



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:28 PM EDT

PDB ID : 2RD7 / pdb_00002rd7
Title : Human Complement Membrane Attack Proteins Share a Common Fold with Bacterial Cytolysins
Authors : Slade, D.J.; Lovelace, L.L.; Chruszcz, M.; Minor, W.; Lebioda, L.; Sodetz, J.M.
Deposited on : 2007-09-21
Resolution : 2.15 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
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

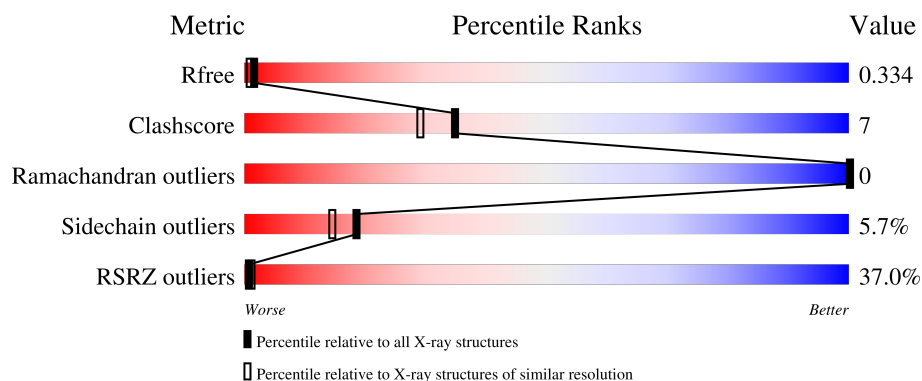
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	367	
2	C	184	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4011 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 Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	7	0
			2633	1671	439	508	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	HIS	-	expression tag	UNP P07357
A	97	HIS	-	expression tag	UNP P07357
A	98	HIS	-	expression tag	UNP P07357
A	99	HIS	-	expression tag	UNP P07357
A	100	HIS	-	expression tag	UNP P07357
A	101	HIS	-	expression tag	UNP P07357
A	102	MET	-	expression tag	UNP P07357

- Molecule 2 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	159	Total	C	N	O	S	0	1	0
			1211	781	206	220	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP P07360
C	0	ALA	-	expression tag	UNP P07360

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		

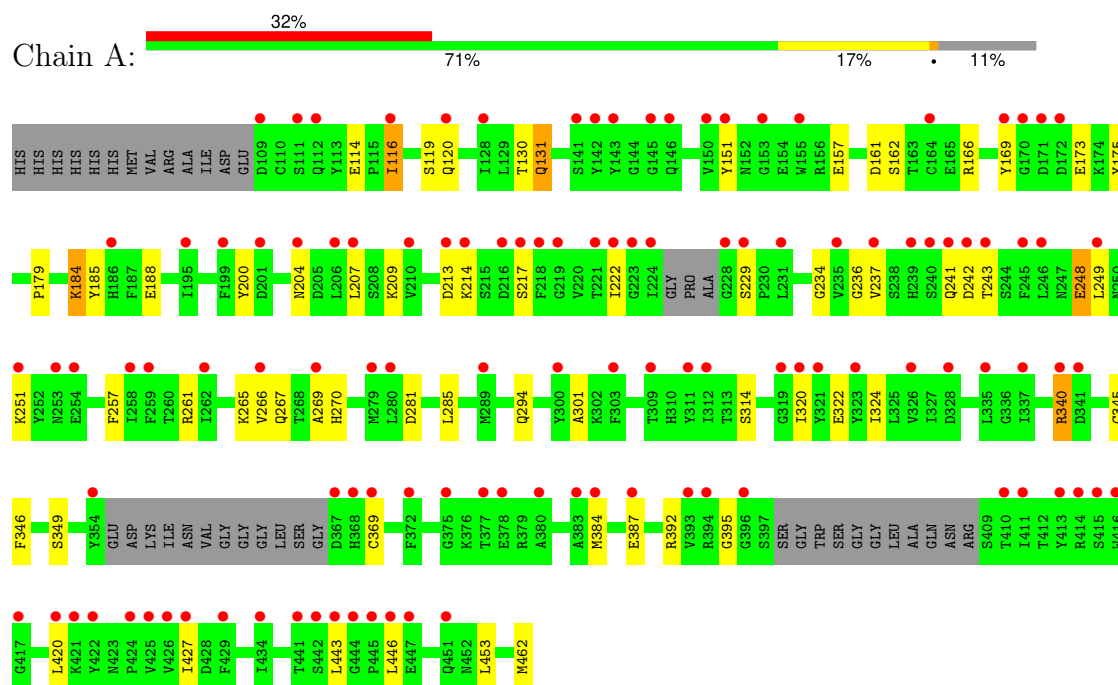
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total 129	O 129	0	0
4	C	37	Total 37	O 37	0	0

