



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2022 – 04:03 PM EST

PDB ID : 8D4V
Title : Crystal Structure of Cathepsin G Inhibited by Eap2 from *S. aureus*
Authors : Gido, C.D.; Herdendorf, T.J.; Geisbrecht, B.V.
Deposited on : 2022-06-02
Resolution : 1.85 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

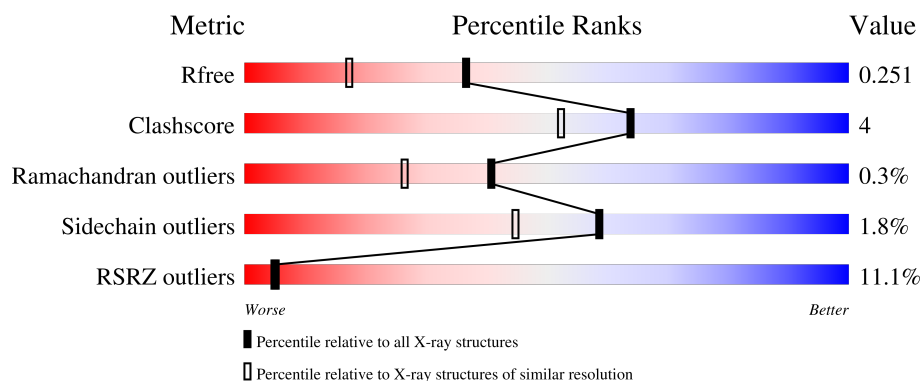
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	223	<div> <div>11%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	223	<div> <div>9%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	100	<div> <div>14%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
2	D	100	<div> <div>12%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5312 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 Cathepsin G, C-terminal truncated form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			
1	C	223	Total	C	N	O	S	0	0	0
			1780	1093	369	308	10			

- Molecule 2 is a protein called Extracellular Adherence Protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	0	0	0
			756	474	131	151			
2	D	98	Total	C	N	O	0	0	0
			762	477	132	153			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	GLY	-	expression tag	UNP Q99QS1
B	156	SER	-	expression tag	UNP Q99QS1
B	157	THR	-	expression tag	UNP Q99QS1
D	155	GLY	-	expression tag	UNP Q99QS1
D	156	SER	-	expression tag	UNP Q99QS1
D	157	THR	-	expression tag	UNP Q99QS1

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

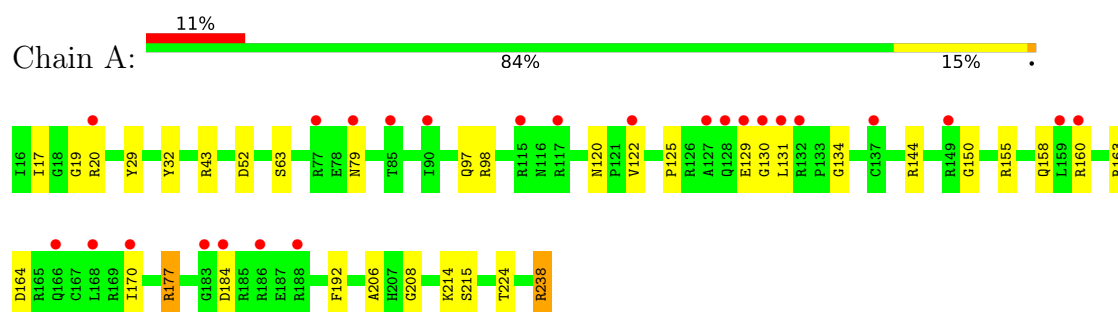
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	C	90	Total	O	0	0
			90	90		
4	B	30	Total	O	0	0
			30	30		
4	D	28	Total	O	0	0
			28	28		

