



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:32 PM UTC

PDB ID : 5L4E / pdb_0000514e
Title : X-ray structure of the 2-22' locally-closed mutant of GLIC in complex with thiopental
Authors : Fourati, Z.; Ruza, R.R.; Delarue, M.
Deposited on : 2016-05-25
Resolution : 3.50 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

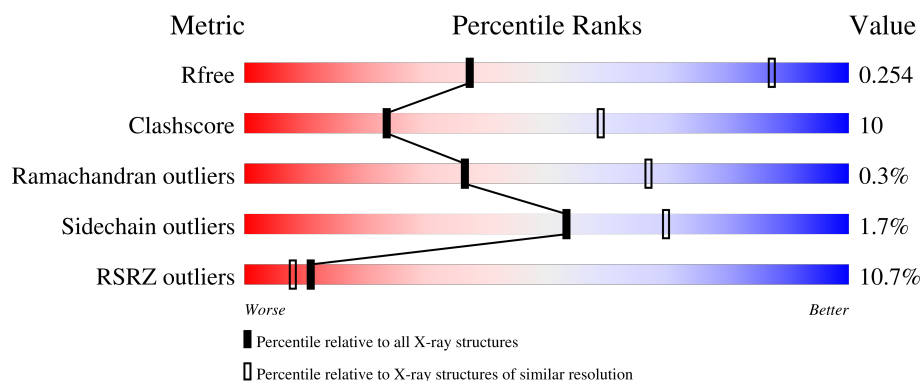
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	317	9% 79% 19% ..
1	B	317	7% 80% 17% ..
1	C	317	16% 73% 23% ..
1	D	317	11% 77% 21% .
1	E	317	10% 77% 21% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12654 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.

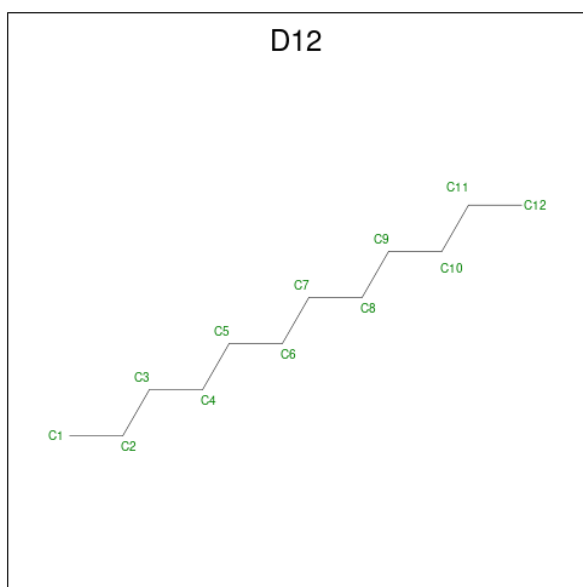
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	B	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	C	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	D	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			
1	E	311	Total	C	N	O	S	0	0	0
			2520	1658	403	454	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	CYS	conflict	UNP Q7NDN8
A	33	CYS	LYS	conflict	UNP Q7NDN8
A	246	CYS	LEU	conflict	UNP Q7NDN8
B	27	SER	CYS	conflict	UNP Q7NDN8
B	33	CYS	LYS	conflict	UNP Q7NDN8
B	246	CYS	LEU	conflict	UNP Q7NDN8
C	27	SER	CYS	conflict	UNP Q7NDN8
C	33	CYS	LYS	conflict	UNP Q7NDN8
C	246	CYS	LEU	conflict	UNP Q7NDN8
D	27	SER	CYS	conflict	UNP Q7NDN8
D	33	CYS	LYS	conflict	UNP Q7NDN8
D	246	CYS	LEU	conflict	UNP Q7NDN8
E	27	SER	CYS	conflict	UNP Q7NDN8
E	33	CYS	LYS	conflict	UNP Q7NDN8
E	246	CYS	LEU	conflict	UNP Q7NDN8

- Molecule 2 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).

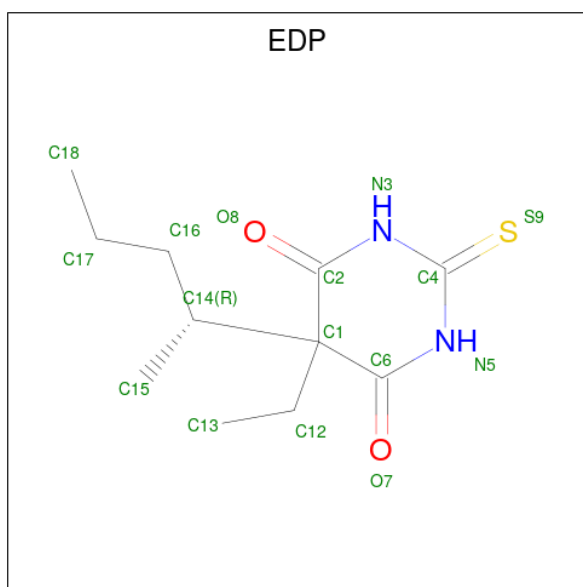


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is 5-ethyl-5-[(2R)-pentan-2-yl]-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (CCD ID: EDP) (formula: C₁₁H₁₈N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	1	0
			16	11	2	2	1		

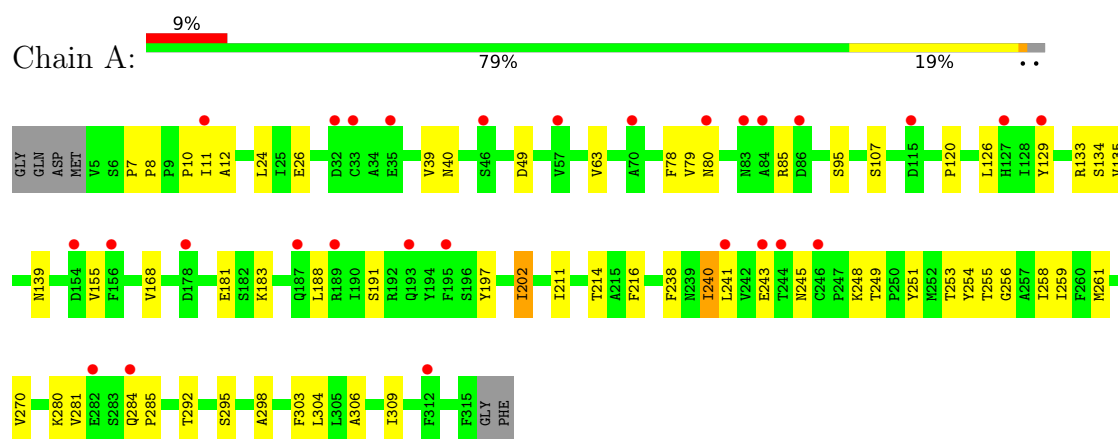
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		
5	C	2	Total	O	0	0
			2	2		
5	D	5	Total	O	0	0
			5	5		
5	E	4	Total	O	0	0
			4	4		

