



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:51 AM UTC

PDB ID : 7RCO / pdb_00007rco
Title : Crystal structure of human TGF-beta-2 bound to 4A11.V2 Fab
Authors : Yin, J.; Lupardus, P.J.; Sudhamsu, J.
Deposited on : 2021-07-07
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

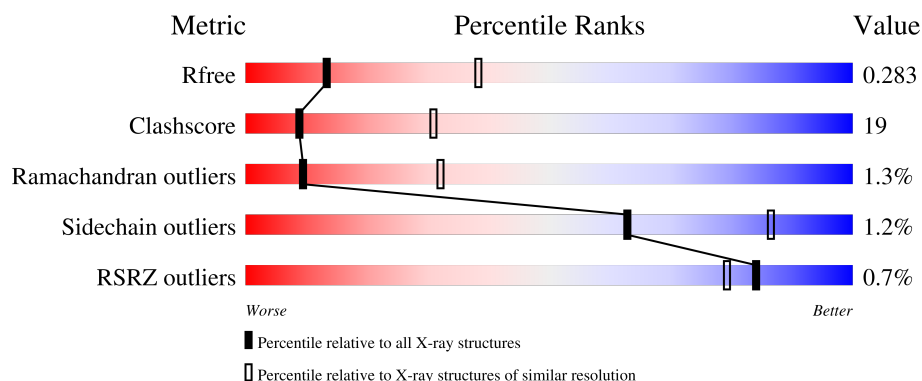
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

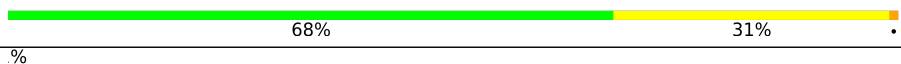
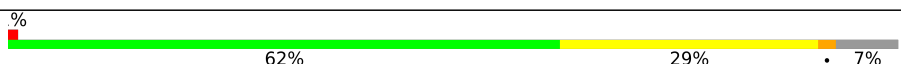
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	112	
1	B	112	
2	C	219	
2	E	219	
3	D	233	

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Mol	Chain	Length	Quality of chain
3	F	233	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (57%), yellow (35%), and red (7%). The segments are labeled with their respective percentages: 57%, 35%, and 7%.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8200 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 Transforming growth factor beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			882	560	148	164	10			
1	B	112	Total	C	N	O	S	0	0	0
			890	566	149	165	10			

- Molecule 2 is a protein called 4A11.V2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1643	1027	273	339	4			
2	E	204	Total	C	N	O	S	0	0	0
			1547	968	255	320	4			

- Molecule 3 is a protein called 4A11.V2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	216	Total	C	N	O	S	0	0	0
			1595	1013	267	308	7			
3	F	216	Total	C	N	O	S	0	0	0
			1595	1013	267	308	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	8	Total	O	0	0
			8	8		
4	C	6	Total	O	0	0
			6	6		
4	D	10	Total	O	0	0
			10	10		

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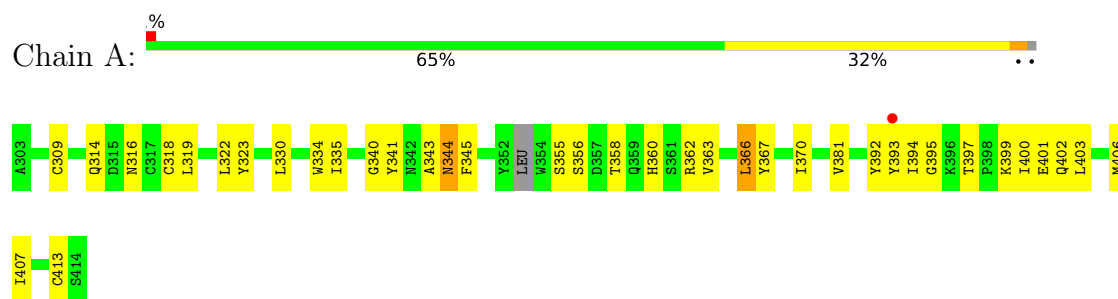
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	10	Total	O	0	0
			10	10		
4	F	9	Total	O	0	0
			9	9		

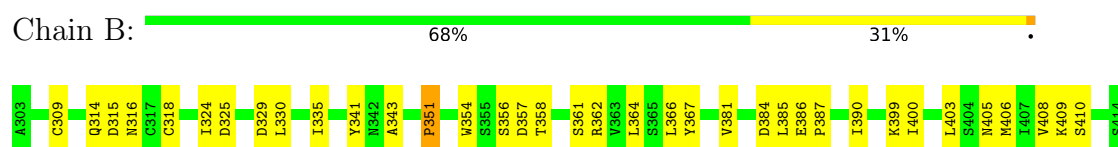
3 Residue-property plots

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.