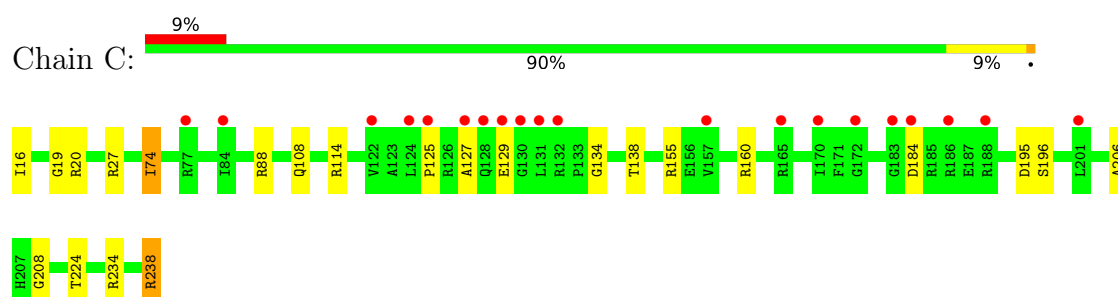
3 Residue-property plots [i](#)

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.

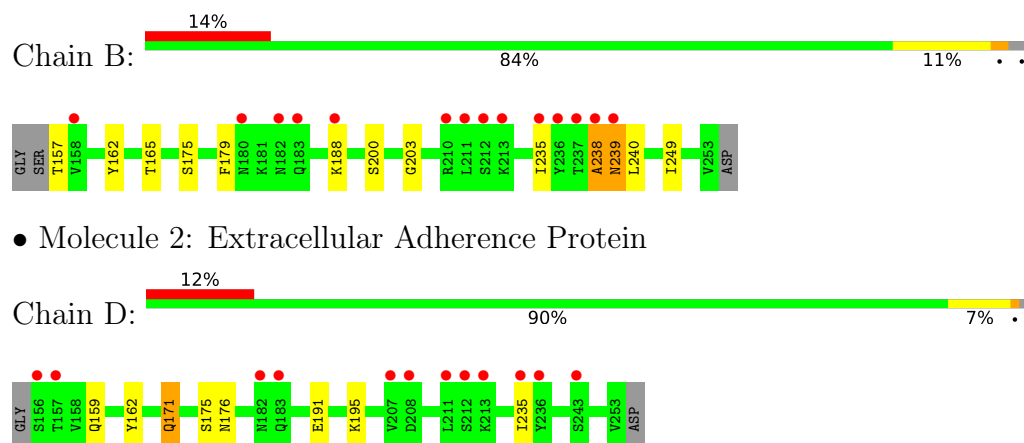
- Molecule 1: Cathepsin G, C-terminal truncated form



- Molecule 1: Cathepsin G, C-terminal truncated form



- Molecule 2: Extracellular Adherence Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.56Å 80.27Å 99.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.24 – 1.85 37.24 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.0 (37.24-1.85) 92.2 (37.24-1.85)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.9.2	Depositor
R, R_{free}	0.207 , 0.251 0.206 , 0.251	Depositor DCC
R_{free} test set	2014 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5312	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1655e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.36	0/1814	0.57	0/2447
1	C	0.37	0/1814	0.58	0/2447
2	B	0.37	0/762	0.56	0/1029
2	D	0.35	0/768	0.54	0/1037
All	All	0.36	0/5158	0.57	0/6960

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1780	0	1793	20	4
1	C	1780	0	1793	13	0
2	B	756	0	788	8	4
2	D	762	0	793	5	0
3	A	5	0	0	0	0
3	C	5	0	0	1	0
4	A	76	0	0	3	0
4	B	30	0	0	1	0
4	C	90	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	0	1	0
All	All	5312	0	5167	43	4

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 4.