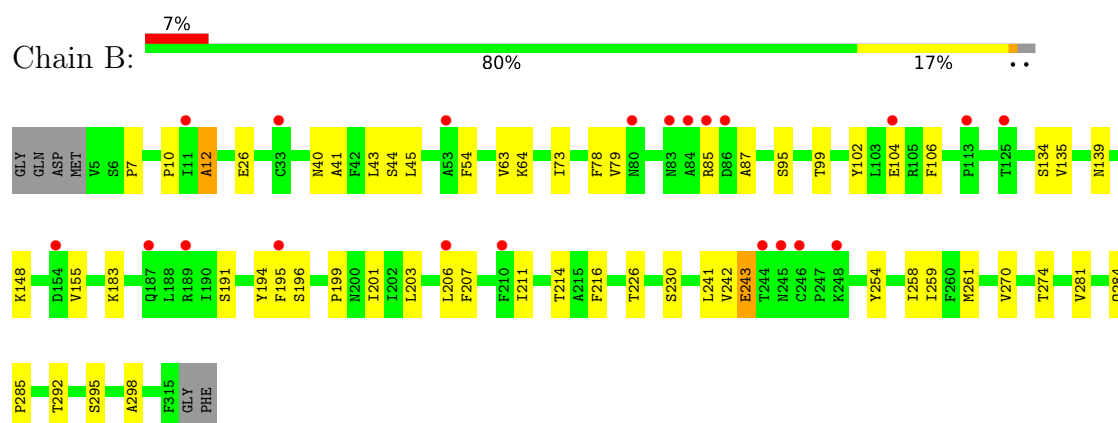
3 Residue-property plots [i](#)

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.

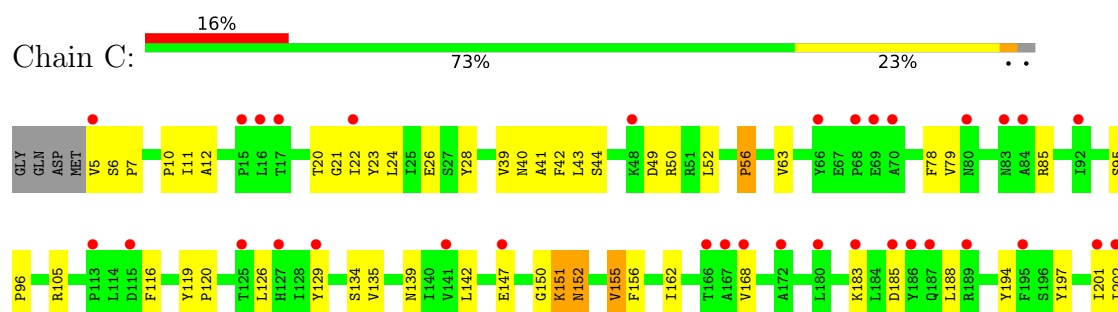
• Molecule 1: Proton-gated ion channel

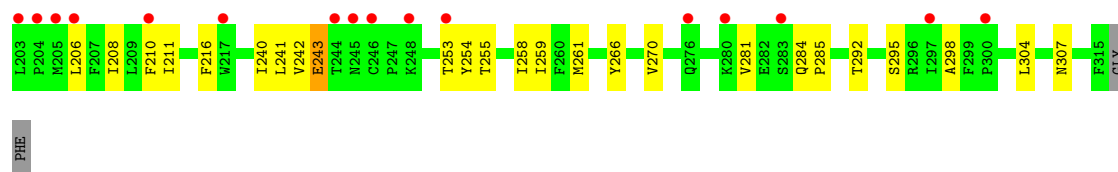


• Molecule 1: Proton-gated ion channel

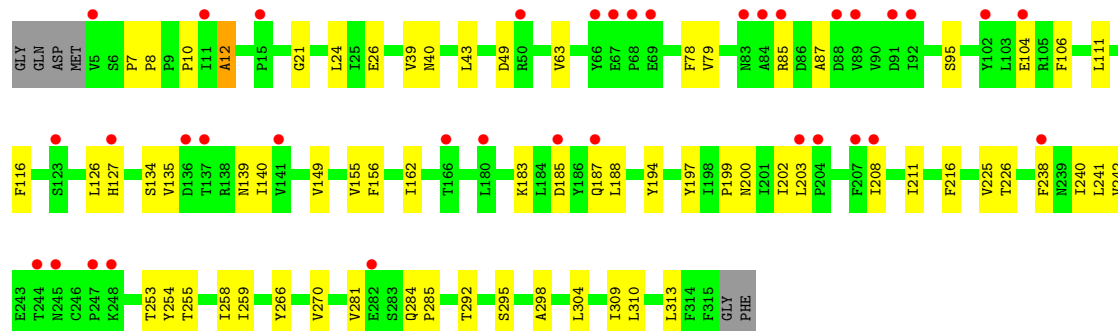
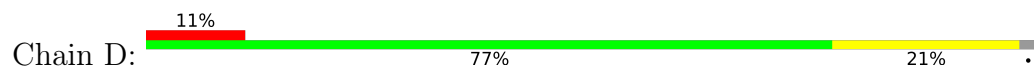


