



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:00 AM UTC

PDB ID : 2F2F / pdb_00002f2f
Title : Crystal structure of cytolethal distending toxin (CDT) from *Actinobacillus actinomycetemcomitans*
Authors : Yamada, T.; Komoto, J.; Saiki, K.; Konishi, K.; Takusagawa, F.
Deposited on : 2005-11-16
Resolution : 2.40 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

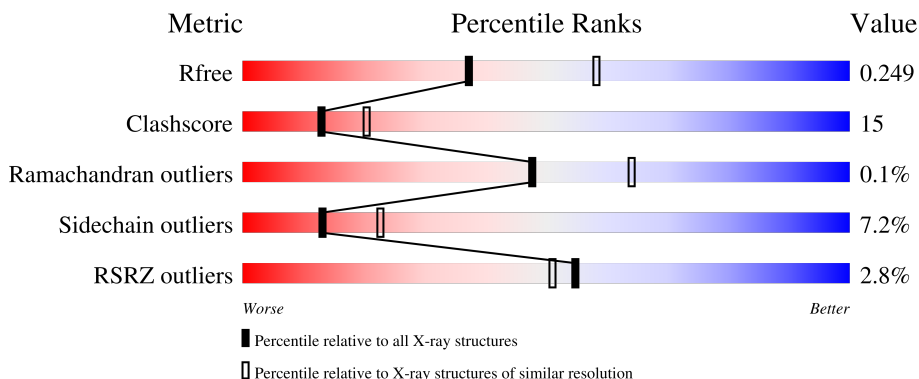
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



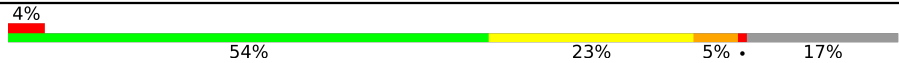
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	222	<p>53% 15% 31%</p>
1	D	222	<p>2% 53% 16% 31%</p>
2	B	283	<p>64% 24% 8%</p>
2	E	283	<p>62% 26% 5% 8%</p>
3	C	186	<p>7% 52% 25% 5% 17%</p>

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Mol	Chain	Length	Quality of chain
3	F	186	 <p>4% 54% 23% 5% 17%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9188 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 Cytolethal distending toxin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1207	770	201	230	6	0	0	0
1	D	153	1207	770	201	230	6	0	0	0

- Molecule 2 is a protein called Cytolethal distending toxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	261	2038	1268	378	388	4	0	0	0
2	E	261	2038	1268	378	388	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	HIS	ARG	see remark 999	UNP Q7DK12
E	281	HIS	ARG	see remark 999	UNP Q7DK12

- Molecule 3 is a protein called cytolethal distending toxin C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	154	1213	781	200	227	5	0	0	0
3	F	154	1213	781	200	227	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	172	PRO	SER	see remark 999	UNP Q7DK11
F	172	PRO	SER	see remark 999	UNP Q7DK11

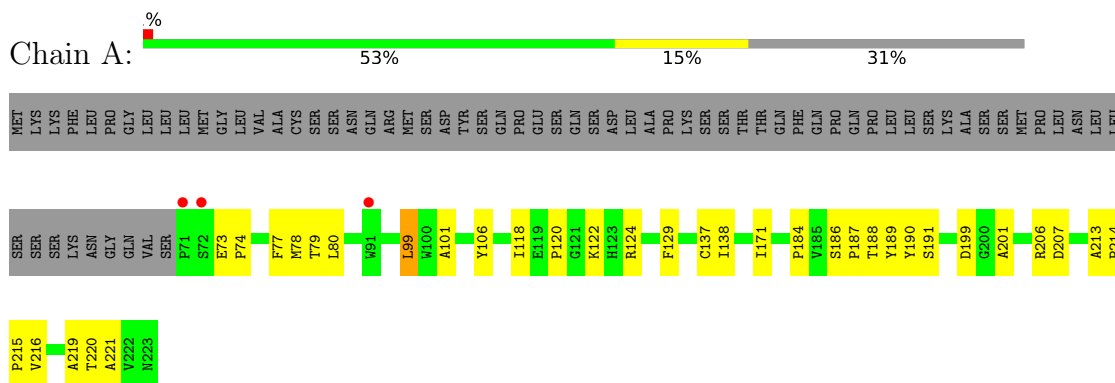
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	60	Total O 60 60	0	0
4	C	32	Total O 32 32	0	0
4	D	41	Total O 41 41	0	0
4	E	64	Total O 64 64	0	0
4	F	38	Total O 38 38	0	0

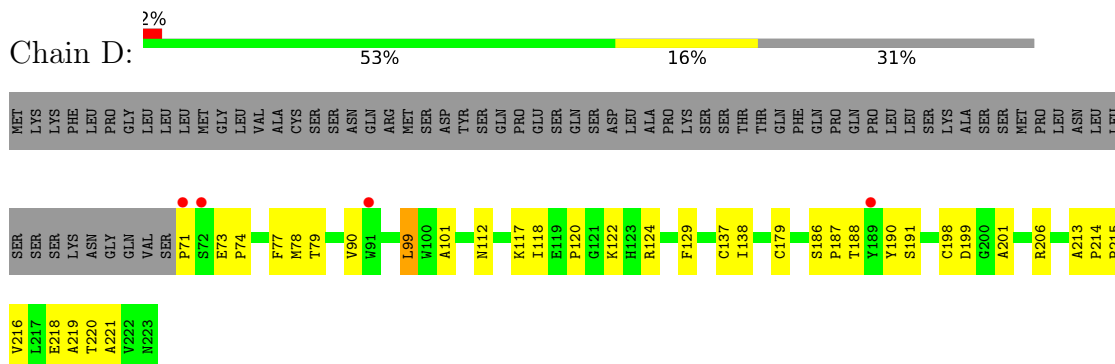
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