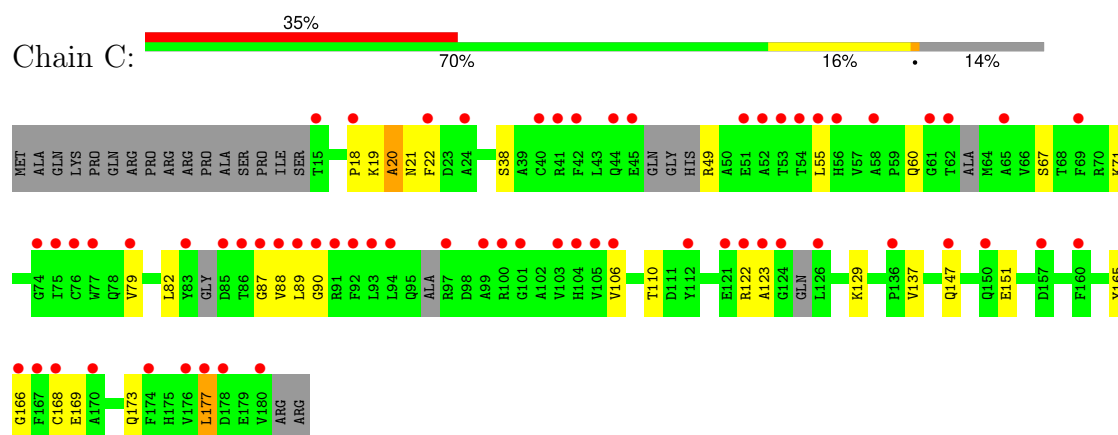
3 Residue-property plots

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: Complement component C8 alpha chain



• Molecule 2: Complement component C8 gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.55Å 126.09Å 51.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 2.15 34.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.9 (34.00-2.15) 91.8 (34.00-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.261 0.282 , 0.334	Depositor DCC
R_{free} test set	1616 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4011	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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:
CL

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	1.10	4/2687 (0.1%)	1.05	6/3624 (0.2%)
2	C	0.94	0/1234	0.94	2/1672 (0.1%)
All	All	1.05	4/3921 (0.1%)	1.02	8/5296 (0.2%)