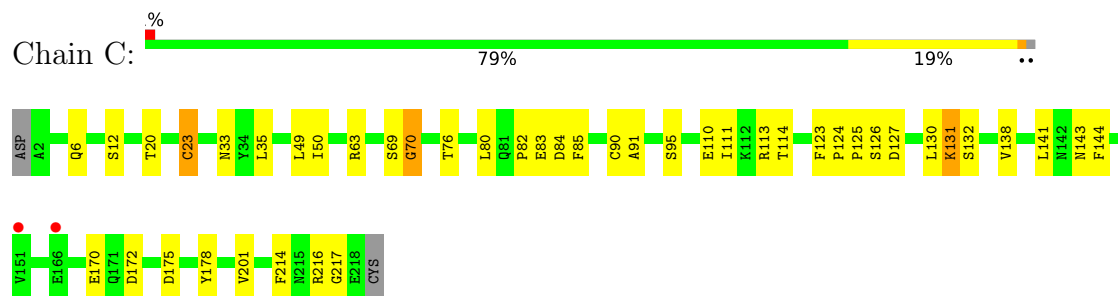
- Molecule 1: Transforming growth factor beta-2



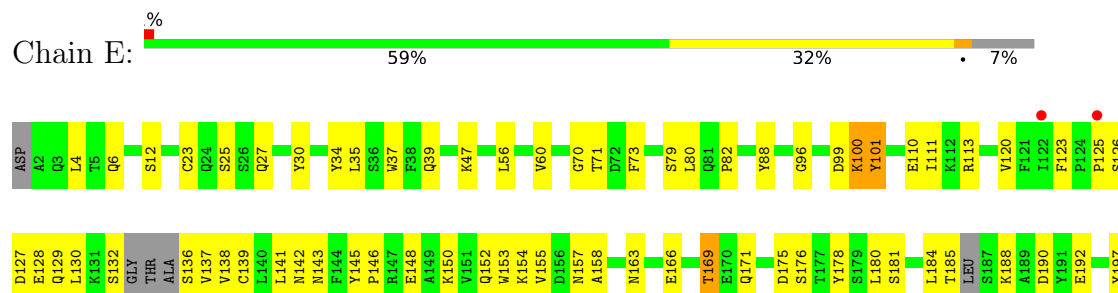
- Molecule 1: Transforming growth factor beta-2



- Molecule 2: 4A11.V2 Fab Light Chain

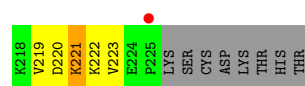
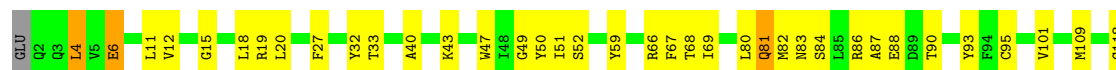


- Molecule 2: 4A11.V2 Fab Light Chain

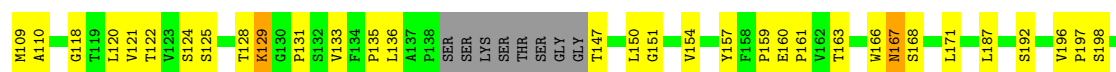
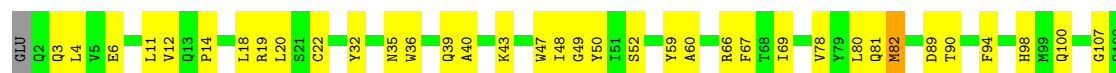




• Molecule 3: 4A11.V2 Fab Heavy Chain



• Molecule 3: 4A11.V2 Fab Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	60.15Å 103.48Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 2.90 45.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.95-2.90) 98.5 (45.95-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.208 , 0.286 0.212 , 0.283	Depositor DCC
R_{free} test set	1335 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8200	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

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	0.75	4/905 (0.4%)	0.71	0/1228
1	B	0.48	0/914	0.66	0/1242
2	C	0.53	2/1679 (0.1%)	0.66	1/2279 (0.0%)
2	E	0.60	2/1580 (0.1%)	0.74	1/2143 (0.0%)
3	D	0.61	1/1637 (0.1%)	0.73	1/2234 (0.0%)
3	F	0.46	1/1637 (0.1%)	0.66	0/2234
All	All	0.57	10/8352 (0.1%)	0.69	3/11360 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	LEU	C-O	-6.56	1.16	1.23
3	F	129	LYS	C-O	-6.14	1.16	1.24
1	A	345	PHE	C-O	-5.95	1.16	1.23
2	E	100	LYS	CA-C	-5.74	1.45	1.52
1	A	343	ALA	CA-C	-5.64	1.45	1.52
2	C	143	ASN	C-O	-5.43	1.17	1.24
2	C	144	PHE	C-O	-5.39	1.17	1.23
2	E	101	TYR	C-O	-5.37	1.17	1.23
1	A	344	ASN	C-O	-5.20	1.17	1.24
1	A	344	ASN	CA-C	-5.04	1.46	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	207	SER	N-CA-C	6.52	118.07	110.97
2	C	131	LYS	CB-CA-C	-6.06	103.34	111.88
3	D	170	ALA	N-CA-C	-5.73	104.41	111.40

