



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:15 AM UTC

PDB ID : 4JDM / pdb_00004jdm
Title : Secreted Chlamydial Protein PGP3, full-length
Authors : Galaledeen, A.; Taylor, A.B.; Chen, D.; Holloway, S.P.; Zhong, G.; Hart, P.J.
Deposited on : 2013-02-25
Resolution : 3.10 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)
Xtrriage (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

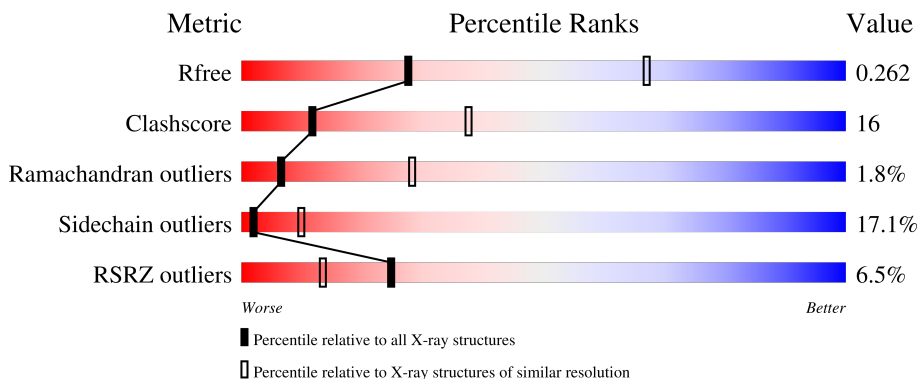
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



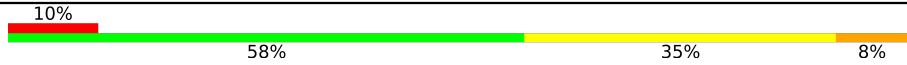
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	269	
1	B	269	
1	C	269	
1	D	269	
1	E	269	

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Mol	Chain	Length	Quality of chain
1	F	269	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '10%', a green segment labeled '58%', a yellow segment labeled '35%', and a small orange segment on the far right labeled '8%'.</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 11712 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 Virulence plasmid protein pGP3-D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	263	1939	1215	317	399	4	4	0	0	0
1	B	263	1941	1217	317	398	4	5	0	0	0
1	C	269	1976	1238	323	406	4	5	0	0	0
1	D	263	1939	1215	317	399	4	4	0	0	0
1	E	263	1941	1217	317	398	4	5	0	0	0
1	F	269	1976	1238	323	406	4	5	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP D7DHH5
A	-3	PRO	-	expression tag	UNP D7DHH5
A	-2	LEU	-	expression tag	UNP D7DHH5
A	-1	GLY	-	expression tag	UNP D7DHH5
A	0	SER	-	expression tag	UNP D7DHH5
B	-4	GLY	-	expression tag	UNP D7DHH5
B	-3	PRO	-	expression tag	UNP D7DHH5
B	-2	LEU	-	expression tag	UNP D7DHH5
B	-1	GLY	-	expression tag	UNP D7DHH5
B	0	SER	-	expression tag	UNP D7DHH5
C	-4	GLY	-	expression tag	UNP D7DHH5
C	-3	PRO	-	expression tag	UNP D7DHH5
C	-2	LEU	-	expression tag	UNP D7DHH5
C	-1	GLY	-	expression tag	UNP D7DHH5
C	0	SER	-	expression tag	UNP D7DHH5
D	-4	GLY	-	expression tag	UNP D7DHH5
D	-3	PRO	-	expression tag	UNP D7DHH5

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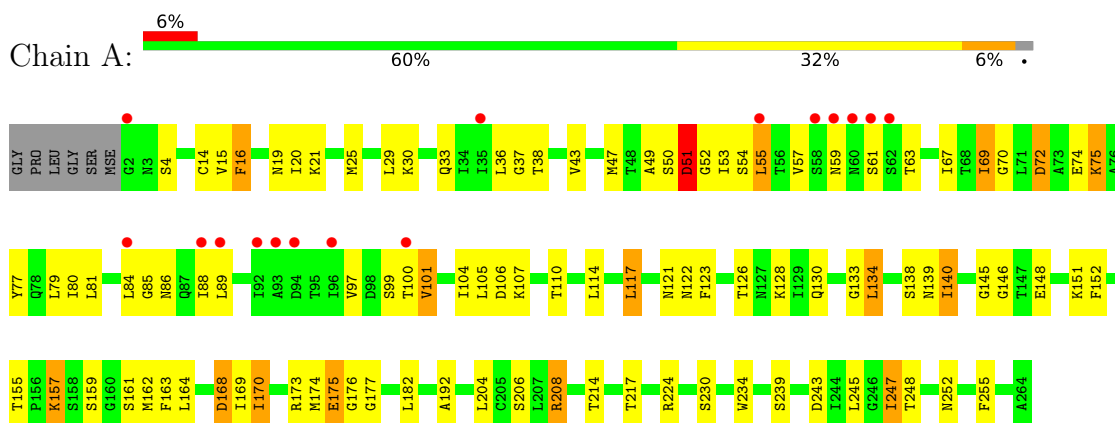
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP D7DHH5
D	-1	GLY	-	expression tag	UNP D7DHH5
D	0	SER	-	expression tag	UNP D7DHH5
E	-4	GLY	-	expression tag	UNP D7DHH5
E	-3	PRO	-	expression tag	UNP D7DHH5
E	-2	LEU	-	expression tag	UNP D7DHH5
E	-1	GLY	-	expression tag	UNP D7DHH5
E	0	SER	-	expression tag	UNP D7DHH5
F	-4	GLY	-	expression tag	UNP D7DHH5
F	-3	PRO	-	expression tag	UNP D7DHH5
F	-2	LEU	-	expression tag	UNP D7DHH5
F	-1	GLY	-	expression tag	UNP D7DHH5
F	0	SER	-	expression tag	UNP D7DHH5

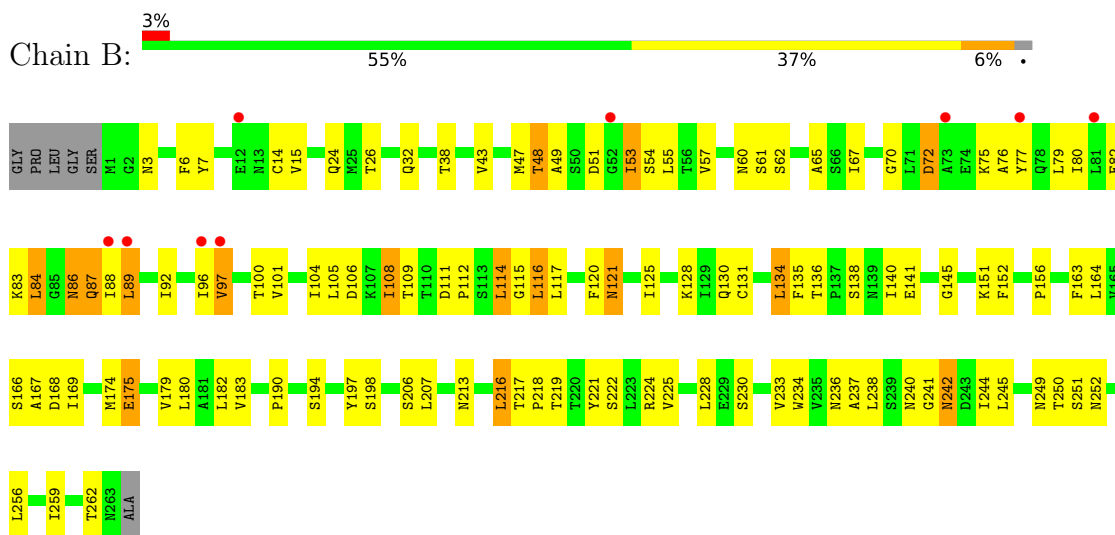
3 Residue-property plots

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.