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
2	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	ALA	C-O	-5.57	1.17	1.23
1	A	301	ALA	C-O	-5.37	1.17	1.24
1	A	266	VAL	N-CA	5.02	1.52	1.46
1	A	314	SER	CA-C	-5.02	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	GLY	N-CA-C	-7.32	103.46	112.68
2	C	38	SER	N-CA-C	6.02	117.56	108.46
1	A	114	GLU	CA-C-N	-5.64	114.44	120.03
1	A	114	GLU	C-N-CA	-5.64	114.44	120.03
1	A	229	SER	N-CA-C	5.47	116.55	109.65
2	C	20	ALA	CA-C-O	5.38	126.83	120.58
1	A	184	LYS	N-CA-C	5.23	117.14	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	TYR	N-CA-C	5.17	118.23	109.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	87	GLY	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	2633	0	2479	40	0
2	C	1211	0	1146	16	0
3	C	1	0	0	0	0
4	A	129	0	0	4	0
4	C	37	0	0	0	0
All	All	4011	0	3625	55	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 (55) 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)
2:C:147:GLN:O	2:C:151:GLU:HG3	1.69	0.92
1:A:340:ARG:HH11	1:A:340:ARG:HG3	1.40	0.85
1:A:345:CYS:HG	1:A:369:CYS:HG	0.87	0.84
2:C:88:VAL:HG12	2:C:89:LEU:H	1.55	0.71
2:C:19:LYS:NZ	2:C:110:THR:O	2.30	0.64
1:A:340:ARG:HH11	1:A:340:ARG:CG	2.11	0.63
1:A:241:GLN:NE2	4:A:525:HOH:O	2.29	0.63
2:C:90:GLY:O	2:C:106:VAL:HA	2.03	0.59
1:A:188[A]:GLU:OE2	1:A:270:HIS:CE1	2.56	0.59
1:A:242:ASP:N	4:A:557:HOH:O	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:HG3	1:A:324:ILE:HD13	1.85	0.57
1:A:294[A]:GLN:HG2	1:A:294[A]:GLN:O	2.03	0.57
2:C:173:GLN:N	2:C:173:GLN:CD	2.63	0.57
1:A:285:LEU:CD2	1:A:443:LEU:HD11	2.36	0.56
1:A:116[A]:ILE:HG22	1:A:119:SER:HB3	1.87	0.56
1:A:130:THR:O	1:A:241:GLN:HG2	2.09	0.52
1:A:116[A]:ILE:HG13	1:A:185:TYR:CE2	2.44	0.52
2:C:71:LYS:HG3	2:C:168:CYS:SG	2.48	0.52
1:A:130:THR:C	1:A:131:GLN:HG2	2.35	0.51
1:A:161:ASP:HB3	1:A:166:ARG:HB3	1.93	0.51
1:A:265:LYS:HE2	1:A:427[B]:ILE:HD13	1.92	0.50
1:A:267:GLN:HG2	1:A:427[B]:ILE:HD11	1.94	0.50
1:A:462:MET:HE2	4:A:496:HOH:O	2.13	0.48
1:A:248:GLU:OE1	1:A:251:LYS:NZ	2.46	0.48
1:A:345:CYS:CB	1:A:369:CYS:HG	2.24	0.48
1:A:116[A]:ILE:HG12	1:A:185:TYR:CG	2.48	0.47
2:C:22:PHE:HB3	2:C:89:LEU:HB3	1.97	0.47
2:C:122:ARG:CG	2:C:123:ALA:H	2.28	0.46
1:A:213:ASP:O	1:A:217:SER:HB2	2.17	0.44
2:C:177:LEU:CD2	2:C:177:LEU:C	2.91	0.44
1:A:157:GLU:OE1	1:A:157:GLU:HA	2.17	0.43
2:C:67:SER:HA	2:C:79:VAL:O	2.18	0.43
1:A:204:ASN:HA	1:A:207:LEU:HD12	1.99	0.43
2:C:18:PRO:O	2:C:19:LYS:C	2.61	0.43
1:A:340:ARG:CG	1:A:340:ARG:NH1	2.75	0.43
2:C:122:ARG:CG	2:C:123:ALA:N	2.81	0.43
1:A:427[A]:ILE:HD12	1:A:427[A]:ILE:HA	1.94	0.42
1:A:257:PHE:HE1	1:A:387:GLU:HG3	1.84	0.42
1:A:257:PHE:CE1	1:A:387:GLU:HG3	2.54	0.42
1:A:151:TYR:HB2	1:A:175:TYR:HE2	1.85	0.42
1:A:234:GLY:HA3	1:A:237:VAL:HG21	2.01	0.42
1:A:116[A]:ILE:CG1	1:A:185:TYR:CD2	3.03	0.42
1:A:270:HIS:HB3	4:A:473:HOH:O	2.20	0.42
2:C:71:LYS:HE3	2:C:166:GLY:O	2.20	0.42
1:A:236:GLY:HA2	1:A:265:LYS:HE3	2.01	0.41
2:C:165:TYR:CD2	2:C:165:TYR:C	2.98	0.41
1:A:162:SER:O	2:C:129:LYS:NZ	2.53	0.41
1:A:346:PHE:O	1:A:349:SER:OG	2.35	0.41
1:A:116[B]:ILE:HG12	1:A:179:PRO:HD3	2.02	0.41
1:A:200:TYR:OH	1:A:209:LYS:HG2	2.20	0.41
1:A:214:LYS:HA	1:A:217:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:CD1	1:A:427[A]:ILE:HD11	2.51	0.41
2:C:20:ALA:O	2:C:21:ASN:HB2	2.20	0.41
1:A:261:ARG:HG3	1:A:324:ILE:CD1	2.51	0.40
1:A:322:GLU:OE2	1:A:392:ARG:NH1	2.54	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	327/367 (89%)	321 (98%)	6 (2%)	0	100	100
2	C	148/184 (80%)	136 (92%)	12 (8%)	0	100	100
All	All	475/551 (86%)	457 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	273/312 (88%)	256 (94%)	17 (6%)	16	12
2	C	119/150 (79%)	112 (94%)	7 (6%)	18	13
All	All	392/462 (85%)	368 (94%)	24 (6%)	18	12