• Molecule 1: Proton-gated ion channel

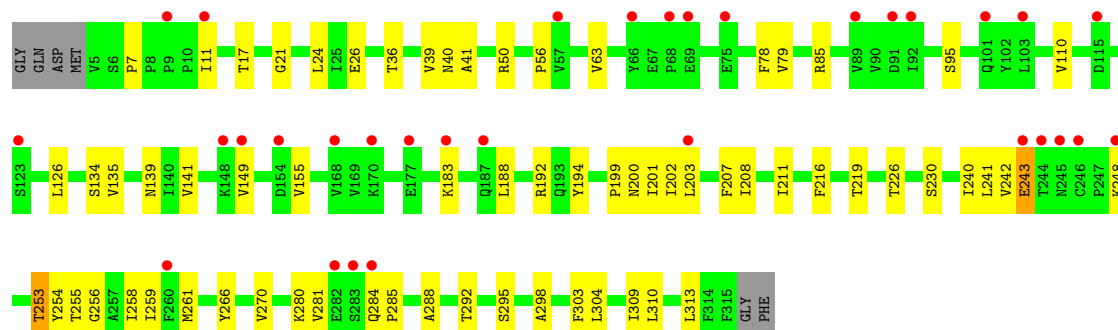
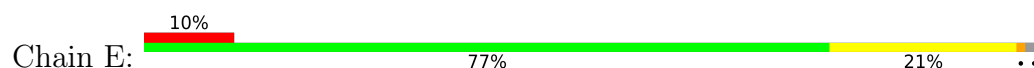




- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.03Å 134.58Å 159.02Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	40.41 – 3.50 40.41 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.41-3.50) 99.1 (40.41-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.229 , 0.249 0.239 , 0.254	Depositor DCC
R_{free} test set	2381 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	105.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12654	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: EDP, D12, 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	0.85	0/2588	1.31	9/3539 (0.3%)
1	B	0.82	0/2588	1.34	9/3539 (0.3%)
1	C	0.86	1/2588 (0.0%)	1.35	11/3539 (0.3%)
1	D	0.80	0/2588	1.32	3/3539 (0.1%)
1	E	0.81	0/2588	1.33	11/3539 (0.3%)
All	All	0.83	1/12940 (0.0%)	1.33	43/17695 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	151	LYS	C-N	6.10	1.41	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	GLU	CA-C-N	8.71	133.09	120.38
1	C	243	GLU	C-N-CA	8.71	133.09	120.38
1	E	243	GLU	CA-C-N	8.71	133.09	120.38
1	E	243	GLU	C-N-CA	8.71	133.09	120.38
1	B	243	GLU	CA-C-N	8.38	132.61	120.38
1	B	243	GLU	C-N-CA	8.38	132.61	120.38
1	B	194	TYR	CA-C-N	7.53	135.91	121.54
1	B	194	TYR	C-N-CA	7.53	135.91	121.54
1	C	152	ASN	CA-CB-CG	7.41	120.01	112.60
1	E	207	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	240	ILE	CA-C-N	6.51	129.00	120.28
1	A	240	ILE	C-N-CA	6.51	129.00	120.28
1	A	240	ILE	N-CA-C	-6.37	104.28	110.72
1	E	202	ILE	N-CA-C	6.20	116.25	110.42
1	A	202	ILE	N-CA-C	6.16	116.32	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ILE	N-CA-C	5.97	116.03	110.42
1	C	168	VAL	CA-C-N	5.83	128.76	120.53
1	C	168	VAL	C-N-CA	5.83	128.76	120.53
1	E	41	ALA	N-CA-C	5.81	116.75	108.74
1	E	194	TYR	CA-C-N	-5.77	112.09	120.29
1	E	194	TYR	C-N-CA	-5.77	112.09	120.29
1	C	41	ALA	N-CA-C	5.66	116.55	108.74
1	B	41	ALA	N-CA-C	5.63	116.52	108.74
1	C	56	PRO	CA-C-N	5.46	127.55	120.88
1	C	56	PRO	C-N-CA	5.46	127.55	120.88
1	C	185	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	225	VAL	N-CA-C	-5.21	105.41	110.42
1	B	196	SER	CA-C-N	5.21	127.51	120.38
1	B	196	SER	C-N-CA	5.21	127.51	120.38
1	C	202	ILE	N-CA-C	5.20	115.97	110.72
1	A	11	ILE	CA-C-N	5.14	128.94	122.16
1	A	11	ILE	C-N-CA	5.14	128.94	122.16
1	A	80	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	168	VAL	CA-C-N	5.07	127.68	120.53
1	A	168	VAL	C-N-CA	5.07	127.68	120.53
1	D	12	ALA	N-CA-C	-5.07	99.28	108.65
1	B	207	PHE	CA-CB-CG	5.06	118.86	113.80
1	E	192	ARG	CA-C-N	5.05	130.24	122.77
1	E	192	ARG	C-N-CA	5.05	130.24	122.77
1	E	56	PRO	CA-C-N	5.02	127.01	120.88
1	E	56	PRO	C-N-CA	5.02	127.01	120.88
1	C	147	GLU	CB-CG-CD	5.01	121.12	112.60
1	B	12	ALA	N-CA-C	-5.00	99.39	108.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2520	0	2529	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2520	0	2529	44	0
1	C	2520	0	2529	76	0
1	D	2520	0	2529	59	0
1	E	2520	0	2529	42	0
2	A	12	0	26	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	D	16	0	18	5	0
5	A	6	0	0	0	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	D	5	0	0	0	0
5	E	4	0	0	0	0
All	All	12654	0	12689	259	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 10.