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	882	0	846	30	0
1	B	890	0	858	30	0
2	C	1643	0	1583	32	0
2	E	1547	0	1484	84	0
3	D	1595	0	1555	65	0
3	F	1595	0	1555	78	0
4	A	5	0	0	0	0
4	B	8	0	0	0	0
4	C	6	0	0	2	0
4	D	10	0	0	4	0
4	E	10	0	0	0	0
4	F	9	0	0	4	0
All	All	8200	0	7881	296	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 19.

All (296) 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:367:TYR:CD2	1:B:324:ILE:HD13	1.96	0.99
2:E:203:HIS:H	2:E:206:LEU:HD11	1.30	0.97
3:D:133:VAL:HG21	3:D:219:VAL:HG11	1.43	0.97
3:F:133:VAL:HG21	3:F:210:VAL:HG11	1.50	0.94
2:C:20:THR:HG22	2:C:76:THR:HG23	1.54	0.89
3:D:90:THR:HG23	3:D:123:VAL:HG22	1.56	0.88
3:D:207:ILE:HB	3:D:221:LYS:O	1.74	0.86
3:F:168:SER:H	3:F:209:ASN:HD21	1.20	0.86
3:D:86:ARG:O	3:D:123:VAL:HG21	1.76	0.85
2:E:130:LEU:HB3	2:E:188:LYS:HZ1	1.42	0.84
3:F:35:ASN:HD21	3:F:98:HIS:CE1	1.96	0.83
3:D:212:HIS:HB3	3:D:217:THR:OG1	1.78	0.82
1:A:356:SER:HB3	1:A:362:ARG:HG2	1.59	0.82
3:D:215:SER:OG	3:D:217:THR:HG23	1.81	0.80
3:D:90:THR:HG22	3:D:122:THR:HA	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:188:LYS:HG2	2:E:192:GLU:CD	2.07	0.78
1:A:367:TYR:CD2	1:B:324:ILE:CD1	2.68	0.77
2:E:203:HIS:N	2:E:206:LEU:HD11	2.00	0.77
2:E:130:LEU:HB3	2:E:188:LYS:NZ	2.01	0.76
2:E:82:PRO:HA	2:E:111:ILE:HD13	1.68	0.75
3:F:90:THR:HG23	3:F:122:THR:HA	1.69	0.74
2:E:96:GLY:O	2:E:100:LYS:HE2	1.86	0.74
2:C:113:ARG:NH1	2:C:114:THR:O	2.20	0.73
2:C:141:LEU:HD11	2:C:201:VAL:HG21	1.71	0.73
3:F:19:ARG:HB2	3:F:81:GLN:NE2	2.04	0.73
2:C:216:ARG:HG2	4:C:301:HOH:O	1.88	0.72
1:A:330:LEU:HD23	1:B:366:LEU:HB3	1.71	0.72
1:B:314:GLN:NE2	1:B:316:ASN:HB2	2.06	0.71
2:E:188:LYS:HG2	2:E:192:GLU:OE1	1.90	0.69
2:C:63:ARG:NH2	2:C:84:ASP:OD2	2.26	0.69
2:E:188:LYS:HE3	2:E:192:GLU:OE2	1.94	0.68
3:F:129:LYS:HD2	3:F:187:LEU:HD21	1.76	0.67
3:D:210:VAL:HG12	3:D:219:VAL:HB	1.76	0.67
3:F:167:ASN:HA	3:F:207:ILE:HG23	1.77	0.67
3:D:129:LYS:HD3	3:D:130:GLY:O	1.93	0.67
3:D:12:VAL:O	3:D:123:VAL:HA	1.97	0.65
2:C:49:LEU:CB	2:C:50:ILE:HD12	2.27	0.65
2:E:154:LYS:NZ	2:E:157:ASN:HA	2.12	0.65
2:E:35:LEU:HD13	2:E:73:PHE:CD1	2.32	0.64
1:A:319:LEU:HD21	1:A:344:ASN:HD22	1.63	0.64
3:D:164:VAL:HG22	3:D:210:VAL:HG23	1.78	0.64
2:E:203:HIS:HB3	2:E:206:LEU:HG	1.79	0.64
2:C:126:SER:O	2:C:130:LEU:HG	1.98	0.63
3:D:207:ILE:HD13	3:D:220:ASP:HB3	1.79	0.63
2:E:206:LEU:HD12	2:E:206:LEU:O	1.99	0.63
3:F:168:SER:N	3:F:209:ASN:HD21	1.93	0.63
3:F:20:LEU:HD11	3:F:82:MET:HE2	1.81	0.62
1:A:314:GLN:HG3	1:A:316:ASN:H	1.64	0.62
2:C:49:LEU:HB2	2:C:50:ILE:HD12	1.82	0.62
3:F:147:THR:N	3:F:198:SER:HB2	2.14	0.62
2:C:12:SER:HA	2:C:110:GLU:O	2.00	0.61
2:E:163:ASN:HD21	2:E:185:THR:H	1.45	0.61
3:F:196:VAL:HG21	3:F:206:TYR:CZ	2.36	0.61