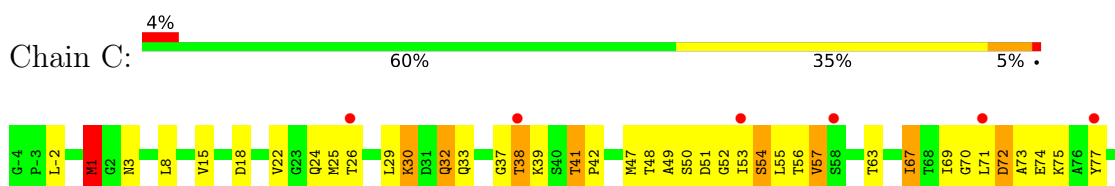
- Molecule 1: Virulence plasmid protein pGP3-D

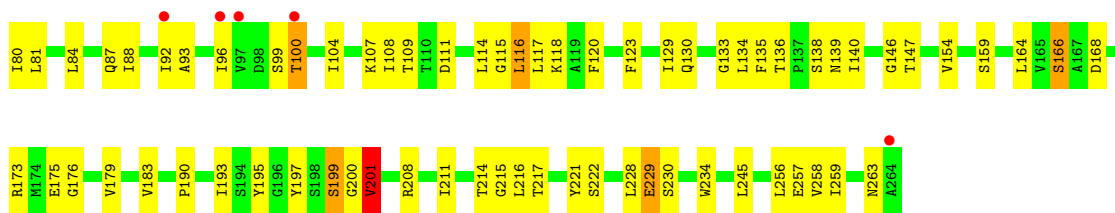


- Molecule 1: Virulence plasmid protein pGP3-D

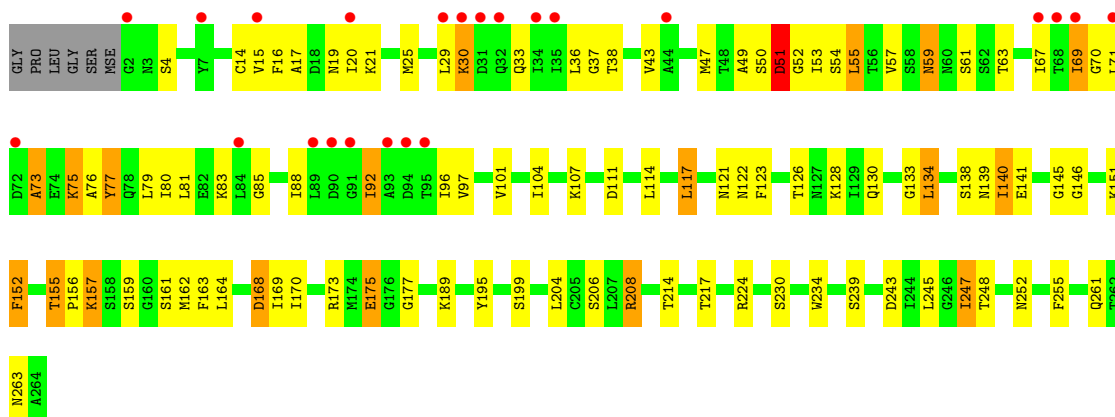


- Molecule 1: Virulence plasmid protein pGP3-D

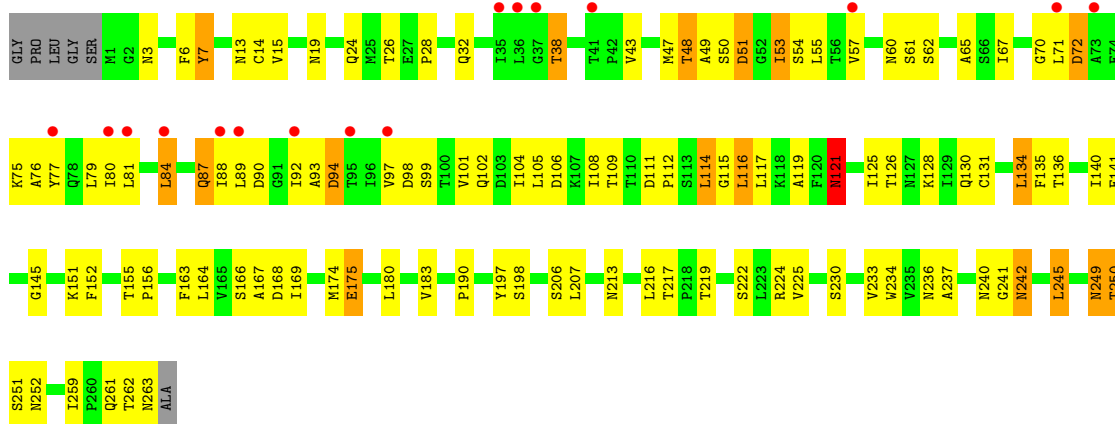




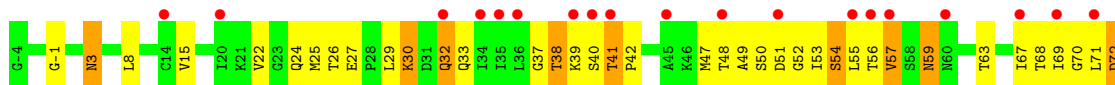
● Molecule 1: Virulence plasmid protein pGP3-D

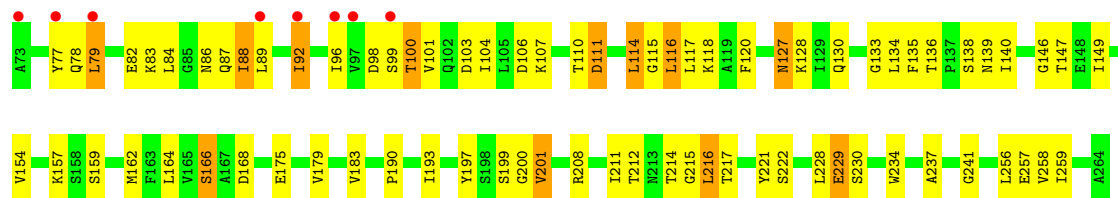


● Molecule 1: Virulence plasmid protein pGP3-D



● Molecule 1: Virulence plasmid protein pGP3-D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.70Å 223.79Å 79.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 3.10 48.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.4 (48.12-3.10) 90.7 (48.12-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.231 , 0.264 0.234 , 0.262	Depositor DCC
R_{free} test set	2828 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtrriage
Anisotropy	0.728	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11712	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 44.12 % 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 1.5988e-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