All (259) 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:B:78:PHE:CD2	1:B:85:ARG:HD2	1.46	1.46
1:C:23:TYR:HE1	1:C:151:LYS:C	1.26	1.42
1:B:78:PHE:HE2	1:B:85:ARG:CZ	1.30	1.41
1:D:127:HIS:CE1	1:D:187:GLN:HE21	1.42	1.36
1:C:23:TYR:CE1	1:C:151:LYS:C	2.02	1.36
1:D:127:HIS:HE1	1:D:187:GLN:NE2	1.26	1.31
1:C:23:TYR:OH	1:C:152:ASN:HA	1.20	1.29
1:B:78:PHE:CE2	1:B:85:ARG:CZ	2.17	1.26
1:C:22:ILE:HB	1:C:42:PHE:O	1.40	1.18
1:C:22:ILE:CG2	1:C:43:LEU:HA	1.74	1.18
1:B:87:ALA:HB1	1:B:104:GLU:OE2	1.44	1.17
1:B:78:PHE:HE2	1:B:85:ARG:NE	1.41	1.15
1:B:78:PHE:CE2	1:B:85:ARG:NH1	2.17	1.12
1:A:238:PHE:CD2	1:A:241:LEU:HD23	1.84	1.10
1:B:78:PHE:CE2	1:B:85:ARG:HD2	1.86	1.10
1:B:85:ARG:NH2	1:B:106:PHE:CD2	2.24	1.06
1:A:248:LYS:HE2	1:E:200:ASN:HB3	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ILE:HG22	1:C:43:LEU:CA	1.85	1.05
1:B:78:PHE:CD2	1:B:85:ARG:CD	2.39	1.04
1:B:78:PHE:CE2	1:B:85:ARG:NE	2.21	1.03
1:E:219:THR:HG22	1:E:280:LYS:NZ	1.74	1.03
1:C:11:ILE:HG13	1:C:50:ARG:CZ	1.89	1.02
1:C:23:TYR:OH	1:C:152:ASN:CA	2.07	1.02
1:D:127:HIS:CE1	1:D:187:GLN:NE2	2.11	1.02
1:A:238:PHE:O	1:A:241:LEU:HB3	1.58	1.02
1:A:249:THR:HG21	1:A:251:TYR:CZ	1.94	1.02
1:C:23:TYR:CE1	1:C:151:LYS:CA	2.43	1.01
1:B:78:PHE:CE2	1:B:85:ARG:CD	2.42	1.01
1:C:22:ILE:CB	1:C:42:PHE:O	2.08	1.00
1:C:11:ILE:HG13	1:C:50:ARG:NH2	1.80	0.96
1:C:23:TYR:HE1	1:C:151:LYS:CA	1.77	0.96
1:A:240:ILE:O	1:A:243:GLU:OE2	1.83	0.95
1:D:85:ARG:NH1	1:D:104:GLU:OE1	2.00	0.95
1:B:85:ARG:NH2	1:B:106:PHE:CG	2.37	0.93
1:C:22:ILE:HG22	1:C:43:LEU:HA	0.92	0.92
1:C:23:TYR:CZ	1:C:152:ASN:HA	2.04	0.91
1:E:219:THR:HG22	1:E:280:LYS:HZ1	1.32	0.91
1:A:238:PHE:CD2	1:A:241:LEU:CD2	2.53	0.91
1:C:23:TYR:CE1	1:C:152:ASN:N	2.39	0.89
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.39	0.88
1:A:249:THR:CG2	1:A:251:TYR:CE1	2.59	0.86
1:B:78:PHE:HE2	1:B:85:ARG:NH1	1.59	0.86
1:C:201:ILE:HG12	1:C:242:VAL:HG21	1.59	0.84
1:D:85:ARG:HH11	1:D:106:PHE:HB3	1.39	0.84
1:A:249:THR:HG21	1:A:251:TYR:CE1	2.12	0.84
1:A:10:PRO:HB2	1:A:12:ALA:O	1.79	0.82
1:D:10:PRO:HB2	1:D:12:ALA:O	1.80	0.81
1:C:23:TYR:HD1	1:C:150:GLY:C	1.89	0.81
1:A:249:THR:HG21	1:A:251:TYR:CE2	2.15	0.81
1:C:10:PRO:HB2	1:C:12:ALA:O	1.80	0.81
1:C:22:ILE:CG2	1:C:42:PHE:O	2.29	0.80
1:D:85:ARG:HH11	1:D:106:PHE:CB	1.93	0.80
1:B:10:PRO:HB2	1:B:12:ALA:O	1.81	0.80
1:B:78:PHE:HD2	1:B:85:ARG:HD2	0.99	0.79
1:C:23:TYR:HE1	1:C:151:LYS:O	1.66	0.78
1:B:43:LEU:HD22	1:B:85:ARG:HH12	1.47	0.78
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.49	0.78
1:D:85:ARG:HD2	1:D:106:PHE:CG	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:TYR:CZ	1:C:152:ASN:CA	2.66	0.76
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.21	0.76
1:A:238:PHE:CE2	1:A:241:LEU:HD23	2.19	0.76
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.51	0.75
1:D:127:HIS:ND1	1:D:187:GLN:HG2	2.02	0.75
1:A:248:LYS:CE	1:E:200:ASN:HB3	2.16	0.75
1:D:309:ILE:O	1:D:313:LEU:HG	1.88	0.74
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.22	0.73
1:D:85:ARG:NH1	1:D:106:PHE:HB3	2.04	0.73
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.52	0.72
1:D:85:ARG:HD2	1:D:106:PHE:CB	2.19	0.72
1:A:240:ILE:O	1:A:243:GLU:HG2	1.90	0.71
1:C:23:TYR:CZ	1:C:152:ASN:N	2.58	0.71
1:E:309:ILE:O	1:E:313:LEU:HG	1.90	0.71
1:A:249:THR:CG2	1:A:251:TYR:CD1	2.74	0.70
1:C:11:ILE:CG1	1:C:50:ARG:CZ	2.70	0.70
1:B:87:ALA:CB	1:B:104:GLU:OE2	2.32	0.70
1:B:78:PHE:HD2	1:B:85:ARG:CD	1.93	0.69
1:C:23:TYR:CE1	1:C:151:LYS:N	2.61	0.69
1:C:11:ILE:CG1	1:C:50:ARG:NH1	2.56	0.69
1:C:23:TYR:CD1	1:C:150:GLY:C	2.72	0.68
1:C:23:TYR:CD1	1:C:151:LYS:N	2.62	0.68
1:E:219:THR:HG22	1:E:280:LYS:HZ3	1.57	0.68
1:C:11:ILE:HG13	1:C:50:ARG:NH1	2.09	0.67
1:E:11:ILE:HD11	1:E:50:ARG:HD2	1.75	0.67
1:C:23:TYR:CD1	1:C:151:LYS:CA	2.79	0.65
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.30	0.65
1:C:23:TYR:CZ	1:C:151:LYS:C	2.74	0.65
1:A:240:ILE:O	1:A:243:GLU:CD	2.39	0.64
1:C:23:TYR:CE1	1:C:151:LYS:O	2.45	0.64
1:E:280:LYS:HG3	1:E:288:ALA:HB1	1.81	0.63
1:A:249:THR:CG2	1:A:251:TYR:CZ	2.75	0.62
1:B:7:PRO:HG3	1:B:135:VAL:HG21	1.83	0.61