1:B:335:ILE:HG12	1:B:390:ILE:HD13	1.83	0.61
3:F:120:LEU:HD12	3:F:121:VAL:H	1.65	0.60
2:E:154:LYS:HZ3	2:E:157:ASN:HA	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:LEU:HD12	2:E:23:CYS:SG	2.40	0.60
2:E:34:TYR:OH	3:F:107:GLY:HA3	2.02	0.60
1:A:366:LEU:HD22	1:A:370:ILE:HD12	1.84	0.60
2:C:141:LEU:HD11	2:C:201:VAL:CG2	2.32	0.59
3:D:150:LEU:HD13	3:D:223:VAL:HG21	1.84	0.59
3:D:206:TYR:O	3:D:223:VAL:HG22	2.03	0.59
3:F:167:ASN:N	3:F:207:ILE:O	2.29	0.59
2:C:80:LEU:HD21	2:C:111:ILE:CD1	2.32	0.59
1:A:381:VAL:HG11	1:B:381:VAL:HG11	1.85	0.59
3:D:154:VAL:HG21	3:D:210:VAL:HG21	1.84	0.59
2:E:56:LEU:HD21	2:E:60:VAL:O	2.03	0.58
2:E:142:ASN:OD1	2:E:143:ASN:ND2	2.36	0.58
3:D:215:SER:OG	3:D:217:THR:CG2	2.51	0.58
3:F:47:TRP:CZ2	3:F:49:GLY:HA2	2.38	0.58
2:E:6:GLN:NE2	2:E:88:TYR:O	2.35	0.58
1:A:397:THR:O	1:A:399:LYS:NZ	2.35	0.57
3:D:90:THR:CG2	3:D:123:VAL:H	2.17	0.57
2:E:129:GLN:OE1	2:E:136:SER:HB3	2.03	0.57
2:E:125:PRO:HD3	2:E:137:VAL:HG12	1.85	0.57
2:E:137:VAL:HG22	2:E:184:LEU:HD23	1.86	0.57
1:B:329:ASP:OD1	2:E:30:TYR:OH	2.22	0.57
2:E:99:ASP:OD1	3:F:60:ALA:HA	2.04	0.57
2:E:154:LYS:NZ	2:E:157:ASN:OD1	2.36	0.57
3:F:163:THR:OG1	3:F:211:ASN:HB3	2.04	0.57
2:E:150:LYS:HB3	2:E:202:THR:OG1	2.05	0.57
2:E:169:THR:HG21	2:E:178:TYR:HA	1.87	0.57
1:A:403:LEU:HB3	1:A:406:MET:HG3	1.87	0.56
1:A:363:VAL:HG13	1:B:330:LEU:HD21	1.87	0.56
2:E:39:GLN:O	2:E:47:LYS:N	2.35	0.56
2:E:154:LYS:NZ	2:E:157:ASN:CA	2.69	0.56
3:D:18:LEU:HD21	3:D:20:LEU:HD23	1.86	0.56
2:E:163:ASN:ND2	2:E:185:THR:H	2.03	0.56
3:D:207:ILE:HG22	3:D:222:LYS:HB2	1.87	0.55
1:A:314:GLN:HG3	1:A:316:ASN:N	2.22	0.55
3:D:86:ARG:NH2	4:D:302:HOH:O	2.36	0.55
2:E:123:PHE:HB2	2:E:138:VAL:HG22	1.89	0.55
3:D:212:HIS:HB3	3:D:217:THR:HG1	1.72	0.55
3:F:211:ASN:ND2	3:F:218:LYS:HE3	2.21	0.55
3:F:120:LEU:HD12	3:F:121:VAL:N	2.22	0.54
2:E:180:LEU:HD12	2:E:181:SER:H	1.72	0.54
3:F:166:TRP:NE1	3:F:192:SER:OG	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:201:LEU:HD13	3:F:206:TYR:HD2	1.73	0.54
1:B:314:GLN:HE21	1:B:316:ASN:HB2	1.72	0.54
3:F:59:TYR:HE1	3:F:69:ILE:HG13	1.72	0.54
2:C:33:ASN:HD21	3:D:109:MET:HE3	1.73	0.54
2:E:139:CYS:HB2	2:E:153:TRP:CH2	2.43	0.53
3:F:12:VAL:HG11	3:F:18:LEU:HD22	1.90	0.53
3:F:204:GLN:OE1	3:F:205:THR:N	2.42	0.53
2:E:146:PRO:HB2	2:E:148:GLU:OE2	2.07	0.53
3:D:33:THR:HG23	3:D:52:SER:HA	1.91	0.53
2:E:139:CYS:HB2	2:E:153:TRP:CZ2	2.44	0.53
2:E:123:PHE:HB2	2:E:138:VAL:CG2	2.39	0.53
2:E:125:PRO:CD	2:E:137:VAL:HG12	2.38	0.53
3:F:196:VAL:HG23	3:F:197:PRO:HD2	1.91	0.53
2:E:113:ARG:HD2	2:E:175:ASP:O	2.09	0.52
3:F:36:TRP:O	3:F:48:ILE:HG12	2.08	0.52
1:A:355:SER:HB2	1:A:413:CYS:H	1.74	0.52
3:D:18:LEU:CD2	3:D:20:LEU:CD2	2.87	0.52
3:D:19:ARG:HD2	3:F:81:GLN:NE2	2.25	0.52
2:E:101:TYR:CE1	3:F:110:ALA:HA	2.44	0.52