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	0.70	0/1960	1.04	6/2660 (0.2%)
1	B	0.75	2/1962 (0.1%)	1.08	4/2663 (0.2%)
1	C	0.73	0/1997	1.07	8/2708 (0.3%)
1	D	0.69	0/1960	1.03	7/2660 (0.3%)
1	E	0.71	2/1962 (0.1%)	1.06	4/2663 (0.2%)
1	F	0.74	1/1997 (0.1%)	1.06	7/2708 (0.3%)
All	All	0.72	5/11838 (0.0%)	1.06	36/16062 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	ASN	CG-ND2	-7.05	1.18	1.33
1	B	121	ASN	CG-OD1	-6.70	1.10	1.23
1	E	121	ASN	CG-ND2	-6.40	1.19	1.33
1	F	149	ILE	CA-CB	5.86	1.61	1.54
1	E	121	ASN	CG-OD1	-5.46	1.13	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASP	CA-C-N	8.37	128.06	119.19
1	C	111	ASP	C-N-CA	8.37	128.06	119.19
1	C	200	GLY	N-CA-C	-8.35	104.54	114.48
1	F	200	GLY	N-CA-C	-8.14	104.80	114.48
1	B	241	GLY	N-CA-C	6.66	121.58	113.79
1	C	201	VAL	CA-C-N	6.61	126.64	119.90
1	C	201	VAL	C-N-CA	6.61	126.64	119.90
1	F	201	VAL	CA-C-N	6.29	126.66	119.93
1	F	201	VAL	C-N-CA	6.29	126.66	119.93
1	F	111	ASP	CA-C-N	5.82	125.35	119.19
1	F	111	ASP	C-N-CA	5.82	125.35	119.19
1	A	252	ASN	N-CA-C	5.79	118.90	109.06
1	A	155	THR	CA-C-N	5.75	125.69	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	THR	C-N-CA	5.75	125.69	119.76
1	F	114	LEU	N-CA-C	5.69	118.69	111.69
1	B	116	LEU	N-CA-C	-5.52	101.30	109.86
1	D	217	THR	CA-C-N	5.51	125.52	119.90
1	D	217	THR	C-N-CA	5.51	125.52	119.90
1	D	155	THR	CA-C-N	5.50	125.45	119.78
1	D	155	THR	C-N-CA	5.50	125.45	119.78
1	E	241	GLY	N-CA-C	5.42	120.14	113.79
1	C	111	ASP	N-CA-C	5.42	117.28	109.04
1	E	216	LEU	N-CA-C	-5.33	103.68	111.30
1	A	43	VAL	CB-CA-C	-5.31	103.91	111.19
1	D	43	VAL	CB-CA-C	-5.24	104.57	111.70
1	B	86	ASN	N-CA-C	5.14	116.88	111.28
1	C	123	PHE	CA-C-N	5.13	125.53	119.99
1	C	123	PHE	C-N-CA	5.13	125.53	119.99
1	B	216	LEU	N-CA-C	-5.11	103.99	111.30
1	D	252	ASN	N-CA-C	5.10	117.73	109.06
1	E	155	THR	CA-C-N	5.07	125.31	119.83
1	E	155	THR	C-N-CA	5.07	125.31	119.83
1	F	216	LEU	N-CA-C	-5.07	106.68	112.92
1	A	217	THR	CA-C-N	5.06	125.06	119.90
1	A	217	THR	C-N-CA	5.06	125.06	119.90
1	D	199	SER	N-CA-C	-5.05	106.81	113.17

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	1939	0	1957	78	0
1	B	1941	0	1964	66	0
1	C	1976	0	1998	60	0
1	D	1939	0	1957	74	0
1	E	1941	0	1964	82	0
1	F	1976	0	1998	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11712	0	11838	375	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 16.