1:C:11:ILE:HG12	1:C:50:ARG:NH1	2.16	0.60
1:B:211:ILE:HG23	1:C:270:VAL:HG11	1.83	0.60
1:E:280:LYS:HG3	1:E:288:ALA:CB	2.32	0.59
1:D:85:ARG:CG	1:D:106:PHE:HB2	2.31	0.59
1:E:201:ILE:HG12	1:E:242:VAL:HG11	1.85	0.59
1:A:240:ILE:O	1:A:243:GLU:CG	2.51	0.59
1:C:23:TYR:HH	1:C:152:ASN:HA	1.57	0.59
1:A:211:ILE:HG23	1:B:270:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ARG:NH2	1:B:106:PHE:CE2	2.71	0.58
1:C:63:VAL:HG22	1:C:95:SER:HA	1.86	0.57
1:A:7:PRO:HG3	1:A:135:VAL:HG21	1.85	0.57
1:B:78:PHE:CZ	1:B:85:ARG:CZ	2.83	0.57
1:C:23:TYR:CD1	1:C:151:LYS:HA	2.39	0.57
2:A:401:D12:H51	1:D:240:ILE:HG21	1.88	0.56
1:C:22:ILE:HG22	1:C:42:PHE:O	2.03	0.56
1:C:23:TYR:CE1	1:C:151:LYS:HA	2.38	0.56
1:B:43:LEU:HD22	1:B:85:ARG:NH1	2.17	0.56
1:D:200:ASN:HB3	1:E:248:LYS:HZ3	1.68	0.56
1:C:201:ILE:HG12	1:C:242:VAL:CG2	2.32	0.56
1:C:22:ILE:O	1:C:22:ILE:HG13	2.06	0.55
1:D:85:ARG:HD2	1:D:106:PHE:HB2	1.88	0.55
1:A:238:PHE:CE2	1:A:241:LEU:CD2	2.86	0.55
1:B:85:ARG:NE	1:B:106:PHE:CD1	2.74	0.55
1:D:7:PRO:HG3	1:D:135:VAL:HG21	1.88	0.55
1:C:254:TYR:CZ	1:C:258:ILE:HD11	2.42	0.54
1:A:249:THR:HG21	1:A:251:TYR:CD1	2.42	0.54
1:D:211:ILE:HG23	1:E:270:VAL:HG11	1.88	0.54
1:D:254:TYR:CZ	1:D:258:ILE:HD11	2.42	0.54
1:C:7:PRO:HG3	1:C:135:VAL:HG21	1.88	0.54
4:D:402:EDP:H12A	1:E:230:SER:OG	2.08	0.54
1:E:7:PRO:HG3	1:E:135:VAL:HG21	1.89	0.53
1:E:254:TYR:CZ	1:E:258:ILE:HD11	2.43	0.53
1:C:211:ILE:HG23	1:D:270:VAL:HG11	1.90	0.53
1:B:254:TYR:CZ	1:B:258:ILE:HD11	2.44	0.53
1:D:127:HIS:CE1	1:D:187:GLN:HG2	2.42	0.53
1:E:24:LEU:HD22	1:E:39:VAL:HG21	1.91	0.52
1:A:254:TYR:CZ	1:A:258:ILE:HD11	2.44	0.52
1:D:185:ASP:OD2	1:D:187:GLN:HG3	2.10	0.52
1:A:249:THR:HG22	1:A:251:TYR:CD1	2.45	0.52
1:B:26:GLU:HB2	1:B:40:ASN:HB3	1.92	0.52
1:B:201:ILE:HG12	1:B:242:VAL:HG11	1.92	0.52
1:D:85:ARG:HH11	1:D:106:PHE:HB2	1.75	0.52
1:E:134:SER:HB3	1:E:139:ASN:HA	1.92	0.51
1:A:270:VAL:HG11	1:E:211:ILE:HG23	1.92	0.51
1:A:249:THR:HG22	1:A:251:TYR:H	1.74	0.51
1:C:56:PRO:HD3	1:C:96:PRO:HB3	1.93	0.51
1:C:241:LEU:HD13	1:D:240:ILE:HG13	1.92	0.51
1:D:309:ILE:HG22	1:D:313:LEU:HD11	1.93	0.51
1:A:238:PHE:C	1:A:241:LEU:HB3	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.93	0.51
1:C:134:SER:HB3	1:C:139:ASN:HA	1.93	0.50
1:C:216:PHE:O	1:C:292:THR:HG22	2.11	0.50
1:E:199:PRO:HA	1:E:203:LEU:HD12	1.93	0.50
1:B:241:LEU:HD13	1:C:240:ILE:HG13	1.94	0.50
1:D:24:LEU:HD22	1:D:39:VAL:HG21	1.92	0.50
1:B:45:LEU:HD12	1:B:102:TYR:CD1	2.45	0.50
1:A:134:SER:HB3	1:A:139:ASN:HA	1.94	0.50
1:B:134:SER:HB3	1:B:139:ASN:HA	1.93	0.50
1:D:85:ARG:CZ	1:D:104:GLU:OE1	2.59	0.50
1:D:116:PHE:O	1:D:253:THR:HG23	2.11	0.50
1:D:79:VAL:HG21	1:D:183:LYS:HE2	1.94	0.50
1:E:11:ILE:HD11	1:E:50:ARG:CD	2.42	0.50
1:E:79:VAL:HG21	1:E:183:LYS:HE2	1.94	0.50
1:E:309:ILE:HG22	1:E:313:LEU:HD11	1.94	0.49
1:A:79:VAL:HG21	1:A:183:LYS:HE2	1.93	0.49
1:D:26:GLU:HB2	1:D:40:ASN:HB3	1.95	0.49
1:D:216:PHE:O	1:D:292:THR:HG22	2.13	0.49
1:E:310:LEU:HA	1:E:313:LEU:HD12	1.94	0.49
1:A:249:THR:HG21	1:A:251:TYR:CD2	2.46	0.48
1:B:79:VAL:HG21	1:B:183:LYS:HE2	1.95	0.48
1:C:208:ILE:HG22	1:C:266:TYR:OH	2.12	0.48
1:C:261:MET:HE1	1:C:307:ASN:ND2	2.28	0.48
1:C:116:PHE:O	1:C:253:THR:HG23	2.13	0.48
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.40	0.48
1:A:63:VAL:HG22	1:A:95:SER:HA	1.95	0.48
1:D:194:TYR:CE2	1:D:197:TYR:HD1	2.32	0.48
1:A:24:LEU:HD22	1:A:39:VAL:HG21	1.94	0.48
1:A:249:THR:HG23	1:A:251:TYR:CE1	2.45	0.48
1:C:23:TYR:HH	1:C:152:ASN:CA	2.20	0.47
1:D:63:VAL:HG22	1:D:95:SER:HA	1.97	0.47
1:D:134:SER:HB3	1:D:139:ASN:HA	1.96	0.47
1:B:226:THR:HG23	4:D:402:EDP:H15	1.97	0.47
1:A:238:PHE:HD2	1:A:241:LEU:CD2	2.19	0.47
1:C:126:LEU:HB2	1:C:188:LEU:HB3	1.95	0.47
1:D:78:PHE:HE2	1:D:85:ARG:CD	2.25	0.47
1:D:85:ARG:NH2	1:D:104:GLU:OE2	2.48	0.47
1:C:49:ASP:HB3	1:C:52:LEU:HD12	1.97	0.47
1:C:26:GLU:HB2	1:C:40:ASN:HB3	1.96	0.47
1:D:241:LEU:HD13	1:E:240:ILE:HG13	1.97	0.47
1:D:85:ARG:CD	1:D:106:PHE:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HB	1:B:274:THR:HG21	1.97	0.46
1:A:216:PHE:O	1:A:292:THR:HG22	2.14	0.46