3:F:22:CYS:HB3	3:F:78:VAL:HG22	1.91	0.52
3:F:39:GLN:NE2	3:F:43:LYS:O	2.39	0.52
2:E:23:CYS:HB2	2:E:37:TRP:CH2	2.44	0.52
2:E:25:SER:OG	2:E:27:GLN:O	2.24	0.52
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.44	0.52
2:E:188:LYS:HE3	2:E:192:GLU:CD	2.33	0.52
3:D:87:ALA:HA	3:D:123:VAL:CG2	2.39	0.52
2:E:203:HIS:CA	2:E:206:LEU:HD11	2.40	0.52
2:E:163:ASN:HD21	2:E:185:THR:N	2.08	0.51
3:D:67:PHE:HD1	3:D:82:MET:HG2	1.74	0.51
2:C:80:LEU:HD21	2:C:111:ILE:HD12	1.90	0.51
2:E:130:LEU:HD22	2:E:188:LYS:NZ	2.26	0.51
3:F:100:GLN:NE2	4:F:301:HOH:O	2.30	0.51
2:E:123:PHE:CE1	3:F:150:LEU:HA	2.47	0.50
2:C:6:GLN:HB3	2:C:23:CYS:SG	2.51	0.50
3:D:18:LEU:HD21	3:D:20:LEU:CD2	2.41	0.50
3:D:93:TYR:O	3:D:118:GLY:HA2	2.11	0.50
3:F:66:ARG:NH1	3:F:89:ASP:OD2	2.44	0.50
3:D:66:ARG:HD3	4:D:302:HOH:O	2.11	0.50
2:E:203:HIS:HB3	2:E:206:LEU:CG	2.41	0.50
3:F:131:PRO:HB2	3:F:154:VAL:HG13	1.92	0.50
3:F:196:VAL:HG21	3:F:206:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:210:VAL:CG1	3:F:219:VAL:HB	2.41	0.49
2:C:35:LEU:HA	2:C:91:ALA:O	2.12	0.49
2:C:85:PHE:HZ	2:C:170:GLU:HB3	1.78	0.49
3:D:151:GLY:HA2	3:D:166:TRP:CZ2	2.47	0.49
2:E:130:LEU:C	2:E:132:SER:H	2.21	0.49
3:F:201:LEU:HD21	3:F:225:PRO:HD3	1.92	0.49
2:C:110:GLU:OE2	2:C:178:TYR:OH	2.25	0.49
3:F:3:GLN:C	3:F:4:LEU:HD12	2.37	0.49
3:F:205:THR:O	3:F:205:THR:OG1	2.28	0.49
1:B:356:SER:HB2	1:B:362:ARG:NH1	2.28	0.49
2:E:101:TYR:HE1	3:F:110:ALA:HA	1.77	0.49
1:A:360:HIS:CE1	1:B:408:VAL:HG23	2.48	0.49
3:F:19:ARG:NH2	4:F:302:HOH:O	2.35	0.49
3:D:40:ALA:HB3	3:D:43:LYS:HB2	1.95	0.49
3:D:67:PHE:CD1	3:D:82:MET:HG2	2.48	0.48
2:E:12:SER:HA	2:E:110:GLU:O	2.13	0.48
2:C:49:LEU:HB3	2:C:50:ILE:HD12	1.95	0.48
2:C:216:ARG:N	4:C:301:HOH:O	2.28	0.48
3:F:19:ARG:NE	4:F:302:HOH:O	2.34	0.48
3:D:18:LEU:HB3	3:D:82:MET:HE3	1.95	0.48
2:E:166:GLU:HB2	2:E:180:LEU:HD11	1.95	0.48
2:E:188:LYS:CG	2:E:192:GLU:OE1	2.62	0.48
2:C:113:ARG:HG3	2:C:114:THR:O	2.14	0.48
3:F:150:LEU:HD13	3:F:223:VAL:HG11	1.94	0.48
1:A:366:LEU:HD22	1:A:370:ILE:CD1	2.44	0.48
2:E:120:VAL:HG13	2:E:141:LEU:HD23	1.95	0.48
2:E:138:VAL:HG21	3:F:136:LEU:HD13	1.95	0.48
3:F:35:ASN:ND2	3:F:98:HIS:CE1	2.74	0.48
1:B:351:PRO:HD2	1:B:354:TRP:HB2	1.96	0.47
2:C:138:VAL:HG21	3:D:136:LEU:HD11	1.95	0.47
2:E:127:ASP:HA	2:E:130:LEU:HD12	1.95	0.47
3:F:50:TYR:C	3:F:50:TYR:CD1	2.91	0.47
3:F:171:LEU:HD12	3:F:171:LEU:HA	1.75	0.47
3:F:6:GLU:OE2	3:F:118:GLY:N	2.46	0.47
2:C:172:ASP:HB3	2:C:175:ASP:OD2	2.14	0.47
3:F:32:TYR:HA	4:F:305:HOH:O	2.13	0.47
3:F:135:PRO:O	3:F:136:LEU:HD23	2.14	0.47
1:A:356:SER:HB3	1:A:362:ARG:CG	2.36	0.47
3:D:172:THR:O	3:D:175:VAL:HG12	2.15	0.47
1:A:334:TRP:CZ3	1:A:335:ILE:HG12	2.50	0.47