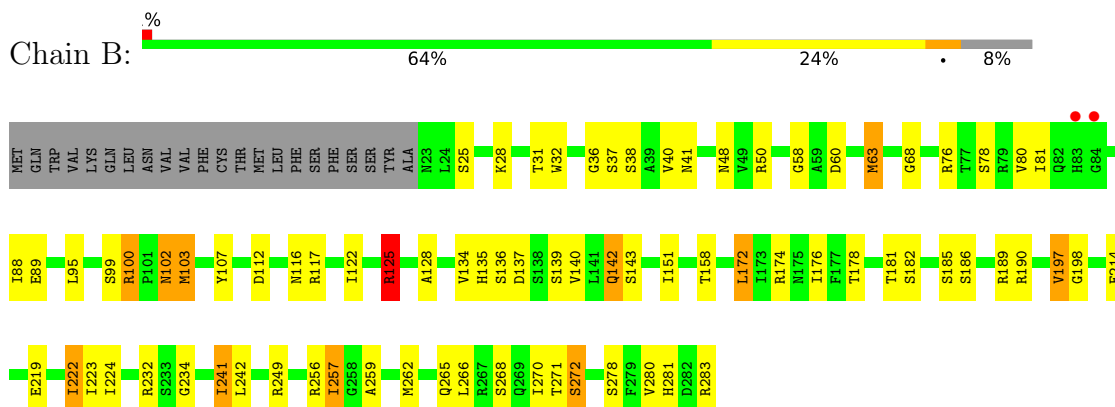
- Molecule 1: Cytolethal distending toxin A



- Molecule 1: Cytolethal distending toxin A

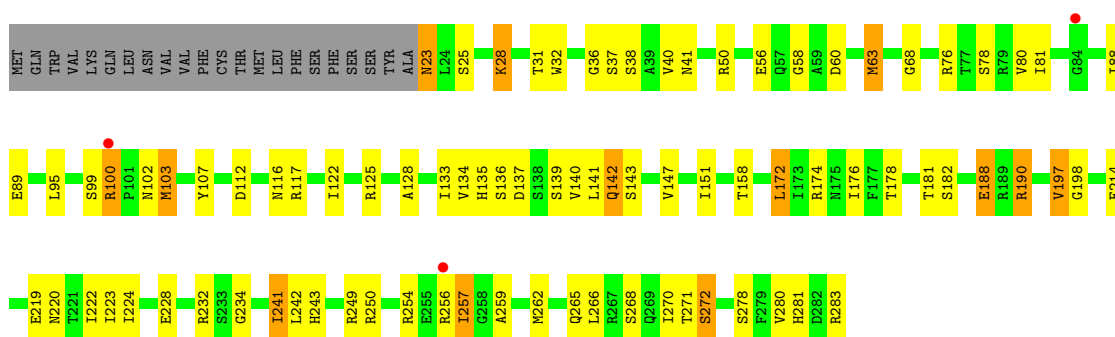


- Molecule 2: Cytolethal distending toxin B



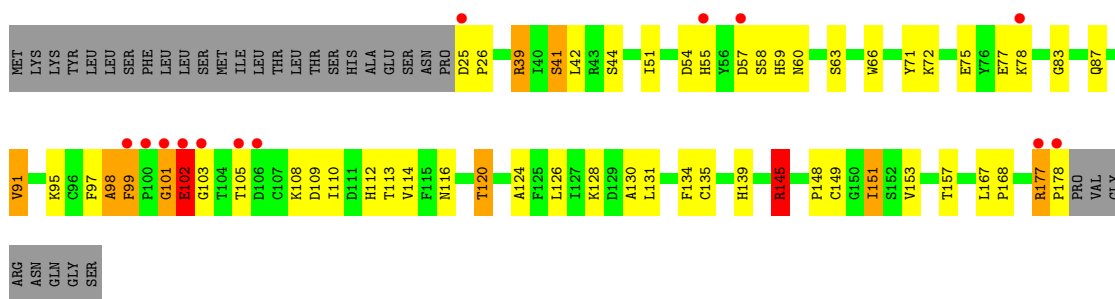
- Molecule 2: Cytolethal distending toxin B

Chain E:  62% 26% 5% 8%



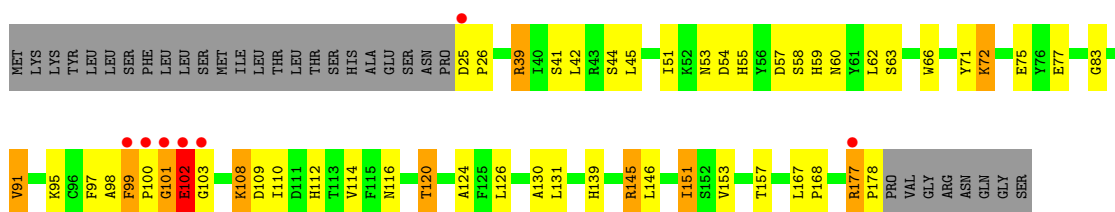
- Molecule 3: cytolethal distending toxin C

