:D:9:PHE:HB3	1:D:12:PHE:HE1	1.65	0.60
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.68	0.59
1:D:85:ASN:ND2	1:D:104:ILE:H	2.01	0.58
1:D:90:ARG:HB2	1:D:91:ILE:HD12	1.86	0.58
1:A:64:ILE:CD1	1:A:206:LEU:HD22	2.28	0.58
1:C:27:PHE:HB3	1:C:37:VAL:HG11	1.86	0.57
1:D:10:GLU:CG	1:D:44:VAL:HG23	2.27	0.57
1:D:119:ARG:HD3	1:D:218:ILE:O	2.05	0.57
1:D:64:ILE:HD12	1:D:206:LEU:HD13	1.87	0.55
1:D:206:LEU:O	1:D:210:GLU:HG2	2.07	0.55
1:A:10:GLU:HB3	1:A:11:PRO:HD2	1.89	0.55
1:A:12:PHE:HE1	1:A:70:LEU:HD23	1.72	0.55
1:A:12:PHE:CE1	1:A:70:LEU:HD23	2.42	0.55
1:D:85:ASN:HD22	1:D:104:ILE:H	1.55	0.55
1:D:112:TYR:OH	1:D:152:HIS:HD2	1.90	0.55
1:B:123:LYS:HD2	1:B:218:ILE:CD1	2.37	0.54
1:C:85:ASN:ND2	1:C:104:ILE:H	2.06	0.53
1:C:17:LYS:HE3	3:C:685:HOH:O	2.10	0.52
1:D:34:ASN:ND2	2:D:624:SO4:O2	2.40	0.52
1:D:119:ARG:HG3	1:D:220:LEU:CD1	2.40	0.51
1:A:35:ALA:HB2	1:A:206:LEU:HD21	1.91	0.51
1:A:44:VAL:HG13	1:A:142:LEU:HD12	1.92	0.51
1:B:119:ARG:HD3	1:B:216:ILE:O	2.11	0.51
1:B:12:PHE:HB2	1:B:44:VAL:HG21	1.93	0.50
1:B:123:LYS:HD2	1:B:218:ILE:HD13	1.94	0.50
1:D:10:GLU:HB2	1:D:11:PRO:CD	2.42	0.50
1:A:51:ILE:HD13	3:A:788:HOH:O	2.12	0.49
1:C:1:MET:N	2:C:623:SO4:O3	2.45	0.49
1:C:125:LEU:CD2	1:C:197:ALA:HA	2.43	0.48
1:A:10:GLU:HB3	1:A:11:PRO:CD	2.44	0.48
1:C:85:ASN:ND2	1:C:105:GLU:H	1.96	0.47
1:D:10:GLU:HG2	1:D:43:PRO:HA	1.97	0.47
1:B:213:ARG:HG2	1:B:213:ARG:NH1	2.31	0.46
1:C:143:CYS:SG	3:C:690:HOH:O	2.61	0.46
1:D:211:LYS:HD3	1:D:213:ARG:NH2	2.25	0.46
1:A:12:PHE:HB3	1:A:44:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HA	1:A:159:TYR:CE2	2.51	0.45
1:B:27:PHE:CE1	1:B:32:ILE:HD11	2.51	0.45
1:C:90:ARG:NH1	1:C:140:THR:H	2.12	0.45
1:A:44:VAL:HA	1:A:142:LEU:CD1	2.46	0.45
1:C:61:LYS:HA	1:C:159:TYR:CE2	2.51	0.45
1:A:90:ARG:HD2	1:B:220:LEU:OXT	2.17	0.45
1:B:211:LYS:O	1:B:212:ASP:C	2.55	0.45
1:B:143:CYS:HB3	1:B:165:PHE:CZ	2.52	0.45
1:C:153:PHE:CZ	1:C:157:GLU:HG3	2.52	0.45
1:D:10:GLU:HG3	1:D:44:VAL:CG2	2.31	0.44
1:C:211:LYS:HB2	1:C:213:ARG:HG3	1.98	0.44
1:D:92:PRO:HB3	1:D:98:GLN:HB2	2.00	0.44
1:C:85:ASN:ND2	1:C:104:ILE:HB	2.32	0.44
1:D:85:ASN:ND2	1:D:104:ILE:N	2.65	0.44
1:B:214:ASP:O	1:B:215:ASP:C	2.56	0.43
1:C:217:LYS:O	1:D:100:ILE:HG21	2.18	0.43
1:C:85:ASN:HD22	1:C:104:ILE:H	1.66	0.43
1:A:87:ILE:HG12	1:A:99:PRO:HG2	2.01	0.43
1:D:12:PHE:CD2	1:D:141:TYR:HE2	2.36	0.43
1:D:87:ILE:HG12	1:D:99:PRO:HG2	1.99	0.43
1:A:151:LEU:O	1:A:155:LYS:HG2	2.18	0.43
1:B:27:PHE:CD1	1:B:32:ILE:HD11	2.54	0.43
1:D:215:ASP:N	3:D:669:HOH:O	2.52	0.42
1:C:35:ALA:HB3	1:C:206:LEU:HD11	2.01	0.42
1:D:207:ASP:O	1:D:211:LYS:HD2	2.19	0.41
1:B:12:PHE:CD1	1:B:44:VAL:HG11	2.56	0.41
1:C:61:LYS:N	1:C:62:PRO:CD	2.84	0.41
1:D:159:TYR:HA	1:D:160:PRO:C	2.40	0.41
1:D:218:ILE:HG22	1:D:219:PRO:O	2.20	0.41
1:D:211:LYS:O	1:D:212:ASP:C	2.57	0.41
1:A:153:PHE:CZ	1:A:157:GLU:HG3	2.55	0.41
1:B:67:ASN:HB2	1:B:165:PHE:CD2	2.56	0.41
1:C:10:GLU:HB2	1:C:11:PRO:CD	2.51	0.41
1:C:125:LEU:HD21	1:C:197:ALA:HA	2.02	0.41