All (375) 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:123:PHE:CE2	1:A:152:PHE:HB3	1.71	1.25
1:D:123:PHE:CE2	1:D:152:PHE:HB3	1.74	1.21
1:A:123:PHE:HE2	1:A:152:PHE:HB3	1.11	0.96
1:A:123:PHE:CD2	1:A:152:PHE:HB3	2.05	0.92
1:E:156:PRO:HG3	1:E:213:ASN:HD22	1.35	0.92
1:A:97:VAL:HG22	1:C:100:THR:HG22	1.52	0.91
1:D:123:PHE:CD2	1:D:152:PHE:HB3	2.05	0.90
1:B:156:PRO:HG3	1:B:213:ASN:HD22	1.38	0.89
1:D:123:PHE:HD2	1:D:152:PHE:HD1	1.21	0.89
1:E:88:ILE:CG2	1:E:92:ILE:HD13	2.03	0.89
1:A:123:PHE:HD2	1:A:152:PHE:CD1	1.91	0.88
1:C:96:ILE:HA	1:C:99:SER:HB2	1.56	0.88
1:D:123:PHE:HD2	1:D:152:PHE:CD1	1.93	0.87
1:A:168:ASP:HB3	1:A:204:LEU:HD21	1.56	0.86
1:E:53:ILE:HG13	1:F:70:GLY:HA2	1.57	0.85
1:E:38:THR:HB	1:F:59:ASN:OD1	1.76	0.84
1:D:123:PHE:HE2	1:D:152:PHE:HB3	1.42	0.83
1:E:111:ASP:HB3	1:E:114:LEU:HG	1.59	0.82
1:D:168:ASP:HB3	1:D:204:LEU:HD21	1.61	0.81
1:B:53:ILE:HG13	1:C:70:GLY:HA2	1.63	0.81
1:B:87:GLN:CD	1:B:87:GLN:H	1.89	0.80
1:E:88:ILE:HG23	1:E:92:ILE:HD13	1.64	0.78
1:E:72:ASP:HB2	1:E:76:ALA:H	1.51	0.75
1:C:136:THR:OG1	1:C:139:ASN:ND2	2.20	0.74
1:C:140:ILE:HD11	1:C:193:ILE:HD13	1.69	0.74
1:E:72:ASP:OD2	1:E:72:ASP:N	2.21	0.73
1:A:123:PHE:HE2	1:A:152:PHE:CB	1.98	0.72
1:B:111:ASP:HB3	1:B:114:LEU:HG	1.71	0.72
1:E:76:ALA:HA	1:E:79:LEU:HD12	1.71	0.72
1:D:195:TYR:OH	1:E:249:ASN:ND2	2.23	0.71
1:D:123:PHE:CD2	1:D:152:PHE:CD1	2.80	0.70
1:C:208:ARG:NH1	1:C:208:ARG:HB3	2.07	0.70
1:A:47:MSE:HG2	1:B:67:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ILE:HG22	1:E:92:ILE:HD13	1.74	0.69
1:F:37:GLY:HA2	1:F:42:PRO:HB3	1.75	0.69
1:A:16:PHE:HD1	1:A:16:PHE:O	1.76	0.69
1:F:136:THR:OG1	1:F:139:ASN:ND2	2.26	0.68
1:B:53:ILE:HD11	1:C:71:LEU:HG	1.75	0.68
1:E:128:LYS:HZ2	1:E:242:ASN:HA	1.59	0.67
1:D:57:VAL:HG12	1:D:67:ILE:HG22	1.76	0.67
1:D:123:PHE:CE2	1:D:152:PHE:CB	2.67	0.67
1:C:37:GLY:HA2	1:C:42:PRO:HB3	1.76	0.67
1:B:128:LYS:HD2	1:B:237:ALA:HB2	1.75	0.67
1:A:67:ILE:HD11	1:C:47:MSE:HE3	1.77	0.66
1:C:208:ARG:HB3	1:C:208:ARG:HH11	1.59	0.66
1:E:128:LYS:HD2	1:E:237:ALA:HB2	1.76	0.65
1:D:47:MSE:HG2	1:E:67:ILE:HD11	1.78	0.65
1:F:140:ILE:HD11	1:F:193:ILE:HD13	1.79	0.65
1:E:183:VAL:HG22	1:E:190:PRO:HA	1.79	0.65
1:F:208:ARG:HB3	1:F:208:ARG:NH1	2.11	0.65
1:E:87:GLN:N	1:E:87:GLN:OE1	2.30	0.64
1:F:72:ASP:OD1	1:F:72:ASP:N	2.30	0.64
1:A:72:ASP:OD1	1:A:72:ASP:N	2.31	0.64
1:E:57:VAL:HG12	1:E:67:ILE:HG22	1.80	0.64
1:E:128:LYS:NZ	1:E:242:ASN:HA	2.13	0.64
1:D:121:ASN:HB3	1:D:123:PHE:CE1	2.33	0.64
1:A:57:VAL:HG12	1:A:67:ILE:HG22	1.80	0.63
1:B:87:GLN:HG3	1:C:77:TYR:OH	1.98	0.63
1:B:49:ALA:HB1	1:B:53:ILE:HB	1.81	0.63
1:A:16:PHE:O	1:A:16:PHE:CD1	2.52	0.63
1:B:72:ASP:N	1:B:72:ASP:OD1	2.30	0.63
1:E:72:ASP:HB3	1:E:75:LYS:HB2	1.81	0.63
1:C:72:ASP:OD1	1:C:72:ASP:N	2.30	0.62
1:F:-1:GLY:O	1:F:3:ASN:ND2	2.33	0.61
1:B:183:VAL:HG22	1:B:190:PRO:HA	1.82	0.61
1:B:57:VAL:HG12	1:B:67:ILE:HG22	1.82	0.61
1:E:49:ALA:HB1	1:E:53:ILE:HB	1.81	0.61
1:E:140:ILE:HG23	1:E:141:GLU:HG2	1.83	0.61
1:A:4:SER:C	1:A:16:PHE:CE1	2.78	0.61
1:E:116:LEU:N	1:E:116:LEU:HD13	2.16	0.61
1:E:125:ILE:O	1:E:236:ASN:ND2	2.34	0.61
1:F:57:VAL:HG12	1:F:67:ILE:HG22	1.80	0.61
1:F:166:SER:HB3	1:F:208:ARG:HD2	1.82	0.61
1:C:32:GLN:HE21	1:C:57:VAL:HG21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG12	1:C:67:ILE:HG22	1.82	0.60
1:B:140:ILE:HG23	1:B:141:GLU:HG2	1.83	0.60
1:A:16:PHE:CD1	1:A:16:PHE:C	2.79	0.59
1:F:208:ARG:HB3	1:F:208:ARG:HH11	1.67	0.59
1:A:4:SER:C	1:A:16:PHE:HE1	2.10	0.59
1:D:122:ASN:C	1:D:123:PHE:HD1	2.09	0.58
1:A:4:SER:HB2	1:B:6:PHE:CD2	2.38	0.58
1:A:16:PHE:HD1	1:A:16:PHE:C	2.10	0.58
1:A:51:ASP:HB2	1:A:79:LEU:HD12	1.85	0.58
1:B:75:LYS:O	1:B:79:LEU:HG	2.02	0.58
1:A:123:PHE:HD2	1:A:152:PHE:HD1	1.48	0.58
1:A:123:PHE:CD2	1:A:152:PHE:CD1	2.83	0.58
1:B:87:GLN:CD	1:B:87:GLN:N	2.61	0.57
1:E:93:ALA:O	1:E:97:VAL:HG23	2.04	0.57
1:F:96:ILE:HA	1:F:99:SER:HB2	1.86	0.57
1:E:109:THR:HA	1:E:117:LEU:HD11	1.87	0.57
1:F:32:GLN:HE21	1:F:57:VAL:HG21	1.68	0.57
1:D:77:TYR:HA	1:D:80:ILE:HD12	1.86	0.57
1:D:245:LEU:HD13	1:F:140:ILE:HD13	1.86	0.57
1:B:125:ILE:O	1:B:236:ASN:ND2	2.38	0.57
1:E:89:LEU:HD12	1:E:90:ASP:N	2.20	0.56
1:F:84:LEU:O	1:F:88:ILE:HB	2.05	0.56
1:A:161:SER:OG	1:A:162:MSE:N	2.38	0.56
1:A:104:ILE:HD11	1:B:101:VAL:HG22	1.86	0.56
1:C:118:LYS:HB3	1:C:257:GLU:HB3	1.88	0.56
1:C:166:SER:HB3	1:C:208:ARG:HD2	1.87	0.56
1:F:130:GLN:HB2	1:F:234:TRP:CH2	2.40	0.56
1:D:130:GLN:HB2	1:D:234:TRP:CZ2	2.41	0.56
1:D:51:ASP:HB2	1:D:79:LEU:HD12	1.86	0.56
1:F:135:PHE:CD2	1:F:179:VAL:HB	2.42	0.55
1:D:97:VAL:HG13	1:F:100:THR:HB	1.88	0.55
1:C:114:LEU:N	1:C:115:GLY:HA2	2.21	0.55
1:D:208:ARG:HH11	1:D:208:ARG:HB3	1.70	0.55
1:D:81:LEU:HA	1:D:85:GLY:HA3	1.88	0.55
1:C:25:MSE:HE1	1:C:29:LEU:HD23	1.89	0.54
1:D:161:SER:OG	1:D:162:MSE:N	2.39	0.54
1:A:133:GLY:C	1:A:146:GLY:HA2	2.33	0.54
1:C:1:MSE:HA	1:C:18:ASP:OD1	2.08	0.54
1:A:173:ARG:NH1	1:A:177:GLY:O	2.41	0.54
1:B:109:THR:HA	1:B:117:LEU:HD11	1.90	0.54
1:D:101:VAL:HG23	1:F:104:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ASN:O	1:B:89:LEU:HG	2.07	0.54
1:D:71:LEU:HD21	1:E:71:LEU:HD21	1.90	0.53
1:E:240:ASN:OD1	1:E:242:ASN:OD1	2.25	0.53
1:F:84:LEU:HB3	1:F:88:ILE:HD13	1.89	0.53
1:D:123:PHE:HE2	1:D:152:PHE:CB	2.16	0.53
1:A:36:LEU:HD11	1:B:32:GLN:HA	1.89	0.53
1:C:183:VAL:HG22	1:C:190:PRO:HA	1.91	0.53
1:D:75:LYS:O	1:D:79:LEU:HG	2.08	0.53
1:E:156:PRO:HG3	1:E:213:ASN:ND2	2.15	0.53
1:C:130:GLN:HB2	1:C:234:TRP:CH2	2.44	0.52
1:F:111:ASP:HB3	1:F:114:LEU:HG	1.92	0.52
1:C:30:LYS:O	1:C:33:GLN:HB2	2.10	0.52