Chain C:  7% 52% 25% 5% 17%



- Molecule 3: cytolethal distending toxin C

Chain F:  4% 54% 23% 5% 17%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.65Å 117.46Å 123.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 99.8 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.31 (at 2.39Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.251 0.216 , 0.249	Depositor DCC
R_{free} test set	6842 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtrriage
Anisotropy	1.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.12 % 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 7.8088e-05. 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

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	0.59	0/1241	0.97	3/1696 (0.2%)
1	D	0.59	0/1241	1.01	6/1696 (0.4%)
2	B	0.59	0/2080	1.05	11/2828 (0.4%)
2	E	0.60	0/2080	1.07	13/2828 (0.5%)
3	C	0.70	2/1249 (0.2%)	1.19	16/1701 (0.9%)
3	F	0.66	1/1249 (0.1%)	1.20	12/1701 (0.7%)
All	All	0.62	3/9140 (0.0%)	1.08	61/12450 (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
2	B	0	1
2	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	99	PHE	C-O	-10.07	1.15	1.24
3	F	99	PHE	C-O	-6.76	1.15	1.23
3	C	99	PHE	N-CA	-5.00	1.43	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	102	GLU	N-CA-C	-13.96	96.07	111.28
3	C	102	GLU	N-CA-C	-13.57	96.49	111.28
3	F	99	PHE	N-CA-C	-13.14	91.06	110.24
3	F	99	PHE	C-N-CD	-9.58	99.51	120.60
3	C	99	PHE	CA-C-N	-9.38	96.15	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	99	PHE	C-N-CA	-9.38	96.15	120.25
3	F	99	PHE	CA-C-N	8.25	146.79	127.00
3	F	99	PHE	C-N-CA	8.25	146.79	127.00
2	B	103	MET	N-CA-C	7.80	122.51	110.42
2	E	103	MET	N-CA-C	7.80	122.73	110.17
1	D	124	ARG	N-CA-C	7.50	123.67	111.37
3	C	99	PHE	CA-C-O	-7.48	112.25	119.13
3	C	77	GLU	N-CA-C	7.08	119.85	111.71
3	F	77	GLU	N-CA-C	7.04	119.03	111.36
3	F	41	SER	N-CA-C	-6.83	97.21	108.76
2	E	140	VAL	N-CA-C	-6.44	106.72	112.90
3	C	126	LEU	N-CA-C	-6.34	99.36	109.76
3	C	98	ALA	CA-C-N	-6.33	112.80	119.83
3	C	98	ALA	C-N-CA	-6.33	112.80	119.83
3	C	99	PHE	C-N-CD	6.23	150.53	125.00
1	A	124	ARG	N-CA-C	6.19	123.99	110.80
3	F	126	LEU	N-CA-C	-6.17	99.64	109.76
3	C	41	SER	N-CA-C	-6.11	98.44	108.76
2	B	60	ASP	N-CA-C	-6.01	105.03	112.90
2	E	271	THR	N-CA-C	5.98	120.09	113.21
3	C	99	PHE	N-CA-CB	5.95	116.05	110.39
3	F	101	GLY	N-CA-C	5.91	127.19	113.18
2	B	271	THR	N-CA-C	5.89	120.17	113.15
2	E	181	THR	N-CA-C	5.87	120.49	112.68
1	D	187	PRO	N-CA-C	-5.86	106.36	114.27
2	B	198	GLY	N-CA-C	5.70	117.86	110.45
2	E	60	ASP	N-CA-C	-5.67	105.08	112.23
1	A	187	PRO	N-CA-C	-5.61	107.34	114.35
2	E	266	LEU	N-CA-C	5.54	118.96	110.20
2	B	48	ASN	N-CA-C	5.54	118.16	111.40
3	C	44	SER	N-CA-C	-5.54	102.08	110.28
1	D	122	LYS	N-CA-C	-5.54	105.32	111.36
3	C	110	ILE	N-CA-C	5.53	116.26	110.62
2	B	266	LEU	N-CA-C	5.52	118.92	110.20
3	F	131	LEU	N-CA-C	5.48	116.94	110.97
2	E	214	GLU	CA-C-N	5.44	125.52	119.32
2	E	214	GLU	C-N-CA	5.44	125.52	119.32
3	C	99	PHE	N-CA-C	5.41	119.52	112.17
2	E	198	GLY	N-CA-C	5.37	117.43	110.45
2	B	181	THR	N-CA-C	5.35	119.80	112.68
2	E	254	ARG	N-CA-C	-5.30	106.76	113.18
1	D	112	ASN	N-CA-C	5.29	120.67	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	131	LEU	N-CA-C	5.27	116.83	111.14
2	E	190	ARG	NE-CZ-NH2	5.25	123.93	119.20
2	B	214	GLU	CA-C-N	5.25	125.30	119.32
2	B	214	GLU	C-N-CA	5.25	125.30	119.32
1	D	71	PRO	N-CA-CB	5.24	108.77	103.00
3	C	145	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	F	44	SER	N-CA-C	-5.11	102.72	110.28
3	F	110	ILE	N-CA-C	5.10	115.82	110.62
2	E	197	VAL	N-CA-C	5.07	115.78	108.48
2	E	28	LYS	N-CA-C	-5.04	99.58	108.20
2	B	197	VAL	N-CA-C	5.03	115.72	108.48
1	A	122	LYS	N-CA-C	-5.03	105.88	111.36
2	B	125	ARG	N-CA-C	-5.01	106.00	111.82
1	D	218	GLU	N-CA-C	-5.00	103.44	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	107	TYR	Sidechain
2	E	107	TYR	Sidechain

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	1207	0	1164	34	0
1	D	1207	0	1164	24	0
2	B	2038	0	2003	57	0
2	E	2038	0	2003	59	0
3	C	1213	0	1185	51	0
3	F	1213	0	1185	56	0
4	A	37	0	0	0	0
4	B	60	0	0	1	0
4	C	32	0	0	0	0
4	D	41	0	0	0	0
4	E	64	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	38	0	0	1	0
All	All	9188	0	8704	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 15.