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116[A]	ILE
1	A	116[B]	ILE
1	A	120	GLN
1	A	131	GLN
1	A	173	GLU
1	A	184	LYS
1	A	222	ILE
1	A	243	THR
1	A	248	GLU
1	A	249	LEU
1	A	281[A]	ASP
1	A	281[B]	ASP
1	A	340	ARG
1	A	384	MET
1	A	420	LEU
1	A	446	LEU
1	A	453	LEU
2	C	49	ARG
2	C	55	LEU
2	C	60	GLN
2	C	82	LEU
2	C	137	VAL
2	C	169	GLU
2	C	177	LEU

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

Mol	Chain	Res	Type
2	C	60	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	328/367 (89%)	1.79	116 (35%)  	20, 51, 73, 89	7 (2%)
2	C	159/184 (86%)	1.83	64 (40%)  	24, 44, 57, 62	1 (0%)
All	All	487/551 (88%)	1.80	180 (36%)  	20, 50, 70, 89	8 (1%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	TRP	6.5
1	A	218[A]	PHE	5.3
1	A	411	ILE	5.0
2	C	85	ASP	4.8
2	C	87	GLY	4.7
1	A	421	LYS	4.6
2	C	103	VAL	4.4
1	A	217	SER	4.4
2	C	89	LEU	4.4
1	A	249	LEU	4.2
1	A	354	TYR	4.1
2	C	90	GLY	4.1
2	C	42	PHE	4.0
2	C	92	PHE	4.0
1	A	312	ILE	3.9
2	C	101	GLY	3.9
1	A	368	HIS	3.9
1	A	224	ILE	3.8
1	A	164	CYS	3.8
2	C	167	PHE	3.8
1	A	207	LEU	3.8
1	A	422	TYR	3.7
2	C	99	ALA	3.7
1	A	213	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	88	VAL	3.7
1	A	228	GLY	3.6
1	A	170	GLY	3.5
2	C	58	ALA	3.4
1	A	415	SER	3.4
2	C	41	ARG	3.4
1	A	172	ASP	3.4
1	A	245	PHE	3.4
1	A	425	VAL	3.4
1	A	426	VAL	3.4
1	A	141	SER	3.4
1	A	201	ASP	3.4
1	A	417	GLY	3.4
1	A	427[A]	ILE	3.4
1	A	216	ASP	3.3
2	C	86	THR	3.3
1	A	446	LEU	3.3
1	A	116[A]	ILE	3.3
1	A	240	SER	3.2
2	C	123	ALA	3.2
1	A	420	LEU	3.2
2	C	75	ILE	3.2
2	C	112	TYR	3.2
1	A	171	ASP	3.2
1	A	237	VAL	3.2
1	A	169	TYR	3.2
1	A	222	ILE	3.1
1	A	199	PHE	3.1
1	A	372	PHE	3.1
2	C	147	GLN	3.0
1	A	186	HIS	3.0
2	C	52	ALA	3.0
1	A	335	LEU	3.0
1	A	424	PRO	3.0
1	A	380	ALA	2.9
1	A	112	GLN	2.9
2	C	170	ALA	2.9
2	C	94	LEU	2.9
2	C	62	THR	2.9
2	C	180	VAL	2.9
1	A	229	SER	2.9
1	A	328	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	40	CYS	2.8
1	A	340	ARG	2.8
2	C	104	HIS	2.8
1	A	145	GLY	2.8
2	C	122	ARG	2.8
1	A	444	GLY	2.8