1:D:67:ILE:HD11	1:F:47:MSE:HE3	1.92	0.52
1:A:247:ILE:HD12	1:A:248:THR:O	2.10	0.52
1:B:156:PRO:HG3	1:B:213:ASN:ND2	2.18	0.52
1:F:114:LEU:N	1:F:115:GLY:HA2	2.24	0.52
1:E:116:LEU:N	1:E:116:LEU:CD1	2.73	0.52
1:E:98:ASP:O	1:E:102:GLN:HB2	2.09	0.51
1:B:96:ILE:O	1:B:100:THR:HG23	2.10	0.51
1:E:131:CYS:HB2	1:E:233:VAL:O	2.10	0.51
1:A:54:SER:O	1:A:69:ILE:HA	2.10	0.51
1:B:76:ALA:O	1:B:80:ILE:HG13	2.11	0.51
1:E:53:ILE:HG12	1:E:72:ASP:OD1	2.09	0.51
1:F:53:ILE:HG23	1:F:70:GLY:O	2.11	0.51
1:C:93:ALA:O	1:C:96:ILE:HG13	2.11	0.51
1:C:211:ILE:HD12	1:C:221:TYR:CE2	2.45	0.51
1:E:134:LEU:HD21	1:E:230:SER:HA	1.91	0.51
1:B:72:ASP:HB3	1:B:75:LYS:HB2	1.93	0.51
1:D:121:ASN:HB3	1:D:123:PHE:HE1	1.74	0.51
1:F:24:GLN:N	1:F:41:THR:OG1	2.44	0.51
1:F:183:VAL:HG22	1:F:190:PRO:HA	1.93	0.51
1:D:133:GLY:C	1:D:146:GLY:HA2	2.36	0.51
1:D:54:SER:O	1:D:69:ILE:HA	2.11	0.51
1:B:104:ILE:HG21	1:C:104:ILE:HD12	1.93	0.50
1:F:53:ILE:CD1	1:F:71:LEU:HD23	2.41	0.50
1:A:97:VAL:HG21	1:C:99:SER:HB3	1.93	0.50
1:B:79:LEU:HA	1:B:82:GLU:HB3	1.92	0.50
1:F:54:SER:O	1:F:69:ILE:HA	2.11	0.50
1:A:106:ASP:O	1:A:110:THR:HG23	2.11	0.50
1:C:77:TYR:O	1:C:81:LEU:HG	2.12	0.50
1:D:19:ASN:HB3	1:E:14:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ALA:O	1:D:76:ALA:HB3	2.10	0.50
1:F:118:LYS:HB3	1:F:257:GLU:HB3	1.94	0.50
1:E:72:ASP:CB	1:E:75:LYS:HB2	2.40	0.50
1:E:87:GLN:OE1	1:E:87:GLN:CA	2.59	0.50
1:A:123:PHE:CD2	1:A:152:PHE:CB	2.90	0.50
1:D:50:SER:C	1:D:52:GLY:H	2.20	0.50
1:A:50:SER:C	1:A:52:GLY:H	2.20	0.50
1:D:263:ASN:OD1	1:E:121:ASN:ND2	2.44	0.50
1:A:130:GLN:HB2	1:A:234:TRP:CZ2	2.46	0.49
1:E:76:ALA:O	1:E:80:ILE:HG13	2.12	0.49
1:A:80:ILE:HD12	1:B:77:TYR:HB2	1.95	0.49
1:A:208:ARG:HH11	1:A:208:ARG:HB3	1.77	0.49
1:D:134:LEU:HD21	1:D:230:SER:HA	1.94	0.49
1:D:123:PHE:CD2	1:D:152:PHE:CB	2.88	0.49
1:E:24:GLN:HB2	1:E:43:VAL:HG12	1.94	0.49
1:A:100:THR:HG22	1:B:97:VAL:HG22	1.94	0.49
1:D:4:SER:HB2	1:E:6:PHE:CD2	2.47	0.49
1:E:135:PHE:CE1	1:E:145:GLY:HA3	2.47	0.49
1:A:4:SER:O	1:A:16:PHE:CE1	2.66	0.49
1:B:108:ILE:HG22	1:B:109:THR:HG23	1.95	0.49
1:E:130:GLN:HG3	1:E:234:TRP:CE2	2.48	0.49
1:F:25:MSE:HE1	1:F:29:LEU:HD23	1.94	0.49
1:D:111:ASP:O	1:D:117:LEU:HD21	2.13	0.48
1:E:89:LEU:HD12	1:E:89:LEU:C	2.38	0.48
1:E:108:ILE:HG23	1:E:116:LEU:HD23	1.94	0.48
1:C:54:SER:O	1:C:69:ILE:HA	2.14	0.48
1:F:78:GLN:O	1:F:82:GLU:HB2	2.14	0.48
1:D:123:PHE:N	1:D:123:PHE:CD1	2.81	0.48
1:D:49:ALA:HB1	1:D:53:ILE:HB	1.94	0.48
1:A:121:ASN:HB3	1:A:123:PHE:CE1	2.49	0.48
1:B:24:GLN:HB2	1:B:43:VAL:HG12	1.94	0.48
1:F:49:ALA:HB1	1:F:53:ILE:N	2.29	0.48
1:A:4:SER:O	1:A:16:PHE:HE1	1.96	0.48
1:A:54:SER:HB3	1:A:70:GLY:N	2.29	0.48
1:A:123:PHE:HE1	1:C:263:ASN:OD1	1.96	0.48
1:A:170:ILE:HD13	1:C:195:TYR:HD1	1.79	0.48
1:E:51:ASP:HB2	1:E:79:LEU:CD1	2.44	0.48
1:F:128:LYS:NZ	1:F:241:GLY:O	2.33	0.48
1:B:180:LEU:HG	1:B:225:VAL:HG22	1.96	0.48
1:B:240:ASN:OD1	1:B:242:ASN:CG	2.57	0.48
1:D:123:PHE:CD2	1:D:152:PHE:HD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ARG:HB3	1:D:208:ARG:NH1	2.28	0.48
1:F:30:LYS:O	1:F:33:GLN:HB2	2.14	0.48
1:F:228:LEU:O	1:F:230:SER:N	2.43	0.47
1:B:182:LEU:HD11	1:B:221:TYR:HB3	1.96	0.47
1:E:106:ASP:OD1	1:E:106:ASP:N	2.47	0.47
1:D:130:GLN:HB2	1:D:234:TRP:CH2	2.49	0.47
1:B:135:PHE:CE1	1:B:145:GLY:HA3	2.50	0.47
1:D:76:ALA:O	1:D:80:ILE:HG13	2.15	0.47
1:D:140:ILE:HG12	1:E:245:LEU:HD23	1.96	0.47
1:A:49:ALA:HB1	1:A:53:ILE:HB	1.96	0.47
1:A:128:LYS:HE2	1:A:243:ASP:CG	2.39	0.47
1:B:111:ASP:HA	1:B:112:PRO:HD3	1.76	0.47
1:D:21:LYS:HE3	1:D:25:MSE:O	2.15	0.47
1:E:169:ILE:HA	1:E:251:SER:HB3	1.97	0.47
1:C:107:LYS:HA	1:C:107:LYS:HD3	1.75	0.47
1:D:247:ILE:HD12	1:D:248:THR:O	2.15	0.47
1:A:140:ILE:HD13	1:A:140:ILE:HA	1.74	0.46
1:D:55:LEU:HD22	1:D:69:ILE:HG22	1.96	0.46
1:A:75:LYS:O	1:A:79:LEU:HG	2.15	0.46
1:B:130:GLN:HG3	1:B:234:TRP:CE2	2.50	0.46
1:F:234:TRP:HB3	1:F:237:ALA:HB3	1.98	0.46
1:A:123:PHE:CD1	1:A:123:PHE:N	2.81	0.46
1:B:83:LYS:HB3	1:B:84:LEU:HG	1.98	0.46
1:C:84:LEU:O	1:C:88:ILE:HD13	2.15	0.46
1:D:104:ILE:HD11	1:E:101:VAL:HG22	1.98	0.46
1:B:167:ALA:HB3	1:B:207:LEU:HB3	1.98	0.46
1:D:134:LEU:HD12	1:D:134:LEU:HA	1.76	0.46
1:E:145:GLY:O	1:E:224:ARG:HD3	2.16	0.46
1:C:32:GLN:HE21	1:C:57:VAL:HG11	1.81	0.46
1:D:145:GLY:O	1:D:224:ARG:HD2	2.16	0.46
1:E:180:LEU:HG	1:E:225:VAL:HG22	1.98	0.46
1:F:38:THR:OG1	1:F:39:LYS:N	2.49	0.46
1:F:127:ASN:OD1	1:F:127:ASN:N	2.48	0.46
1:F:211:ILE:HD12	1:F:221:TYR:CE2	2.50	0.46
1:C:72:ASP:HB2	1:C:75:LYS:HB2	1.98	0.45
1:E:90:ASP:O	1:E:94:ASP:HB3	2.16	0.45
1:E:197:TYR:CE2	1:F:197:TYR:HE2	2.34	0.45
1:F:166:SER:HB3	1:F:208:ARG:CD	2.46	0.45
1:C:24:GLN:N	1:C:41:THR:OG1	2.48	0.45
1:C:108:ILE:HG22	1:C:109:THR:HG23	1.98	0.45
1:C:135:PHE:CD2	1:C:179:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASP:HB2	1:A:79:LEU:CD1	2.47	0.45
1:A:134:LEU:HD21	1:A:230:SER:HA	1.97	0.45
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.32	0.45
1:B:105:LEU:O	1:B:109:THR:HG23	2.16	0.45
1:D:75:LYS:H	1:D:75:LYS:HG2	1.44	0.45
1:E:72:ASP:CG	1:E:76:ALA:HB2	2.41	0.45
1:E:88:ILE:HG23	1:E:92:ILE:CD1	2.42	0.45
1:B:238:LEU:HD21	1:B:244:ILE:HG23	1.99	0.45
1:B:197:TYR:CE2	1:C:197:TYR:HE2	2.34	0.45
1:E:61:SER:O	1:E:65:ALA:HB2	2.17	0.45
1:D:17:ALA:HB1	1:E:13:ASN:O	2.17	0.45
1:E:51:ASP:HB2	1:E:79:LEU:HD11	1.97	0.45
1:A:72:ASP:HB2	1:A:75:LYS:HG3	1.99	0.45
1:E:261:GLN:HB3	1:F:157:LYS:HE3	1.99	0.45
1:A:37:GLY:O	1:B:32:GLN:N	2.47	0.45
1:A:134:LEU:HA	1:A:134:LEU:HD12	1.68	0.45
1:B:54:SER:HB3	1:B:70:GLY:C	2.42	0.45
1:D:54:SER:HB3	1:D:70:GLY:N	2.32	0.45