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)
3:F:177:ARG:HE	3:F:177:ARG:HA	1.11	1.08
3:F:177:ARG:HA	3:F:177:ARG:NE	1.83	0.94
3:F:25:ASP:HB3	3:F:26:PRO:CD	1.98	0.93
2:E:135:HIS:HD2	2:E:139:SER:HB2	1.34	0.92
3:C:25:ASP:HB3	3:C:26:PRO:CD	2.01	0.90
2:B:135:HIS:HD2	2:B:139:SER:HB2	1.38	0.86
3:C:99:PHE:O	3:C:101:GLY:N	2.10	0.84
2:E:95:LEU:HB2	2:E:102:ASN:HD22	1.44	0.83
3:C:151:ILE:H	3:C:151:ILE:HD13	1.43	0.82
1:A:219:ALA:HB1	3:C:120:THR:HG21	1.60	0.81
3:C:25:ASP:HB3	3:C:26:PRO:HD2	1.60	0.81
3:F:25:ASP:HB3	3:F:26:PRO:HD2	1.63	0.81
2:B:135:HIS:CD2	2:B:139:SER:HB2	2.17	0.80
2:B:102:ASN:HD21	2:B:125:ARG:HH22	1.28	0.80
2:E:135:HIS:CD2	2:E:139:SER:HB2	2.16	0.80
3:F:151:ILE:HD13	3:F:151:ILE:H	1.48	0.79
1:A:220:THR:O	3:C:120:THR:HG22	1.87	0.75
2:B:136:SER:HB3	2:B:172:LEU:HD13	1.69	0.75
3:C:54:ASP:OD2	3:C:103:GLY:HA3	1.86	0.75
2:E:136:SER:HB3	2:E:172:LEU:HD13	1.68	0.74
1:D:188:THR:HG23	1:D:190:TYR:H	1.52	0.74
1:A:106:TYR:CE2	1:A:189:TYR:HD2	2.06	0.74
1:A:188:THR:HG23	1:A:190:TYR:H	1.52	0.73
2:B:219:GLU:OE1	2:B:249:ARG:HD3	1.88	0.73
3:F:99:PHE:CE1	3:F:146:LEU:HB2	2.25	0.72
3:F:177:ARG:HE	3:F:177:ARG:CA	1.97	0.72
2:B:224:ILE:HG22	2:B:259:ALA:HB2	1.72	0.72
2:B:102:ASN:ND2	2:B:125:ARG:HH22	1.88	0.71
2:E:219:GLU:OE1	2:E:249:ARG:HD3	1.91	0.71
1:A:78:MET:HE3	1:A:118:ILE:HD11	1.72	0.70
2:B:262:MET:HG3	2:B:278:SER:HB3	1.73	0.70
3:F:25:ASP:CB	3:F:26:PRO:CD	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:PHE:C	3:C:99:PHE:CD2	2.69	0.70
2:E:262:MET:HG3	2:E:278:SER:HB3	1.73	0.70
2:B:142:GLN:OE1	2:B:143:SER:N	2.24	0.69
3:C:99:PHE:HZ	3:C:145:ARG:HA	1.57	0.69
3:C:25:ASP:CB	3:C:26:PRO:CD	2.71	0.69
2:E:224:ILE:HG22	2:E:259:ALA:HB2	1.75	0.68
1:A:186:SER:OG	1:A:188:THR:HG22	1.95	0.67
1:D:220:THR:C	3:F:120:THR:HG22	2.21	0.66
2:E:63:MET:HB3	2:E:158:THR:HB	1.77	0.66
3:F:99:PHE:HD2	3:F:100:PRO:HA	1.61	0.66
1:A:101:ALA:HB3	1:A:191:SER:HB2	1.78	0.65
2:E:23:ASN:N	2:E:23:ASN:HD22	1.93	0.65
1:A:220:THR:C	3:C:120:THR:HG22	2.22	0.65
2:E:190:ARG:HD2	4:E:343:HOH:O	1.97	0.64
1:D:78:MET:HE3	1:D:118:ILE:HD11	1.79	0.64
1:A:220:THR:OG1	3:C:157:THR:HG22	1.98	0.64
1:A:79:THR:HG23	1:A:215:PRO:HA	1.79	0.64
2:B:270:ILE:HD12	2:B:270:ILE:H	1.62	0.63
1:D:186:SER:OG	1:D:188:THR:HG22	1.98	0.63
2:E:25:SER:HA	2:E:257:ILE:HD11	1.80	0.63
3:F:54:ASP:OD2	3:F:103:GLY:HA3	1.99	0.63
1:A:106:TYR:CD2	1:A:189:TYR:HD2	2.17	0.62
1:D:79:THR:HG23	1:D:215:PRO:HA	1.80	0.62
2:B:63:MET:HB3	2:B:158:THR:HB	1.80	0.62
3:F:25:ASP:CG	3:F:26:PRO:HD3	2.25	0.61
1:D:101:ALA:HB3	1:D:191:SER:HB2	1.83	0.60
1:A:219:ALA:HB1	3:C:120:THR:CG2	2.32	0.60
2:E:270:ILE:HD12	2:E:270:ILE:H	1.67	0.60
1:A:73:GLU:N	1:A:74:PRO:CD	2.65	0.60
2:E:25:SER:CA	2:E:257:ILE:HD11	2.31	0.60
3:F:120:THR:OG1	3:F:124:ALA:O	2.21	0.59
3:F:177:ARG:NH1	3:F:178:PRO:HD3	2.18	0.59
1:A:219:ALA:CB	3:C:120:THR:HG21	2.31	0.59
1:D:220:THR:OG1	3:F:157:THR:HG22	2.02	0.59
3:C:167:LEU:HB3	3:C:168:PRO:HD2	1.83	0.59
3:C:54:ASP:CG	3:C:103:GLY:HA3	2.29	0.58
3:F:167:LEU:HB3	3:F:168:PRO:HD2	1.85	0.57
1:A:120:PRO:O	2:B:283:ARG:NH1	2.37	0.57
3:F:66:TRP:CH2	3:F:97:PHE:HB2	2.40	0.57
3:F:71:TYR:OH	3:F:75:GLU:OE2	2.18	0.57
3:F:99:PHE:HE1	3:F:145:ARG:C	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLY:HA3	2:B:41:ASN:ND2	2.20	0.57
2:B:262:MET:HE2	2:B:265:GLN:HG3	1.86	0.57
3:F:151:ILE:H	3:F:151:ILE:CD1	2.19	0.56
2:E:68:GLY:HA2	2:E:117:ARG:HA	1.87	0.56
2:E:262:MET:HE2	2:E:265:GLN:HG3	1.87	0.56
1:D:220:THR:O	3:F:120:THR:HG22	2.06	0.56
2:B:25:SER:HA	2:B:257:ILE:HD11	1.87	0.55
2:B:68:GLY:HA2	2:B:117:ARG:HA	1.88	0.55
1:D:179:CYS:HG	1:D:198:CYS:CB	2.18	0.55
2:E:28:LYS:NZ	2:E:56:GLU:O	2.29	0.55
3:C:151:ILE:H	3:C:151:ILE:CD1	2.16	0.55
2:B:128:ALA:HA	2:B:151:ILE:HD13	1.89	0.55
3:C:71:TYR:OH	3:C:75:GLU:OE2	2.20	0.55
3:C:66:TRP:CH2	3:C:97:PHE:HB2	2.42	0.55
1:D:120:PRO:O	2:E:283:ARG:NH1	2.40	0.55