3:F:59:TYR:CE1	3:F:69:ILE:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:CYS:SG	1:A:318:CYS:CB	3.03	0.47
1:B:403:LEU:HB2	1:B:406:MET:HG3	1.97	0.47
3:D:50:TYR:CD1	3:D:50:TYR:C	2.93	0.47
1:A:367:TYR:CE2	1:B:324:ILE:HD13	2.46	0.47
2:C:124:PRO:HB3	2:C:214:PHE:CE2	2.50	0.47
3:D:200:SER:HA	3:D:203:THR:HB	1.96	0.47
2:E:136:SER:HA	2:E:184:LEU:O	2.15	0.47
2:E:137:VAL:HG22	2:E:184:LEU:HB3	1.96	0.47
3:F:36:TRP:HD1	3:F:69:ILE:HD13	1.79	0.47
3:F:128:THR:HG21	3:F:214:PRO:O	2.15	0.47
3:D:81:GLN:OE1	3:D:83:ASN:ND2	2.43	0.47
2:C:125:PRO:HB2	2:C:130:LEU:HD21	1.96	0.46
2:E:155:VAL:HG12	2:E:197:TYR:CD1	2.49	0.46
2:C:83:GLU:CD	2:C:83:GLU:H	2.22	0.46
3:D:86:ARG:HD3	4:D:302:HOH:O	2.16	0.46
3:D:88:GLU:OE1	3:D:88:GLU:N	2.39	0.46
2:E:171:GLN:HG3	2:E:176:SER:HA	1.96	0.46
1:B:357:ASP:CG	1:B:358:THR:H	2.23	0.46
1:A:330:LEU:HD23	1:B:366:LEU:HD23	1.98	0.46
2:E:190:ASP:N	2:E:190:ASP:OD2	2.49	0.46
3:D:86:ARG:CD	4:D:302:HOH:O	2.64	0.46
3:D:221:LYS:HD2	3:D:221:LYS:HA	1.49	0.45
2:C:127:ASP:HA	2:C:130:LEU:HD12	1.99	0.45
3:F:201:LEU:HD13	3:F:206:TYR:CD2	2.50	0.45
2:E:188:LYS:O	2:E:192:GLU:HG2	2.16	0.45
1:B:357:ASP:HB3	1:B:361:SER:CB	2.47	0.45
1:A:392:TYR:CD1	1:A:399:LYS:HD3	2.52	0.45
2:E:126:SER:C	2:E:128:GLU:H	2.23	0.45
2:E:154:LYS:CE	2:E:157:ASN:HA	2.47	0.45
2:C:85:PHE:CZ	2:C:170:GLU:HB3	2.52	0.44
3:D:6:GLU:OE1	3:D:95:CYS:N	2.50	0.44
1:B:386:GLU:HG2	1:B:387:PRO:HD2	2.00	0.44
3:D:11:LEU:HD11	3:D:124:SER:OG	2.17	0.44
3:F:128:THR:HG23	3:F:159:PRO:HD3	1.98	0.44
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.78	0.44
3:D:27:PHE:HB2	3:D:32:TYR:CD2	2.53	0.44
2:E:202:THR:HG22	2:E:209:PRO:HG3	1.99	0.44
3:D:151:GLY:HA2	3:D:166:TRP:CH2	2.52	0.44
2:E:113:ARG:HG3	2:E:176:SER:OG	2.18	0.44
1:A:392:TYR:CE1	1:A:399:LYS:HD3	2.53	0.44
1:B:309:CYS:HG	1:B:318:CYS:CB	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:87:ALA:HA	3:D:123:VAL:HG23	1.99	0.44
3:D:222:LYS:HB2	3:D:222:LYS:HE2	1.76	0.44
3:D:154:VAL:CG2	3:D:210:VAL:HG21	2.46	0.44
3:D:207:ILE:CB	3:D:221:LYS:O	2.57	0.44
1:A:393:TYR:O	1:A:395:GLY:N	2.51	0.43
3:D:15:GLY:HA2	3:D:84:SER:HA	2.00	0.43
1:B:325:ASP:O	1:B:329:ASP:HB2	2.17	0.43
3:D:200:SER:O	3:D:202:GLY:N	2.51	0.43
2:C:82:PRO:HA	2:C:111:ILE:HG13	2.01	0.43
1:B:399:LYS:HD3	1:B:400:ILE:H	1.84	0.43
3:F:11:LEU:HD12	3:F:12:VAL:H	1.83	0.43
2:E:128:GLU:OE1	3:F:221:LYS:NZ	2.52	0.43
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.84	0.43
2:C:123:PHE:HA	2:C:124:PRO:HD3	1.84	0.43
3:F:20:LEU:CD1	3:F:82:MET:HE2	2.49	0.43
3:F:221:LYS:HD3	3:F:222:LYS:O	2.18	0.43
3:D:27:PHE:HB2	3:D:32:TYR:CE2	2.54	0.43
3:F:20:LEU:HD12	3:F:20:LEU:N	2.33	0.43
3:F:157:TYR:C	3:F:157:TYR:CD1	2.97	0.43
1:A:341:TYR:HE2	1:A:407:ILE:HG13	1.83	0.42
2:C:69:SER:OG	2:C:70:GLY:N	2.51	0.42
2:C:124:PRO:HB3	2:C:214:PHE:CZ	2.54	0.42