1:E:50:SER:N	1:F:68:THR:HG22	2.32	0.45
1:A:130:GLN:HB2	1:A:234:TRP:CH2	2.52	0.44
1:B:48:THR:HG22	1:B:49:ALA:H	1.81	0.44
1:C:120:PHE:HD2	1:C:256:LEU:HD13	1.82	0.44
1:A:123:PHE:CD2	1:A:152:PHE:HD1	2.30	0.44
1:B:128:LYS:NZ	1:B:242:ASN:HA	2.31	0.44
1:E:104:ILE:HG21	1:F:104:ILE:HD12	1.99	0.44
1:A:55:LEU:HD22	1:A:69:ILE:HG22	2.00	0.44
1:A:139:ASN:ND2	1:A:145:GLY:HA2	2.32	0.44
1:C:77:TYR:HA	1:C:80:ILE:HD12	1.99	0.44
1:F:228:LEU:C	1:F:230:SER:H	2.25	0.44
1:E:183:VAL:HG22	1:E:190:PRO:CA	2.47	0.44
1:F:79:LEU:O	1:F:83:LYS:HG2	2.17	0.44
1:B:61:SER:O	1:B:65:ALA:HB2	2.18	0.44
1:A:145:GLY:O	1:A:224:ARG:HD2	2.18	0.44
1:B:131:CYS:HB2	1:B:233:VAL:O	2.17	0.44
1:C:92:ILE:O	1:C:96:ILE:HG23	2.17	0.44
1:A:21:LYS:HE3	1:A:25:MSE:O	2.17	0.44
1:C:96:ILE:HD12	1:C:96:ILE:C	2.43	0.44
1:D:128:LYS:HE2	1:D:243:ASP:CG	2.43	0.44
1:F:214:THR:OG1	1:F:215:GLY:N	2.50	0.44
1:A:97:VAL:HG13	1:C:100:THR:HA	1.99	0.44
1:C:49:ALA:HB1	1:C:53:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:O	1:B:224:ARG:HD3	2.17	0.43
1:C:114:LEU:H	1:C:115:GLY:HA2	1.83	0.43
1:A:19:ASN:HB3	1:B:14:CYS:SG	2.58	0.43
1:B:240:ASN:OD1	1:B:242:ASN:OD1	2.35	0.43
1:A:84:LEU:O	1:A:86:ASN:N	2.49	0.43
1:A:122:ASN:C	1:A:123:PHE:HD1	2.26	0.43
1:A:245:LEU:HD13	1:C:140:ILE:HD13	2.00	0.43
1:F:99:SER:O	1:F:103:ASP:HB2	2.18	0.43
1:B:115:GLY:HA2	1:B:259:ILE:HD13	2.00	0.43
1:F:140:ILE:O	1:F:140:ILE:HG13	2.19	0.43
1:B:105:LEU:O	1:B:108:ILE:HG22	2.19	0.43
1:B:106:ASP:N	1:B:106:ASP:OD1	2.51	0.43
1:C:133:GLY:O	1:C:146:GLY:HA2	2.18	0.43
1:D:29:LEU:HD22	1:D:33:GLN:HB3	2.01	0.43
1:D:117:LEU:HD12	1:D:157:LYS:HB3	2.01	0.43
1:E:101:VAL:O	1:E:105:LEU:HG	2.17	0.43
1:B:88:ILE:H	1:B:88:ILE:HG13	1.52	0.43
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.86	0.43
1:B:120:PHE:HD1	1:B:256:LEU:HD13	1.84	0.42
1:D:173:ARG:NH1	1:D:177:GLY:O	2.52	0.42
1:A:148:GLU:HA	1:A:224:ARG:HA	2.01	0.42
1:C:245:LEU:HD23	1:C:245:LEU:HA	1.86	0.42
1:D:133:GLY:O	1:D:146:GLY:HA2	2.18	0.42
1:E:126:THR:HG22	1:E:250:THR:HG22	2.02	0.42
1:F:134:LEU:HD23	1:F:230:SER:HA	2.01	0.42
1:A:29:LEU:HD22	1:A:33:GLN:HB3	2.01	0.42
1:B:174:MSE:O	1:B:175:GLU:C	2.62	0.42
1:C:214:THR:OG1	1:C:215:GLY:N	2.52	0.42
1:C:228:LEU:O	1:C:230:SER:N	2.45	0.42
1:E:48:THR:HG22	1:E:49:ALA:H	1.84	0.42
1:B:134:LEU:HD21	1:B:230:SER:HA	2.01	0.42
1:D:36:LEU:HD11	1:E:32:GLN:HA	2.00	0.42
1:D:92:ILE:HD12	1:D:92:ILE:HA	1.87	0.42
1:C:228:LEU:C	1:C:230:SER:H	2.26	0.42
1:D:140:ILE:HD13	1:D:140:ILE:HA	1.71	0.42
1:D:51:ASP:OD2	1:E:71:LEU:HD12	2.20	0.42
1:C:50:SER:C	1:C:52:GLY:H	2.27	0.42
1:D:96:ILE:HD11	1:E:93:ALA:HB2	2.02	0.42
1:E:19:ASN:CG	1:E:28:PRO:HB2	2.44	0.42
1:F:32:GLN:HE21	1:F:57:VAL:HG11	1.83	0.42
1:B:256:LEU:HA	1:B:256:LEU:HD12	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ASN:ND2	1:D:145:GLY:HA2	2.35	0.42
1:D:155:THR:HA	1:D:156:PRO:HD2	1.81	0.42
1:A:117:LEU:HD12	1:A:157:LYS:HB3	2.01	0.42
1:A:123:PHE:HD2	1:A:152:PHE:CG	2.35	0.42
1:A:170:ILE:HD13	1:C:195:TYR:CD1	2.54	0.42
1:D:163:PHE:CD1	1:D:255:PHE:HB3	2.54	0.42
1:A:173:ARG:CZ	1:A:176:GLY:HA3	2.50	0.41
1:D:141:GLU:O	1:D:189:LYS:HB3	2.20	0.41
1:E:115:GLY:O	1:E:259:ILE:HD12	2.19	0.41
1:E:174:MSE:O	1:E:175:GLU:C	2.63	0.41
1:F:86:ASN:O	1:F:89:LEU:HG	2.20	0.41
1:B:47:MSE:HE3	1:C:67:ILE:HD12	2.02	0.41
1:F:79:LEU:HD13	1:F:79:LEU:HA	1.92	0.41
1:F:89:LEU:HA	1:F:92:ILE:HD12	2.02	0.41
1:D:37:GLY:O	1:E:32:GLN:N	2.52	0.41
1:D:83:LYS:HD3	1:D:83:LYS:HA	1.95	0.41
1:A:101:VAL:O	1:A:105:LEU:HG	2.20	0.41
1:F:50:SER:C	1:F:52:GLY:H	2.28	0.41
1:C:38:THR:OG1	1:C:39:LYS:N	2.52	0.41
1:D:59:ASN:OD1	1:D:59:ASN:N	2.54	0.41
1:E:47:MSE:HE3	1:F:67:ILE:HD12	2.03	0.41
1:E:104:ILE:O	1:E:108:ILE:HD13	2.20	0.41
1:F:106:ASP:O	1:F:110:THR:OG1	2.31	0.41
1:F:133:GLY:O	1:F:146:GLY:HA2	2.21	0.41
1:A:123:PHE:CE1	1:C:263:ASN:OD1	2.73	0.41
1:E:167:ALA:HB3	1:E:207:LEU:HB3	2.03	0.41
1:F:32:GLN:HE21	1:F:57:VAL:CG2	2.34	0.41
1:A:174:MSE:O	1:A:175:GLU:C	2.63	0.41
1:B:169:ILE:HA	1:B:251:SER:HB3	2.02	0.41
1:F:53:ILE:HD13	1:F:53:ILE:HA	1.94	0.41
1:F:120:PHE:HD2	1:F:256:LEU:HD13	1.86	0.41
1:A:104:ILE:HD11	1:B:101:VAL:HA	2.03	0.41
1:B:128:LYS:HZ2	1:B:242:ASN:HA	1.86	0.41
1:B:194:SER:HB2	1:B:207:LEU:HD12	2.03	0.41
1:D:107:LYS:HE3	1:D:107:LYS:HB2	1.82	0.41
1:A:182:LEU:HB3	1:A:192:ALA:HB3	2.03	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.88	0.41
1:E:7:TYR:CE1	1:E:14:CYS:HB2	2.55	0.41
1:F:107:LYS:HA	1:F:107:LYS:HD3	1.83	0.41
1:F:162:MSE:HG2	1:F:212:THR:HA	2.03	0.41
1:B:179:VAL:HG23	1:B:228:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:LEU:HA	1:D:71:LEU:HD23	1.88	0.40
1:D:261:GLN:HG3	1:E:119:ALA:HB1	2.01	0.40
1:A:163:PHE:CD1	1:A:255:PHE:HB3	2.55	0.40
1:E:54:SER:HB3	1:E:70:GLY:C	2.46	0.40
1:C:134:LEU:HD23	1:C:230:SER:HA	2.03	0.40
1:C:173:ARG:CZ	1:C:176:GLY:HA3	2.51	0.40
1:C:199:SER:OG	1:C:201:VAL:HG13	2.20	0.40
1:D:30:LYS:O	1:D:33:GLN:HB2	2.21	0.40
1:A:122:ASN:C	1:A:123:PHE:CD1	3.00	0.40
1:B:114:LEU:HD22	1:B:114:LEU:HA	1.82	0.40
1:E:77:TYR:CZ	1:E:81:LEU:HD11	2.57	0.40
1:E:84:LEU:HB3	1:E:87:GLN:NE2	2.36	0.40
1:E:111:ASP:HA	1:E:112:PRO:HD3	1.77	0.40
1:F:25:MSE:HE2	1:F:27:GLU:O	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	261/269 (97%)	244 (94%)	12 (5%)	5 (2%)	6	27
1	B	261/269 (97%)	245 (94%)	13 (5%)	3 (1%)	11	39
1	C	267/269 (99%)	243 (91%)	18 (7%)	6 (2%)	5	24
1	D	261/269 (97%)	243 (93%)	13 (5%)	5 (2%)	6	27
1	E	261/269 (97%)	241 (92%)	17 (6%)	3 (1%)	11	39
1	F	267/269 (99%)	240 (90%)	21 (8%)	6 (2%)	5	24
All	All	1578/1614 (98%)	1456 (92%)	94 (6%)	28 (2%)	6	28