3:C:25:ASP:CG	3:C:26:PRO:HD3	2.31	0.55
1:D:99:LEU:HD21	1:D:138:ILE:HG12	1.89	0.55
3:C:135:CYS:HG	3:C:149:CYS:CB	2.18	0.54
3:C:99:PHE:C	3:C:99:PHE:HD2	2.15	0.54
2:E:28:LYS:HE3	2:E:58:GLY:O	2.07	0.54
3:F:99:PHE:HZ	3:F:145:ARG:HA	1.73	0.54
3:C:177:ARG:NH1	3:C:178:PRO:HD2	2.23	0.54
3:F:99:PHE:HD2	3:F:100:PRO:CA	2.20	0.54
2:B:140:VAL:HG23	2:E:190:ARG:HH22	1.73	0.54
2:B:223:ILE:HG13	2:B:241:ILE:HD12	1.89	0.54
2:E:234:GLY:O	3:F:178:PRO:HA	2.08	0.54
3:F:25:ASP:CB	3:F:26:PRO:HD3	2.37	0.53
2:B:190:ARG:NH2	2:E:141:LEU:CD1	2.71	0.53
2:B:31:THR:HB	2:B:197:VAL:HG12	1.89	0.53
3:F:167:LEU:HB3	3:F:168:PRO:CD	2.39	0.53
2:E:31:THR:HB	2:E:197:VAL:HG12	1.89	0.53
1:D:73:GLU:N	1:D:74:PRO:CD	2.71	0.53
2:E:76:ARG:NH1	2:E:89:GLU:HB3	2.23	0.53
3:F:42:LEU:HD23	3:F:51:ILE:HG13	1.89	0.53
3:C:91:VAL:HG12	3:C:91:VAL:O	2.09	0.53
3:C:99:PHE:CZ	3:C:145:ARG:HA	2.42	0.53
3:C:134:PHE:CZ	3:C:148:PRO:HG3	2.45	0.52
2:B:25:SER:CA	2:B:257:ILE:HD11	2.40	0.52
3:C:101:GLY:O	3:C:102:GLU:C	2.51	0.52
3:F:139:HIS:CG	3:F:145:ARG:HH11	2.27	0.52
2:B:234:GLY:O	3:C:178:PRO:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:ASN:O	3:C:63:SER:OG	2.22	0.52
3:F:177:ARG:HH11	3:F:178:PRO:HD3	1.73	0.52
2:E:174:ARG:NH1	4:E:316:HOH:O	2.38	0.52
3:C:167:LEU:HB3	3:C:168:PRO:CD	2.40	0.51
1:A:99:LEU:HD21	1:A:138:ILE:HG12	1.91	0.51
3:C:114:VAL:HG12	3:C:130:ALA:HB2	1.93	0.51
3:C:139:HIS:CG	3:C:145:ARG:HH11	2.28	0.51
2:E:142:GLN:OE1	2:E:143:SER:N	2.44	0.51
3:F:99:PHE:CD2	3:F:100:PRO:HA	2.42	0.51
1:D:199:ASP:CG	1:D:206:ARG:HH12	2.18	0.51
2:E:63:MET:HG3	2:E:197:VAL:HB	1.92	0.51
1:D:221:ALA:HB3	3:F:153:VAL:O	2.11	0.51
1:A:199:ASP:CG	1:A:206:ARG:HH12	2.19	0.51
2:B:178:THR:HA	2:B:182:SER:OG	2.11	0.50
3:F:60:ASN:O	3:F:63:SER:OG	2.16	0.50
2:B:242:LEU:C	2:B:242:LEU:HD12	2.36	0.50
2:E:36:GLY:HA3	2:E:41:ASN:ND2	2.27	0.50
2:B:63:MET:HG3	2:B:197:VAL:HB	1.93	0.50
2:B:112:ASP:O	2:B:116:ASN:HA	2.12	0.50
2:B:174:ARG:O	2:B:178:THR:HG23	2.12	0.50
2:E:25:SER:HA	2:E:257:ILE:CD1	2.42	0.50
2:E:219:GLU:HB3	2:E:249:ARG:HG2	1.94	0.50
3:F:62:LEU:HD22	4:F:208:HOH:O	2.12	0.50
3:F:98:ALA:O	3:F:101:GLY:HA3	2.12	0.49
2:B:219:GLU:HB3	2:B:249:ARG:HG2	1.94	0.49
1:D:219:ALA:HB1	3:F:120:THR:HG21	1.94	0.49
1:A:213:ALA:HB1	1:A:214:PRO:CD	2.43	0.49
3:C:120:THR:OG1	3:C:124:ALA:O	2.29	0.49
2:E:112:ASP:O	2:E:116:ASN:HA	2.13	0.49
3:F:54:ASP:CG	3:F:103:GLY:HA3	2.38	0.49
2:E:76:ARG:HG3	2:E:76:ARG:HH11	1.77	0.49
3:C:98:ALA:HB2	3:C:105:THR:HG22	1.94	0.48
1:A:106:TYR:CD2	1:A:189:TYR:CD2	3.00	0.48
2:B:63:MET:CE	2:B:122:ILE:HG12	2.44	0.48
2:E:134:VAL:HG11	2:E:176:ILE:HG13	1.94	0.48
3:F:139:HIS:ND1	3:F:145:ARG:HD2	2.28	0.48
3:F:91:VAL:O	3:F:91:VAL:HG12	2.13	0.48
1:D:129:PHE:O	1:D:137:CYS:HA	2.13	0.48
1:D:199:ASP:OD1	1:D:201:ALA:HB2	2.14	0.48
2:B:140:VAL:HG22	4:E:347:HOH:O	2.13	0.48
1:A:106:TYR:CE2	1:A:189:TYR:CD2	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ALA:HB1	1:A:214:PRO:HD2	1.95	0.47
3:F:99:PHE:CE1	3:F:145:ARG:C	2.91	0.47
2:E:63:MET:HE2	2:E:158:THR:HB	1.96	0.47
3:C:99:PHE:C	3:C:101:GLY:N	2.69	0.47
2:E:242:LEU:C	2:E:242:LEU:HD12	2.39	0.47
2:B:134:VAL:HG11	2:B:176:ILE:HG13	1.95	0.47
3:F:75:GLU:CD	3:F:75:GLU:H	2.22	0.47
3:F:101:GLY:O	3:F:102:GLU:C	2.57	0.47
1:A:73:GLU:N	1:A:74:PRO:HD2	2.30	0.47
2:B:50:ARG:NH2	2:B:95:LEU:O	2.47	0.47
3:C:39:ARG:NH1	3:C:39:ARG:HG2	2.30	0.47
3:F:39:ARG:HH11	3:F:39:ARG:HG2	1.79	0.47
2:B:280:VAL:HG12	2:B:281:HIS:N	2.30	0.46
3:F:39:ARG:HG2	3:F:39:ARG:NH1	2.29	0.46
2:B:256:ARG:HG3	2:B:256:ARG:HH11	1.80	0.46
2:E:223:ILE:HG13	2:E:241:ILE:HD12	1.97	0.46
3:F:114:VAL:HG12	3:F:130:ALA:HB2	1.98	0.46
1:A:106:TYR:CE1	1:A:189:TYR:CE2	3.03	0.46
2:B:37:SER:H	2:B:41:ASN:HD22	1.64	0.46
2:E:256:ARG:O	2:E:281:HIS:HD2	1.98	0.46
2:B:63:MET:HE2	2:B:158:THR:HB	1.98	0.46
2:B:88:ILE:HG23	2:B:88:ILE:O	2.16	0.46
2:B:135:HIS:HD2	2:B:139:SER:CB	2.18	0.46
2:B:222:ILE:HD12	2:B:223:ILE:N	2.32	0.46