1:C:5:VAL:HG23	1:C:6:SER:H	1.81	0.46
1:C:79:VAL:HG21	1:C:183:LYS:HE2	1.96	0.46
1:D:126:LEU:HD12	1:D:188:LEU:HD23	1.97	0.46
1:B:216:PHE:O	1:B:292:THR:HG22	2.14	0.46
1:D:85:ARG:NH2	1:D:87:ALA:HB2	2.31	0.46
1:E:208:ILE:HG22	1:E:266:TYR:OH	2.16	0.46
1:E:126:LEU:HB2	1:E:188:LEU:HB3	1.97	0.46
1:D:85:ARG:CZ	1:D:87:ALA:HB2	2.46	0.46
1:A:295:SER:HA	1:A:298:ALA:HB3	1.98	0.46
1:C:24:LEU:HD22	1:C:39:VAL:HG21	1.98	0.46
1:A:126:LEU:HB2	1:A:188:LEU:HB3	1.97	0.46
1:C:119:TYR:OH	1:C:197:TYR:HE1	1.99	0.46
1:B:63:VAL:HG12	1:B:95:SER:HA	1.98	0.46
1:C:295:SER:HA	1:C:298:ALA:HB3	1.98	0.45
1:D:310:LEU:HA	1:D:313:LEU:HD12	1.97	0.45
1:D:85:ARG:HG2	1:D:106:PHE:HB2	1.99	0.45
1:A:26:GLU:HB2	1:A:40:ASN:HB3	1.98	0.45
1:D:199:PRO:HA	1:D:203:LEU:HD12	1.97	0.45
1:D:21:GLY:HA2	1:D:149:VAL:HG22	1.99	0.45
1:E:295:SER:HA	1:E:298:ALA:HB3	1.98	0.44
1:A:197:TYR:CE2	1:A:202:ILE:HD11	2.51	0.44
1:D:43:LEU:HB3	1:D:104:GLU:HG3	2.00	0.44
1:B:295:SER:HA	1:B:298:ALA:HB3	2.00	0.44
1:D:295:SER:HA	1:D:298:ALA:HB3	1.99	0.44
1:C:120:PRO:O	1:C:194:TYR:HB3	2.18	0.44
1:E:63:VAL:HG22	1:E:95:SER:HA	1.98	0.44
4:D:402:EDP:H12	1:E:226:THR:HG23	2.00	0.44
1:C:284:GLN:N	1:C:285:PRO:HD3	2.33	0.43
1:B:199:PRO:HA	1:B:203:LEU:HD12	2.00	0.43
1:D:226:THR:HG23	4:D:402:EDP:C13	2.48	0.43
1:D:284:GLN:N	1:D:285:PRO:HD3	2.33	0.43
1:C:261:MET:HE1	1:C:307:ASN:HD21	1.84	0.43
1:C:20:THR:HG21	1:C:142:LEU:HD22	2.00	0.43
1:D:127:HIS:CE1	1:D:187:GLN:CD	2.88	0.43
1:D:8:PRO:HB3	1:D:49:ASP:OD1	2.19	0.43
1:C:23:TYR:HE1	1:C:151:LYS:N	2.07	0.43
1:B:284:GLN:N	1:B:285:PRO:HD3	2.34	0.42
1:D:255:THR:O	1:D:259:ILE:HG12	2.19	0.42
1:E:36:THR:HA	1:E:110:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLY:O	1:C:44:SER:OG	2.31	0.42
1:C:105:ARG:HH22	1:D:79:VAL:HA	1.83	0.42
1:A:284:GLN:N	1:A:285:PRO:HD3	2.34	0.42
1:B:54:PHE:CG	1:B:64:LYS:HE2	2.54	0.42
1:E:216:PHE:O	1:E:292:THR:HG22	2.18	0.42
1:E:255:THR:O	1:E:259:ILE:HG12	2.20	0.42
1:E:284:GLN:N	1:E:285:PRO:HD3	2.34	0.42
1:D:208:ILE:HG22	1:D:266:TYR:OH	2.20	0.42
1:A:306:ALA:HA	1:A:309:ILE:HD12	2.02	0.42
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.86	0.42
1:E:253:THR:HG23	1:E:256:GLY:HA3	2.02	0.42
1:A:255:THR:O	1:A:259:ILE:HG12	2.20	0.42
2:A:401:D12:H52	1:C:240:ILE:HG21	2.02	0.42
1:B:226:THR:O	1:B:230:SER:HB2	2.20	0.42
1:A:8:PRO:HB3	1:A:49:ASP:OD1	2.20	0.42
1:C:255:THR:O	1:C:259:ILE:HG12	2.20	0.41
1:A:133:ARG:HD2	1:A:181:GLU:OE2	2.20	0.41
1:C:152:ASN:HB3	1:C:155:VAL:HG23	2.03	0.41
1:A:261:MET:HE3	1:A:303:PHE:CE2	2.55	0.41
1:B:261:MET:HE2	1:B:261:MET:HB3	1.94	0.41
1:C:206:LEU:HD22	1:C:210:PHE:CZ	2.56	0.41
1:E:21:GLY:HA2	1:E:149:VAL:HG22	2.03	0.41
1:C:156:PHE:HA	1:C:162:ILE:HD11	2.02	0.41
1:D:238:PHE:O	1:D:242:VAL:HG22	2.19	0.41
1:A:240:ILE:HG13	1:E:241:LEU:HD13	2.03	0.41
1:E:17:THR:HA	1:E:141:VAL:O	2.21	0.41
1:E:261:MET:HE3	1:E:303:PHE:CE2	2.56	0.41
1:C:79:VAL:HB	1:C:129:TYR:HB2	2.02	0.40
1:A:253:THR:HG23	1:A:256:GLY:HA3	2.02	0.40
1:C:28:TYR:HB3	1:D:111:LEU:HD22	2.02	0.40
1:A:248:LYS:HE2	1:E:200:ASN:CB	2.29	0.40
1:D:156:PHE:HA	1:D:162:ILE:HD11	2.03	0.40
4:D:402:EDP:H12	4:D:402:EDP:H16A	1.89	0.40
1:A:39:VAL:O	1:A:107:SER:HA	2.21	0.40
1:A:79:VAL:HB	1:A:129:TYR:HB2	2.04	0.40
1:B:44:SER:HB2	1:B:148:LYS:HD3	2.03	0.40
1:A:120:PRO:HG3	1:A:197:TYR:CE2	2.57	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	309/317 (98%)	296 (96%)	13 (4%)	0	100	100
1	B	309/317 (98%)	294 (95%)	13 (4%)	2 (1%)	21	54
1	C	309/317 (98%)	296 (96%)	12 (4%)	1 (0%)	36	67
1	D	309/317 (98%)	296 (96%)	13 (4%)	0	100	100
1	E	309/317 (98%)	296 (96%)	12 (4%)	1 (0%)	36	67
All	All	1545/1585 (98%)	1478 (96%)	63 (4%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	PHE
1	B	243	GLU
1	E	243	GLU
1	C	243	GLU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/284 (99%)	274 (98%)	6 (2%)	47	66
1	B	280/284 (99%)	273 (98%)	7 (2%)	42	63
1	C	280/284 (99%)	277 (99%)	3 (1%)	65	74
1	D	280/284 (99%)	276 (99%)	4 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	280/284 (99%)	276 (99%)	4 (1%)	59 71
All	All	1400/1420 (99%)	1376 (98%)	24 (2%)	53 70