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	C	175	GLU
1	D	114	LEU
1	F	175	GLU
1	A	85	GLY
1	A	117	LEU
1	B	51	ASP
1	C	116	LEU
1	D	117	LEU
1	A	175	GLU
1	C	32	GLN
1	C	229	GLU
1	E	51	ASP
1	F	32	GLN
1	F	101	VAL
1	F	229	GLU
1	A	51	ASP
1	B	175	GLU
1	C	1	MSE
1	D	175	GLU
1	E	175	GLU
1	F	116	LEU
1	C	73	ALA
1	D	51	ASP
1	E	99	SER
1	D	73	ALA
1	F	40	SER
1	B	218	PRO

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	223/222 (100%)	186 (83%)	37 (17%)	2 10
1	B	224/222 (101%)	183 (82%)	41 (18%)	2 8
1	C	227/222 (102%)	187 (82%)	40 (18%)	2 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	223/222 (100%)	189 (85%)	34 (15%)	3	13
1	E	224/222 (101%)	187 (84%)	37 (16%)	2	11
1	F	227/222 (102%)	185 (82%)	42 (18%)	1	8
All	All	1348/1332 (101%)	1117 (83%)	231 (17%)	2	10

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	15	VAL
1	A	16	PHE
1	A	20	ILE
1	A	30	LYS
1	A	38	THR
1	A	51	ASP
1	A	55	LEU
1	A	59	ASN
1	A	61	SER
1	A	63	THR
1	A	69	ILE
1	A	72	ASP
1	A	74	GLU
1	A	75	LYS
1	A	77	TYR
1	A	81	LEU
1	A	88	ILE
1	A	89	LEU
1	A	99	SER
1	A	101	VAL
1	A	126	THR
1	A	134	LEU
1	A	138	SER
1	A	140	ILE
1	A	151	LYS
1	A	157	LYS
1	A	159	SER
1	A	164	LEU
1	A	168	ASP
1	A	169	ILE
1	A	170	ILE
1	A	206	SER

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Mol	Chain	Res	Type
1	A	208	ARG
1	A	214	THR
1	A	239	SER
1	A	247	ILE
1	B	3	ASN
1	B	7	TYR
1	B	15	VAL
1	B	26	THR
1	B	38	THR
1	B	48	THR
1	B	53	ILE
1	B	55	LEU
1	B	60	ASN
1	B	62	SER
1	B	72	ASP
1	B	84	LEU
1	B	87	GLN
1	B	89	LEU
1	B	92	ILE
1	B	97	VAL
1	B	108	ILE
1	B	114	LEU
1	B	116	LEU
1	B	121	ASN
1	B	134	LEU
1	B	136	THR
1	B	138	SER
1	B	151	LYS
1	B	152	PHE
1	B	163	PHE
1	B	164	LEU
1	B	166	SER
1	B	168	ASP
1	B	198	SER
1	B	206	SER
1	B	216	LEU
1	B	217	THR
1	B	219	THR
1	B	222	SER
1	B	242	ASN
1	B	245	LEU
1	B	249	ASN

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Mol	Chain	Res	Type
1	B	250	THR
1	B	252	ASN
1	B	262	THR
1	C	-2	LEU
1	C	1	MSE
1	C	3	ASN
1	C	8	LEU
1	C	15	VAL
1	C	22	VAL
1	C	26	THR
1	C	30	LYS
1	C	38	THR
1	C	41	THR
1	C	48	THR
1	C	51	ASP
1	C	54	SER
1	C	55	LEU
1	C	56	THR
1	C	57	VAL
1	C	63	THR
1	C	67	ILE
1	C	72	ASP
1	C	74	GLU
1	C	87	GLN
1	C	100	THR
1	C	116	LEU
1	C	117	LEU
1	C	129	ILE
1	C	138	SER
1	C	147	THR
1	C	154	VAL
1	C	159	SER
1	C	164	LEU
1	C	166	SER
1	C	168	ASP
1	C	199	SER
1	C	201	VAL
1	C	216	LEU
1	C	217	THR
1	C	222	SER
1	C	229	GLU
1	C	258	VAL