2:E:88:ILE:O	2:E:88:ILE:HG23	2.15	0.46
2:B:256:ARG:O	2:B:281:HIS:HD2	1.98	0.45
2:E:174:ARG:O	2:E:178:THR:HG23	2.16	0.45
2:B:31:THR:HB	2:B:197:VAL:CG1	2.47	0.45
3:C:25:ASP:CB	3:C:26:PRO:HD3	2.45	0.45
2:E:178:THR:HA	2:E:182:SER:OG	2.16	0.45
2:E:50:ARG:NH2	2:E:95:LEU:O	2.49	0.45
2:B:256:ARG:HG3	2:B:256:ARG:NH1	2.32	0.45
1:D:73:GLU:N	1:D:74:PRO:HD2	2.31	0.45
2:E:63:MET:CE	2:E:122:ILE:HG12	2.47	0.45
3:F:83:GLY:HA3	3:F:116:ASN:OD1	2.17	0.45
1:D:73:GLU:HG3	1:D:77:PHE:HE2	1.81	0.45
2:E:31:THR:HB	2:E:197:VAL:CG1	2.47	0.45
2:E:128:ALA:HA	2:E:151:ILE:HD13	1.98	0.45
2:E:280:VAL:HG12	2:E:281:HIS:N	2.32	0.45
2:B:76:ARG:NH1	2:B:89:GLU:HB3	2.32	0.45
3:F:109:ASP:OD2	3:F:112:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:H	1:A:74:PRO:CD	2.30	0.45
3:C:39:ARG:HG2	3:C:39:ARG:HH11	1.81	0.44
3:C:57:ASP:C	3:C:59:HIS:H	2.25	0.44
3:F:108:LYS:HA	3:F:108:LYS:HD3	1.63	0.44
1:D:213:ALA:HB1	1:D:214:PRO:CD	2.47	0.44
2:B:28:LYS:HE2	2:B:58:GLY:O	2.18	0.44
3:C:91:VAL:O	3:C:91:VAL:CG1	2.64	0.44
2:B:32:TRP:CZ2	2:B:272:SER:HB3	2.52	0.44
1:D:179:CYS:SG	1:D:198:CYS:CB	3.05	0.44
1:A:106:TYR:CZ	1:A:189:TYR:CD2	3.05	0.44
1:A:186:SER:HG	1:A:188:THR:HG22	1.81	0.44
2:E:232:ARG:HG2	2:E:232:ARG:HH11	1.82	0.44
2:B:76:ARG:HG3	2:B:76:ARG:HH11	1.82	0.44
1:D:220:THR:HA	3:F:157:THR:HA	1.99	0.44
2:B:158:THR:HA	2:B:197:VAL:O	2.18	0.44
1:A:129:PHE:O	1:A:137:CYS:HA	2.18	0.44
3:C:83:GLY:HA3	3:C:116:ASN:OD1	2.18	0.44
2:E:158:THR:HA	2:E:197:VAL:O	2.18	0.44
3:F:57:ASP:C	3:F:59:HIS:H	2.25	0.44
1:D:213:ALA:HB1	1:D:214:PRO:HD2	1.99	0.43
2:E:37:SER:H	2:E:41:ASN:HD22	1.66	0.43
2:E:142:GLN:OE1	2:E:142:GLN:N	2.52	0.43
2:E:188:GLU:H	2:E:188:GLU:CD	2.26	0.43
2:B:135:HIS:CD2	2:B:139:SER:CB	2.97	0.43
3:C:42:LEU:HD23	3:C:51:ILE:HG13	2.00	0.43
2:E:256:ARG:HG3	2:E:256:ARG:HH11	1.83	0.43
1:A:199:ASP:OD1	1:A:201:ALA:HB2	2.18	0.43
2:B:37:SER:N	2:B:41:ASN:HD22	2.16	0.43
2:B:100:ARG:HE	2:B:100:ARG:HB3	1.45	0.43
3:C:57:ASP:C	3:C:59:HIS:N	2.77	0.43
2:B:140:VAL:CG2	4:E:347:HOH:O	2.67	0.43
2:B:142:GLN:OE1	2:B:142:GLN:CA	2.67	0.43
1:A:80:LEU:HD22	1:A:171:ILE:HD11	2.00	0.42
3:C:75:GLU:CD	3:C:75:GLU:H	2.27	0.42
3:F:151:ILE:HD13	3:F:151:ILE:N	2.24	0.42
3:F:139:HIS:CE1	3:F:145:ARG:HD2	2.54	0.42
2:E:37:SER:N	2:E:41:ASN:HD22	2.17	0.42
1:A:221:ALA:HB3	3:C:153:VAL:O	2.20	0.42
2:B:103:MET:HE3	2:B:103:MET:HB3	1.87	0.42
2:E:100:ARG:HE	2:E:100:ARG:HB3	1.46	0.42
1:A:220:THR:HA	3:C:157:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:57:ASP:C	3:F:59:HIS:N	2.78	0.42
2:E:249:ARG:C	2:E:250:ARG:HG3	2.45	0.42
2:B:257:ILE:HD13	4:B:298:HOH:O	2.19	0.42
3:C:109:ASP:OD2	3:C:112:HIS:HD2	2.02	0.42
2:E:256:ARG:HG3	2:E:256:ARG:NH1	2.35	0.42
1:A:73:GLU:HG3	1:A:77:PHE:HE2	1.85	0.41
2:B:186:SER:OG	2:B:189:ARG:HG3	2.20	0.41
3:C:87:GLN:HG2	3:C:113:THR:O	2.20	0.41
3:C:128:LYS:HA	3:C:134:PHE:O	2.20	0.41
1:A:184:PRO:CG	1:A:207:ASP:HB2	2.50	0.41
2:E:133:ILE:HD13	2:E:147:VAL:HG22	2.02	0.41
3:F:53:ASN:HB3	3:F:66:TRP:CH2	2.55	0.41
3:F:102:GLU:H	3:F:102:GLU:HG3	1.14	0.41
1:D:214:PRO:HG2	3:F:45:LEU:HD11	2.02	0.41
2:E:32:TRP:CZ2	2:E:272:SER:HB3	2.55	0.41
2:B:232:ARG:HH11	2:B:232:ARG:HG2	1.86	0.41
2:E:220:ASN:O	2:E:243:HIS:ND1	2.45	0.41
1:A:219:ALA:O	3:C:157:THR:HA	2.20	0.40
3:F:72:LYS:HE2	3:F:72:LYS:HB3	1.81	0.40
2:E:41:ASN:HD21	2:E:68:GLY:HA3	1.86	0.40
2:E:103:MET:HB3	2:E:103:MET:HE3	1.80	0.40
3:C:151:ILE:HD13	3:C:151:ILE:N	2.21	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	151/222 (68%)	145 (96%)	6 (4%)	0	100	100
1	D	151/222 (68%)	145 (96%)	6 (4%)	0	100	100
2	B	259/283 (92%)	248 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	259/283 (92%)	247 (95%)	12 (5%)	0	100	100
3	C	152/186 (82%)	147 (97%)	4 (3%)	1 (1%)	18	28
3	F	152/186 (82%)	147 (97%)	5 (3%)	0	100	100
All	All	1124/1382 (81%)	1079 (96%)	44 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	101	GLY