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

Mol	Chain	Res	Type
1	A	155	VAL
1	A	191	SER
1	A	245	ASN
1	A	280	LYS
1	A	281	VAL
1	A	304	LEU
1	B	73	ILE
1	B	99	THR
1	B	155	VAL
1	B	191	SER
1	B	214	THR
1	B	259	ILE
1	B	281	VAL
1	C	155	VAL
1	C	281	VAL
1	C	304	LEU
1	D	140	ILE
1	D	155	VAL
1	D	281	VAL
1	D	304	LEU
1	E	155	VAL
1	E	253	THR
1	E	281	VAL
1	E	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	239	ASN
1	B	40	ASN
1	B	239	ASN
1	C	40	ASN
1	D	127	HIS
1	D	187	GLN

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Mol	Chain	Res	Type
1	E	40	ASN
1	E	193	GLN
1	E	239	ASN
1	E	276	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDP	D	402	-	15,16,16	0.31	0	18,23,23	2.35	3 (16%)
2	D12	A	401	-	11,11,11	0.26	0	10,10,10	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDP	D	402	-	-	8/12/32/32	0/1/1/1
2	D12	A	401	-	-	0/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	EDP	C12-C1-C2	-8.66	100.34	108.41
4	D	402	EDP	C12-C1-C6	2.83	111.05	108.41
4	D	402	EDP	C14-C1-C2	2.57	111.97	107.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	EDP	C2-C1-C14-C15
4	D	402	EDP	C2-C1-C14-C16
4	D	402	EDP	C6-C1-C14-C15
4	D	402	EDP	C6-C1-C14-C16
4	D	402	EDP	C12-C1-C14-C15
4	D	402	EDP	C12-C1-C14-C16
4	D	402	EDP	C1-C14-C16-C17
4	D	402	EDP	C15-C14-C16-C17