1	A	279	MET	2.8
2	C	65	ALA	2.8
1	A	146	GLN	2.7
1	A	109	ASP	2.7
1	A	219	GLY	2.7
1	A	142	TYR	2.7
2	C	55	LEU	2.7
2	C	53	THR	2.7
1	A	204	ASN	2.7
2	C	56[A]	HIS	2.7
1	A	266	VAL	2.7
2	C	106	VAL	2.7
1	A	128	ILE	2.7
2	C	157	ASP	2.7
1	A	259	PHE	2.7
1	A	337	ILE	2.7
2	C	91	ARG	2.7
1	A	377	THR	2.6
1	A	393	VAL	2.6
1	A	369	CYS	2.6
1	A	153	GLY	2.6
1	A	383	ALA	2.6
1	A	210	VAL	2.6
1	A	289	MET	2.6
1	A	269	ALA	2.6
1	A	416	TRP	2.6
1	A	239	HIS	2.6
2	C	178	ASP	2.6
1	A	280	LEU	2.6
2	C	77	TRP	2.6
1	A	429	PHE	2.5
2	C	61	GLY	2.5
1	A	253	ASN	2.5
2	C	44	GLN	2.5
2	C	150	GLN	2.5
1	A	323	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	76	CYS	2.5
1	A	367	ASP	2.5
1	A	206	LEU	2.5
1	A	451[A]	GLN	2.4
2	C	168	CYS	2.4
1	A	445	PRO	2.4
2	C	24	ALA	2.4
1	A	319	GLY	2.4
1	A	241	GLN	2.4
1	A	143	TYR	2.4
1	A	309	THR	2.4
1	A	414	ARG	2.4
2	C	174	PHE	2.4
2	C	54	THR	2.4
1	A	235	VAL	2.4
2	C	105	VAL	2.4
1	A	378	GLU	2.3
1	A	231	LEU	2.3
1	A	375	GLY	2.3
1	A	384	MET	2.3
2	C	22	PHE	2.3
1	A	195	ILE	2.3
1	A	221	THR	2.3
2	C	83	TYR	2.3
2	C	126	LEU	2.3
1	A	242	ASP	2.3
1	A	262	ILE	2.3
1	A	243	THR	2.3
1	A	311	TYR	2.3
2	C	124	GLY	2.3
1	A	214	LYS	2.3
2	C	121	GLU	2.3
1	A	320	ILE	2.3
1	A	341	ASP	2.3
1	A	413	TYR	2.3
1	A	120	GLN	2.2
1	A	303	PHE	2.2
1	A	434	ILE	2.2
2	C	15	THR	2.2
1	A	151	TYR	2.2
2	C	45	GLU	2.2
2	C	69	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	326	VAL	2.2
1	A	254	GLU	2.2
2	C	93	LEU	2.2
1	A	300	TYR	2.2
2	C	97	ARG	2.2
2	C	100	ARG	2.2
1	A	410	THR	2.2
2	C	160	PHE	2.2
1	A	442	SER	2.2
1	A	251	LYS	2.2
2	C	166	GLY	2.1
1	A	443	LEU	2.1
1	A	447	GLU	2.1
1	A	321	TYR	2.1
2	C	136	PRO	2.1
1	A	258	ILE	2.1
1	A	150	VAL	2.1
2	C	79	VAL	2.1
2	C	176	VAL	2.1
1	A	111	SER	2.1
1	A	394	ARG	2.0
1	A	441	THR	2.0
2	C	18	PRO	2.0
1	A	396	GLY	2.0
2	C	74	GLY	2.0
1	A	387	GLU	2.0
2	C	51	GLU	2.0
1	A	246	LEU	2.0
2	C	177	LEU	2.0
1	A	223	GLY	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
3	CL	C	183	1/1	0.92	0.12	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.