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	132/195 (68%)	130 (98%)	2 (2%)	57	77
1	D	132/195 (68%)	128 (97%)	4 (3%)	36	58
2	B	223/244 (91%)	204 (92%)	19 (8%)	10	16
2	E	223/244 (91%)	203 (91%)	20 (9%)	9	15
3	C	135/164 (82%)	121 (90%)	14 (10%)	7	10
3	F	135/164 (82%)	123 (91%)	12 (9%)	9	15
All	All	980/1206 (81%)	909 (93%)	71 (7%)	13	23

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	216	VAL
2	B	38	SER
2	B	40	VAL
2	B	63	MET
2	B	78	SER
2	B	80	VAL

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Mol	Chain	Res	Type
2	B	81	ILE
2	B	99	SER
2	B	100	ARG
2	B	102	ASN
2	B	125	ARG
2	B	137	ASP
2	B	142	GLN
2	B	172	LEU
2	B	185	SER
2	B	222	ILE
2	B	241	ILE
2	B	257	ILE
2	B	268	SER
2	B	272	SER
3	C	39	ARG
3	C	41	SER
3	C	55	HIS
3	C	58	SER
3	C	72	LYS
3	C	78	LYS
3	C	91	VAL
3	C	95	LYS
3	C	102	GLU
3	C	108	LYS
3	C	120	THR
3	C	145	ARG
3	C	151	ILE
3	C	177	ARG
1	D	90	VAL
1	D	99	LEU
1	D	117	LYS
1	D	216	VAL
2	E	23	ASN
2	E	38	SER
2	E	40	VAL
2	E	63	MET
2	E	78	SER
2	E	80	VAL
2	E	81	ILE
2	E	99	SER
2	E	100	ARG
2	E	125	ARG