1:A:67:ASN:O	1:A:165:PHE:HA	2.22	0.40
1:A:65:VAL:O	1:A:163:ALA:HA	2.22	0.40
1:D:6:ILE:HD12	1:D:37:VAL:HG11	2.03	0.40
1:D:143:CYS:HB3	1:D:165:PHE:CZ	2.56	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	220/220 (100%)	212 (96%)	7 (3%)	1 (0%)	29	12
1	B	220/220 (100%)	215 (98%)	4 (2%)	1 (0%)	29	12
1	C	221/220 (100%)	217 (98%)	4 (2%)	0	100	100
1	D	221/220 (100%)	210 (95%)	9 (4%)	2 (1%)	17	5
All	All	882/880 (100%)	854 (97%)	24 (3%)	4 (0%)	29	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLY
1	B	215	ASP
1	D	13	GLY
1	D	215	ASP

### 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	194/192 (101%)	188 (97%)	6 (3%)	40	16
1	B	194/192 (101%)	189 (97%)	5 (3%)	46	22
1	C	195/192 (102%)	191 (98%)	4 (2%)	53	30
1	D	195/192 (102%)	190 (97%)	5 (3%)	46	22
All	All	778/768 (101%)	758 (97%)	20 (3%)	46	22

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	191	LEU
1	A	192	GLU
1	A	206	LEU
1	A	207	ASP
1	A	214	ASP
1	B	22	GLN
1	B	54	LYS
1	B	161	LEU
1	B	213	ARG
1	B	216	ILE
1	C	34	ASN
1	C	50	THR
1	C	55	ARG
1	C	85	ASN
1	D	85	ASN
1	D	90	ARG
1	D	206	LEU
1	D	209	LEU
1	D	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	67	ASN
1	A	144	ASN
1	A	185	ASN
1	B	22	GLN
1	B	34	ASN
1	B	67	ASN
1	C	34	ASN
1	C	67	ASN
1	C	85	ASN
1	D	67	ASN
1	D	85	ASN
1	D	94	ASN
1	D	144	ASN
1	D	152	HIS
1	D	185	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
2	SO4	B	622	-	4,4,4	0.63	0	6,6,6	0.10	0
2	SO4	C	623	-	4,4,4	0.61	0	6,6,6	0.15	0
2	SO4	A	621	-	4,4,4	0.62	0	6,6,6	0.15	0
2	SO4	D	624	-	4,4,4	0.61	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	623	SO4	1	0
2	D	624	SO4	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/220 (100%)	-0.15	10 (4%) 33 38	10, 17, 39, 61	0
1	B	220/220 (100%)	-0.16	8 (3%) 42 48	11, 17, 38, 49	0
1	C	220/220 (100%)	-0.24	7 (3%) 47 53	11, 18, 34, 52	0
1	D	220/220 (100%)	-0.01	15 (6%) 17 21	11, 17, 45, 69	0
All	All	880/880 (100%)	-0.14	40 (4%) 33 38	10, 17, 40, 69	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	ILE	5.4
1	D	214	ASP	5.3
1	D	91	ILE	5.1
1	A	214	ASP	4.9
1	A	13	GLY	4.9
1	D	220	LEU	4.5
1	A	91	ILE	4.4
1	D	96	GLY	4.4
1	B	14	GLY	4.3
1	D	213	ARG	4.3
1	B	214	ASP	4.3
1	A	12	PHE	4.2
1	B	12	PHE	4.0
1	A	96	GLY	3.9
1	B	212	ASP	3.6
1	D	90	ARG	3.5
1	C	13	GLY	3.4
1	A	213	ARG	3.0
1	B	13	GLY	2.8
1	A	92	PRO	2.8
1	B	34	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	90	ARG	2.7
1	C	218	ILE	2.7
1	C	220	LEU	2.7
1	D	212	ASP	2.7
1	D	107	ASP	2.6
1	C	217	LYS	2.5
1	D	217	LYS	2.5
1	C	213	ARG	2.4
1	D	12	PHE	2.4
1	B	91	ILE	2.4
1	C	90	ARG	2.4
1	D	44	VAL	2.3
1	D	98	GLN	2.3
1	D	97	TYR	2.3
1	A	211	LYS	2.3
1	B	210	GLU	2.3
1	A	34	ASN	2.2
1	D	95	ASP	2.1
1	C	219	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	C	623	5/5	0.31	0.75	154,154,155,155	0
2	SO4	A	621	5/5	0.75	0.24	101,102,102,103	0
2	SO4	B	622	5/5	0.86	0.41	105,106,106,107	0
2	SO4	D	624	5/5	0.86	0.25	71,71,75,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.