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Mol	Chain	Res	Type
1	C	259	ILE
1	D	14	CYS
1	D	15	VAL
1	D	16	PHE
1	D	20	ILE
1	D	30	LYS
1	D	38	THR
1	D	51	ASP
1	D	55	LEU
1	D	59	ASN
1	D	61	SER
1	D	63	THR
1	D	69	ILE
1	D	75	LYS
1	D	77	TYR
1	D	88	ILE
1	D	92	ILE
1	D	126	THR
1	D	134	LEU
1	D	138	SER
1	D	140	ILE
1	D	151	LYS
1	D	152	PHE
1	D	157	LYS
1	D	159	SER
1	D	164	LEU
1	D	168	ASP
1	D	169	ILE
1	D	170	ILE
1	D	175	GLU
1	D	206	SER
1	D	208	ARG
1	D	214	THR
1	D	239	SER
1	D	247	ILE
1	E	3	ASN
1	E	7	TYR
1	E	15	VAL
1	E	26	THR
1	E	38	THR
1	E	48	THR
1	E	53	ILE

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Mol	Chain	Res	Type
1	E	55	LEU
1	E	60	ASN
1	E	62	SER
1	E	72	ASP
1	E	84	LEU
1	E	87	GLN
1	E	94	ASP
1	E	114	LEU
1	E	116	LEU
1	E	121	ASN
1	E	134	LEU
1	E	136	THR
1	E	151	LYS
1	E	152	PHE
1	E	163	PHE
1	E	164	LEU
1	E	166	SER
1	E	168	ASP
1	E	198	SER
1	E	206	SER
1	E	217	THR
1	E	219	THR
1	E	222	SER
1	E	242	ASN
1	E	245	LEU
1	E	249	ASN
1	E	250	THR
1	E	252	ASN
1	E	262	THR
1	E	263	ASN
1	F	3	ASN
1	F	8	LEU
1	F	15	VAL
1	F	22	VAL
1	F	26	THR
1	F	30	LYS
1	F	38	THR
1	F	41	THR
1	F	48	THR
1	F	51	ASP
1	F	54	SER
1	F	55	LEU

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Mol	Chain	Res	Type
1	F	56	THR
1	F	57	VAL
1	F	59	ASN
1	F	63	THR
1	F	72	ASP
1	F	77	TYR
1	F	79	LEU
1	F	87	GLN
1	F	88	ILE
1	F	92	ILE
1	F	98	ASP
1	F	100	THR
1	F	116	LEU
1	F	117	LEU
1	F	127	ASN
1	F	138	SER
1	F	147	THR
1	F	154	VAL
1	F	159	SER
1	F	164	LEU
1	F	166	SER
1	F	168	ASP
1	F	199	SER
1	F	201	VAL
1	F	216	LEU
1	F	217	THR
1	F	222	SER
1	F	229	GLU
1	F	258	VAL
1	F	259	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	121	ASN
1	A	122	ASN
1	A	130	GLN
1	A	132	ASN
1	A	252	ASN
1	B	213	ASN
1	C	32	GLN

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	87	GLN
1	C	139	ASN
1	D	121	ASN
1	D	122	ASN
1	D	130	GLN
1	D	132	ASN
1	D	252	ASN
1	E	213	ASN
1	E	249	ASN
1	F	3	ASN
1	F	32	GLN
1	F	139	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 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	259/269 (96%)	0.11	16 (6%) 26 14	22, 51, 133, 151	0
1	B	258/269 (95%)	0.11	9 (3%) 47 27	26, 49, 141, 158	0
1	C	264/269 (98%)	0.19	11 (4%) 40 22	22, 53, 136, 146	0
1	D	259/269 (96%)	0.22	23 (8%) 15 8	23, 54, 145, 152	0
1	E	258/269 (95%)	0.26	16 (6%) 26 14	31, 55, 145, 159	0
1	F	264/269 (98%)	0.30	27 (10%) 12 6	25, 52, 143, 152	0
All	All	1562/1614 (96%)	0.20	102 (6%) 25 13	22, 53, 142, 159	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	THR	4.7
1	F	55	LEU	4.7
1	D	71	LEU	4.3
1	A	92	ILE	4.2
1	F	35	ILE	4.1
1	F	73	ALA	4.0
1	E	35	ILE	3.9
1	D	32	GLN	3.9
1	D	89	LEU	3.9
1	F	97	VAL	3.7
1	D	2	GLY	3.6
1	F	32	GLN	3.5
1	E	77	TYR	3.5
1	A	89	LEU	3.4
1	A	93	ALA	3.4
1	B	73	ALA	3.3
1	F	96	ILE	3.3
1	A	88	ILE	3.2
1	B	89	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	97	VAL	3.2
1	C	97	VAL	3.1
1	A	60	ASN	3.1
1	F	57	VAL	3.1
1	F	45	ALA	3.1
1	D	93	ALA	3.0
1	F	48	THR	3.0
1	C	58	SER	3.0
1	D	84	LEU	3.0
1	B	97	VAL	3.0
1	C	96	ILE	3.0
1	E	73	ALA	2.9
1	A	94	ASP	2.9
1	A	2	GLY	2.9
1	F	36	LEU	2.8
1	D	34	ILE	2.8
1	F	56	THR	2.8
1	D	31	ASP	2.7
1	D	7	TYR	2.7
1	F	14	CYS	2.7
1	C	92	ILE	2.7
1	F	71	LEU	2.7
1	F	41	THR	2.7
1	E	71	LEU	2.7
1	E	89	LEU	2.7
1	B	88	ILE	2.7
1	D	35	ILE	2.6
1	A	96	ILE	2.6
1	E	57	VAL	2.6
1	A	100	THR	2.6
1	F	34	ILE	2.5
1	F	67	ILE	2.5
1	C	77	TYR	2.5
1	A	59	ASN	2.5
1	F	51	ASP	2.5
1	D	20	ILE	2.4
1	D	91	GLY	2.4
1	A	58	SER	2.4
1	A	62	SER	2.4
1	E	36	LEU	2.4
1	E	80	ILE	2.4
1	C	53	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	52	GLY	2.4
1	E	88	ILE	2.4
1	B	81	LEU	2.4
1	D	67	ILE	2.3
1	E	81	LEU	2.3
1	F	89	LEU	2.3
1	D	29	LEU	2.3
1	A	61	SER	2.3
1	F	77	TYR	2.3
1	F	39	LYS	2.2
1	D	94	ASP	2.2
1	E	84	LEU	2.2
1	F	79	LEU	2.2
1	B	77	TYR	2.2
1	A	35	ILE	2.2
1	F	20	ILE	2.2
1	F	92	ILE	2.2
1	F	40	SER	2.2
1	D	72	ASP	2.2
1	C	38	THR	2.2
1	D	68	THR	2.2
1	C	264	ALA	2.2
1	F	60	ASN	2.2
1	E	37	GLY	2.2
1	D	90	ASP	2.2
1	C	100	THR	2.1
1	E	92	ILE	2.1
1	F	69	ILE	2.1
1	A	84	LEU	2.1
1	A	55	LEU	2.1
1	B	96	ILE	2.1
1	D	30	LYS	2.1
1	D	95	THR	2.1
1	E	95	THR	2.1
1	F	99	SER	2.1
1	D	15	VAL	2.1
1	C	71	LEU	2.1
1	D	44	ALA	2.1
1	B	12	GLU	2.1
1	D	69	ILE	2.0
1	E	41	THR	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.