All (43) 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:129:GLU:HG3	1:A:130:GLY:O	1.98	0.63
2:B:157:THR:N	2:B:179:PHE:O	2.34	0.60
1:A:98:ARG:NH1	2:B:203:GLY:O	2.37	0.58
2:D:171:GLN:HG2	4:D:311:HOH:O	2.03	0.58
1:C:127:ALA:HB2	4:C:482:HOH:O	2.03	0.56
2:D:235:ILE:H	2:D:235:ILE:HD12	1.72	0.55
2:B:188:LYS:NZ	4:B:301:HOH:O	2.41	0.54
1:A:32:TYR:OH	1:A:43:ARG:NE	2.44	0.50
1:C:19:GLY:O	1:C:155:ARG:NH2	2.45	0.48
1:C:114:ARG:NE	4:C:402:HOH:O	2.22	0.48
1:A:134:GLY:HA2	1:A:160:ARG:NE	2.29	0.46
1:A:215:SER:HB3	2:B:165:THR:OG1	2.16	0.46
1:C:129:GLU:O	4:C:401:HOH:O	2.21	0.45
1:C:16:ILE:N	1:C:195:ASP:OD2	2.49	0.45
1:A:238:ARG:NH1	3:C:301:SO4:O4	2.33	0.45
1:A:163:ARG:NH1	1:A:164:ASP:HB2	2.32	0.45
2:B:239:ASN:HD22	2:B:240:LEU:H	1.65	0.44
1:A:63:SER:OG	4:A:401:HOH:O	2.21	0.44
1:C:88:ARG:NH1	1:C:108:GLN:OE1	2.47	0.43
1:C:208:GLY:HA2	1:C:224:THR:O	2.19	0.43
1:C:74:ILE:H	1:C:74:ILE:HG13	1.67	0.42
1:A:52:ASP:N	1:A:52:ASP:OD1	2.52	0.42
1:C:234:ARG:O	1:C:238:ARG:HB3	2.19	0.42
1:A:79:ASN:OD1	4:A:402:HOH:O	2.22	0.42
2:B:162:TYR:CZ	2:B:175:SER:HB3	2.55	0.42
1:A:97:GLN:NE2	2:B:200:SER:O	2.53	0.41
2:B:162:TYR:HA	2:B:249:ILE:O	2.20	0.41
2:D:191:GLU:HG2	2:D:195:LYS:HE3	2.03	0.41
1:A:144:ARG:HA	1:A:150:GLY:HA2	2.02	0.41
1:C:134:GLY:HA2	1:C:160:ARG:CZ	2.50	0.41
1:A:131:LEU:HA	1:A:131:LEU:HD12	1.78	0.41
1:A:170:ILE:CG2	1:A:214:LYS:HE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PRO:HD3	1:C:206:ALA:O	2.21	0.41
1:A:125:PRO:HD3	1:A:206:ALA:O	2.20	0.41
1:C:27:ARG:NH2	1:C:138:THR:HG21	2.36	0.41
1:A:17:ILE:HG13	1:A:192:PHE:HB2	2.02	0.40
1:A:19:GLY:O	1:A:155:ARG:NH2	2.54	0.40
1:A:177:ARG:NH2	4:A:404:HOH:O	2.42	0.40
1:A:208:GLY:HA2	1:A:224:THR:O	2.21	0.40
1:C:19:GLY:O	1:C:20:ARG:HD2	2.21	0.40
2:D:162:TYR:CZ	2:D:175:SER:HB3	2.56	0.40
2:D:159:GLN:HB3	2:D:176:ASN:HB3	2.04	0.40
1:A:29:TYR:CG	1:A:122:VAL:HB	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLN:NE2	2:B:239:ASN:ND2[4_654]	1.17	1.03
1:A:158:GLN:CD	2:B:239:ASN:ND2[4_654]	1.66	0.54
1:A:20:ARG:NH2	2:B:238:ALA:N[4_654]	1.90	0.30
1:A:20:ARG:NE	2:B:238:ALA:CB[4_654]	2.11	0.09

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	221/223 (99%)	216 (98%)	5 (2%)	0	100	100
1	C	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
2	B	95/100 (95%)	91 (96%)	2 (2%)	2 (2%)	7	1
2	D	96/100 (96%)	93 (97%)	3 (3%)	0	100	100
All	All	633/646 (98%)	613 (97%)	18 (3%)	2 (0%)	41	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	238	ALA
2	B	235	ILE