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402	EDP	5	0
2	A	401	D12	2	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	311/317 (98%)	0.71	28 (9%) 15 10	88, 121, 167, 197	0
1	B	311/317 (98%)	0.61	21 (6%) 23 14	86, 121, 154, 169	0
1	C	311/317 (98%)	0.93	50 (16%) 4 4	86, 122, 161, 202	0
1	D	311/317 (98%)	0.84	36 (11%) 9 6	84, 131, 182, 221	0
1	E	311/317 (98%)	0.73	32 (10%) 12 8	89, 125, 173, 206	0
All	All	1555/1585 (98%)	0.76	167 (10%) 11 8	84, 124, 168, 221	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	GLN	6.7
1	C	127	HIS	6.1
1	D	89	VAL	5.3
1	C	129	TYR	5.3
1	C	185	ASP	5.2
1	D	68	PRO	4.8
1	E	244	THR	4.7
1	D	187	GLN	4.6
1	C	244	THR	4.6
1	B	154	ASP	4.5
1	D	92	ILE	4.4
1	D	67	GLU	4.3
1	A	243	GLU	4.2
1	A	282	GLU	4.1
1	D	69	GLU	4.1
1	A	244	THR	4.0
1	B	84	ALA	3.9
1	B	244	THR	3.9
1	B	83	ASN	3.9
1	A	84	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	85	ARG	3.7
1	A	187	GLN	3.6
1	E	91	ASP	3.6
1	B	187	GLN	3.5
1	B	246	CYS	3.5
1	D	84	ALA	3.5
1	D	11	ILE	3.5
1	A	284	GLN	3.5
1	C	115	ASP	3.4
1	D	127	HIS	3.4
1	C	186	TYR	3.4
1	C	166	THR	3.4
1	A	127	HIS	3.4
1	A	80	ASN	3.3
1	A	312	PHE	3.3
1	D	83	ASN	3.3
1	A	195	PHE	3.3
1	C	5	VAL	3.3
1	C	189	ARG	3.3
1	D	185	ASP	3.3
1	E	282	GLU	3.2
1	C	80	ASN	3.2
1	E	246	CYS	3.2
1	E	11	ILE	3.1
1	C	167	ALA	3.1
1	E	89	VAL	3.1
1	C	16	LEU	3.1
1	D	244	THR	3.1
1	C	206	LEU	3.1
1	A	129	TYR	3.1
1	B	104	GLU	3.1
1	C	168	VAL	3.1
1	D	66	TYR	3.1
1	D	203	LEU	3.0
1	E	187	GLN	3.0
1	A	86	ASP	3.0
1	C	245	ASN	3.0
1	E	103	LEU	3.0
1	C	210	PHE	3.0
1	A	154	ASP	3.0
1	C	125	THR	2.9
1	E	284	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	248	LYS	2.9
1	A	33	CYS	2.9
1	D	204	PRO	2.9
1	D	137	THR	2.8
1	C	15	PRO	2.8
1	C	113	PRO	2.8
1	C	69	GLU	2.8
1	E	245	ASN	2.8
1	B	33	CYS	2.8
1	B	195	PHE	2.8
1	A	189	ARG	2.8
1	C	203	LEU	2.8
1	D	207	PHE	2.8
1	E	69	GLU	2.8
1	B	189	ARG	2.7
1	B	245	ASN	2.7
1	D	180	LEU	2.7
1	A	83	ASN	2.7
1	B	206	LEU	2.7
1	A	32	ASP	2.7
1	D	104	GLU	2.7
1	C	202	ILE	2.6
1	D	123	SER	2.6
1	C	48	LYS	2.6
1	D	102	TYR	2.6
1	D	88	ASP	2.6
1	E	9	PRO	2.6
1	C	83	ASN	2.6
1	A	35	GLU	2.5
1	C	276	GLN	2.5
1	C	246	CYS	2.5
1	B	86	ASP	2.5
1	B	210	PHE	2.5
1	C	248	LYS	2.5
1	E	203	LEU	2.5
1	E	154	ASP	2.5
1	E	101	GLN	2.5
1	D	15	PRO	2.5
1	D	136	ASP	2.5
1	C	141	VAL	2.5
1	A	115	ASP	2.4
1	A	156	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	68	PRO	2.4
1	C	283	SER	2.4
1	D	141	VAL	2.4
1	C	22	ILE	2.4
1	C	205	MET	2.4
1	C	297	ILE	2.4
1	C	300	PRO	2.4
1	D	245	ASN	2.4
1	E	168	VAL	2.4
1	E	115	ASP	2.4
1	C	204	PRO	2.3
1	C	183	LYS	2.3
1	A	241	LEU	2.3
1	A	11	ILE	2.3
1	C	195	PHE	2.3
1	D	91	ASP	2.3
1	E	75	GLU	2.3
1	E	248	LYS	2.3
1	E	243	GLU	2.3
1	E	149	VAL	2.3
1	E	183	LYS	2.3
1	B	53	ALA	2.2
1	B	11	ILE	2.2
1	E	92	ILE	2.2
1	C	217	TRP	2.2
1	C	92	ILE	2.2
1	E	177	GLU	2.2
1	D	166	THR	2.2
1	D	238	PHE	2.2
1	A	178	ASP	2.2
1	E	66	TYR	2.2
1	B	125	THR	2.2
1	C	253	THR	2.2
1	C	70	ALA	2.1
1	A	57	VAL	2.1
1	C	68	PRO	2.1
1	E	170	LYS	2.1
1	E	57	VAL	2.1
1	A	70	ALA	2.1
1	C	84	ALA	2.1
1	E	283	SER	2.1
1	D	208	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	66	TYR	2.1
1	C	17	THR	2.1
1	D	50	ARG	2.1
1	B	248	LYS	2.1
1	C	280	LYS	2.1
1	B	80	ASN	2.1
1	C	180	LEU	2.1
1	D	282	GLU	2.1
1	A	246	CYS	2.1
1	D	5	VAL	2.1
1	D	247	PRO	2.0
1	C	201	ILE	2.0
1	A	46	SER	2.0
1	C	172	ALA	2.0
1	B	113	PRO	2.0
1	D	85	ARG	2.0
1	E	148	LYS	2.0
1	E	123	SER	2.0
1	A	193	GLN	2.0
1	C	147	GLU	2.0
1	E	260	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	E	401	1/1	0.65	0.21	127,127,127,127	0
3	CL	D	401	1/1	0.75	0.33	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	402	1/1	0.83	0.13	142,142,142,142	0
3	CL	B	401	1/1	0.85	0.17	123,123,123,123	0
4	EDP	D	402	16/16	0.85	0.32	132,141,144,146	4
3	CL	C	401	1/1	0.93	0.09	107,107,107,107	0
2	D12	A	401	12/12	0.94	0.18	79,83,87,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.