2:E:145:TYR:CD1	2:E:146:PRO:HA	2.54	0.42
2:E:154:LYS:HZ3	2:E:157:ASN:CG	2.26	0.42
3:F:40:ALA:HB3	3:F:43:LYS:HB2	2.00	0.42
1:B:357:ASP:HB3	1:B:361:SER:HB2	2.01	0.42
1:B:385:LEU:HD13	1:B:405:ASN:HB3	2.01	0.42
2:E:34:TYR:CD1	3:F:109:MET:HA	2.54	0.42
2:E:188:LYS:CD	2:E:192:GLU:OE1	2.67	0.42
1:B:324:ILE:HG21	1:B:330:LEU:HD11	2.01	0.42
1:A:401:GLU:CG	1:A:402:GLN:N	2.83	0.42
2:E:148:GLU:OE2	2:E:148:GLU:N	2.41	0.42
2:E:188:LYS:HE3	2:E:192:GLU:OE1	2.19	0.42
3:F:150:LEU:HD12	3:F:151:GLY:N	2.34	0.42
1:B:314:GLN:HG3	1:B:315:ASP:N	2.35	0.42
3:D:32:TYR:CZ	3:D:101:VAL:HG12	2.55	0.42
3:F:150:LEU:HD11	3:F:166:TRP:CZ3	2.55	0.42
3:F:133:VAL:CG2	3:F:210:VAL:HG11	2.37	0.42
2:E:126:SER:O	2:E:130:LEU:HG	2.20	0.41
1:A:323:TYR:CZ	1:A:340:GLY:HA3	2.55	0.41
3:D:11:LEU:HD12	3:D:11:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:GLY:O	3:D:194:VAL:HA	2.21	0.41
3:F:6:GLU:OE2	3:F:94:PHE:HA	2.20	0.41
3:F:48:ILE:HG21	3:F:48:ILE:HD13	1.79	0.41
3:F:67:PHE:CE2	3:F:82:MET:HB3	2.54	0.41
1:B:341:TYR:CZ	1:B:343:ALA:HB2	2.56	0.41
3:D:59:TYR:OH	3:D:68:THR:HA	2.21	0.41
2:E:79:SER:O	2:E:80:LEU:C	2.63	0.41
2:E:154:LYS:HE2	2:E:157:ASN:C	2.44	0.41
3:F:14:PRO:HD3	3:F:124:SER:C	2.44	0.41
3:F:19:ARG:HB2	3:F:81:GLN:HE22	1.83	0.41
3:D:90:THR:HG22	3:D:123:VAL:H	1.84	0.41
2:E:123:PHE:HB3	3:F:136:LEU:HB3	2.01	0.41
1:B:384:ASP:HB2	1:B:410:SER:OG	2.21	0.41
3:D:136:LEU:HD23	3:D:136:LEU:HA	1.75	0.41
2:E:145:TYR:CG	2:E:146:PRO:HA	2.54	0.41
3:F:50:TYR:HE1	3:F:52:SER:HB3	1.86	0.41
2:C:126:SER:CB	3:D:135:PRO:HG2	2.50	0.41
2:E:25:SER:O	2:E:71:THR:OG1	2.39	0.41
2:E:154:LYS:HE2	2:E:158:ALA:N	2.35	0.41
2:E:201:VAL:HG13	2:E:206:LEU:HD21	2.03	0.41
3:F:67:PHE:HD2	3:F:80:LEU:HD11	1.85	0.41
3:F:160:GLU:OE1	3:F:161:PRO:HA	2.21	0.41
3:D:4:LEU:HD22	3:D:95:CYS:SG	2.60	0.41
2:E:203:HIS:HB3	2:E:206:LEU:CD1	2.50	0.41
1:A:401:GLU:HG2	1:A:402:GLN:N	2.36	0.41
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.77	0.41
3:F:47:TRP:HZ2	3:F:50:TYR:CD2	2.38	0.41
3:F:207:ILE:HD12	3:F:221:LYS:O	2.20	0.41
1:B:409:LYS:HA	1:B:409:LYS:HD2	1.97	0.40
3:D:20:LEU:HD12	3:D:80:LEU:HD23	2.02	0.40
1:A:322:LEU:HD11	1:B:367:TYR:CE1	2.57	0.40
3:D:51:ILE:HB	3:D:69:ILE:HG22	2.03	0.40
2:E:180:LEU:HD12	2:E:181:SER:N	2.34	0.40
3:F:35:ASN:OD1	3:F:98:HIS:HE1	2.04	0.40
2:E:80:LEU:HD23	2:E:80:LEU:HA	1.77	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	107/112 (96%)	93 (87%)	11 (10%)	3 (3%)	4	15
1	B	110/112 (98%)	103 (94%)	6 (6%)	1 (1%)	14	41
2	C	215/219 (98%)	198 (92%)	13 (6%)	4 (2%)	6	23
2	E	198/219 (90%)	174 (88%)	22 (11%)	2 (1%)	12	39
3	D	212/233 (91%)	203 (96%)	8 (4%)	1 (0%)	24	54
3	F	212/233 (91%)	187 (88%)	22 (10%)	3 (1%)	9	30
All	All	1054/1128 (93%)	958 (91%)	82 (8%)	14 (1%)	9	32