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Mol	Chain	Res	Type
2	E	137	ASP
2	E	142	GLN
2	E	172	LEU
2	E	188	GLU
2	E	222	ILE
2	E	228	GLU
2	E	241	ILE
2	E	257	ILE
2	E	268	SER
2	E	272	SER
3	F	39	ARG
3	F	55	HIS
3	F	58	SER
3	F	72	LYS
3	F	91	VAL
3	F	95	LYS
3	F	102	GLU
3	F	108	LYS
3	F	120	THR
3	F	145	ARG
3	F	151	ILE
3	F	177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	ASN
2	B	57	GLN
2	B	102	ASN
2	B	135	HIS
2	B	281	HIS
3	C	55	HIS
3	C	112	HIS
1	D	108	GLN
2	E	41	ASN
2	E	57	GLN
2	E	102	ASN
2	E	135	HIS
2	E	281	HIS
3	F	55	HIS
3	F	112	HIS

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](#)

There are no ligands in this entry.

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	153/222 (68%)	-0.13	3 (1%) 65 60	2, 8, 23, 51	0
1	D	153/222 (68%)	-0.12	4 (2%) 57 53	2, 8, 23, 47	0
2	B	261/283 (92%)	-0.21	2 (0%) 82 80	2, 6, 25, 44	0
2	E	261/283 (92%)	-0.21	3 (1%) 78 74	2, 7, 26, 44	0
3	C	154/186 (82%)	0.29	13 (8%) 17 14	3, 15, 39, 65	0
3	F	154/186 (82%)	0.13	7 (4%) 38 34	3, 11, 33, 50	0
All	All	1136/1382 (82%)	-0.07	32 (2%) 55 51	2, 8, 29, 65	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	PRO	9.3
3	F	100	PRO	9.3
1	A	71	PRO	8.0
1	D	72	SER	7.6
3	F	102	GLU	6.3
3	C	102	GLU	6.1
1	A	72	SER	6.0
3	F	101	GLY	5.8
3	C	101	GLY	5.4
3	C	100	PRO	4.8
3	C	103	GLY	4.8
3	C	99	PHE	3.8
3	F	103	GLY	3.6
3	F	99	PHE	3.6
3	C	57	ASP	3.5
2	B	83	HIS	2.8
3	C	105	THR	2.7
3	C	78	LYS	2.6
2	E	256	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	25	ASP	2.5
1	D	189	TYR	2.4
2	E	84	GLY	2.3
3	C	106	ASP	2.3
3	F	25	ASP	2.3
1	D	91	TRP	2.3
3	C	178	PRO	2.2
3	C	177	ARG	2.2
3	F	177	ARG	2.2
1	A	91	TRP	2.1
3	C	55	HIS	2.1
2	E	100	ARG	2.0
2	B	84	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.