5.3.2 Protein sidechains [i](#)

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	190/190 (100%)	186 (98%)	4 (2%)	53	38
1	C	190/190 (100%)	186 (98%)	4 (2%)	53	38
2	B	90/92 (98%)	89 (99%)	1 (1%)	73	65
2	D	91/92 (99%)	90 (99%)	1 (1%)	73	65
All	All	561/564 (100%)	551 (98%)	10 (2%)	59	45

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	177	ARG
1	A	184	ASP
1	A	238	ARG
1	C	74	ILE
1	C	184	ASP
1	C	196	SER
1	C	238	ARG
2	B	239	ASN
2	D	171	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	239	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](#)

2 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	$\# Z > 2$
3	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	C	301	-	4,4,4	0.19	0	6,6,6	0.23	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	SO4	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	223/223 (100%)	0.85	25 (11%) 5 5	22, 40, 72, 84	0
1	C	223/223 (100%)	0.69	20 (8%) 9 9	23, 37, 64, 80	0
2	B	97/100 (97%)	1.16	14 (14%) 2 2	30, 45, 79, 110	0
2	D	98/100 (98%)	0.89	12 (12%) 4 4	28, 42, 68, 85	0
All	All	641/646 (99%)	0.85	71 (11%) 5 5	22, 40, 72, 110	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	237	THR	12.9
2	B	238	ALA	8.6
1	A	129	GLU	6.8
2	B	236	TYR	6.1
1	C	129	GLU	5.0
1	A	20	ARG	4.9
2	B	212	SER	4.7
1	A	127	ALA	4.6
2	D	235	ILE	4.6
2	B	235	ILE	4.6
1	C	127	ALA	4.5
2	D	236	TYR	4.5
1	C	188	ARG	4.4
2	D	211	LEU	4.2
2	B	182	ASN	4.1
2	B	211	LEU	4.0
1	A	149	ARG	4.0
1	A	170	ILE	4.0
1	A	132	ARG	3.9
1	A	77	ARG	3.8
1	A	117	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLN	3.8
1	A	188	ARG	3.8
2	D	243	SER	3.6
2	B	213	LYS	3.6
1	C	131	LEU	3.6
1	C	77	ARG	3.5
2	B	239	ASN	3.4
1	A	184	ASP	3.3
2	D	207	VAL	3.2
1	C	186	ARG	3.2
2	D	156	SER	3.0
1	C	84	ILE	2.9
2	B	158	VAL	2.9
2	D	208	ASP	2.8
1	C	201	LEU	2.8
1	C	172	GLY	2.8
2	D	182	ASN	2.8
1	A	168	LEU	2.7
1	A	115	ARG	2.7
2	B	188	LYS	2.7
1	C	128	GLN	2.6
2	B	210	ARG	2.6
1	A	183	GLY	2.5
1	C	183	GLY	2.5
1	A	79	ASN	2.5
1	C	170	ILE	2.5
1	A	85	THR	2.4
1	C	132	ARG	2.4
1	C	157	VAL	2.4
1	C	165	ARG	2.4
2	D	157	THR	2.3
1	A	160	ARG	2.3
1	A	90	ILE	2.3
1	A	122	VAL	2.3
1	C	130	GLY	2.3
1	A	186	ARG	2.3
1	A	128	GLN	2.2
2	B	183	GLN	2.2
1	A	137	CYS	2.2
2	D	183	GLN	2.2
1	C	122	VAL	2.2
1	A	131	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	125	PRO	2.2
1	A	130	GLY	2.2
2	D	213	LYS	2.2
2	B	180	ASN	2.1
1	C	124	LEU	2.1
1	A	159	LEU	2.1
1	C	184	ASP	2.0
2	D	212	SER	2.0

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, 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(\AA^2)	Q<0.9
3	SO4	A	301	5/5	0.98	0.12	34,41,47,48	0
3	SO4	C	301	5/5	0.98	0.14	49,56,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.