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	169	THR
1	A	394	ILE
2	E	70	GLY
2	C	132	SER
3	D	201	LEU
1	A	358	THR
2	C	95	SER
3	F	125	SER
2	C	70	GLY
3	F	167	ASN
1	B	351	PRO
2	C	217	GLY
3	F	213	LYS
1	A	400	ILE

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	99/100 (99%)	98 (99%)	1 (1%)	68	89
1	B	100/100 (100%)	100 (100%)	0	100	100
2	C	187/189 (99%)	184 (98%)	3 (2%)	55	83
2	E	177/189 (94%)	175 (99%)	2 (1%)	65	88
3	D	175/190 (92%)	171 (98%)	4 (2%)	44	76
3	F	175/190 (92%)	174 (99%)	1 (1%)	78	93
All	All	913/958 (95%)	902 (99%)	11 (1%)	63	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	LEU
2	C	23	CYS
2	C	90	CYS
2	C	131	LYS
3	D	6	GLU
3	D	81	GLN
3	D	155	LYS
3	D	221	LYS
2	E	152	GLN
2	E	206	LEU
3	F	82	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	B	314	GLN
1	B	336	HIS
1	B	360	HIS
2	C	33	ASN
2	C	160	GLN
2	C	165	GLN
2	E	32	ASN
2	E	142	ASN
2	E	143	ASN
2	E	163	ASN

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Mol	Chain	Res	Type
3	F	81	GLN
3	F	209	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	111/112 (99%)	0.01	1 (0%) 81 75	54, 78, 120, 131	0
1	B	112/112 (100%)	-0.22	0 100 100	50, 66, 82, 94	0
2	C	217/219 (99%)	-0.15	2 (0%) 81 75	52, 69, 99, 110	0
2	E	204/219 (93%)	0.01	2 (0%) 79 73	36, 78, 121, 127	0
3	D	216/233 (92%)	-0.02	3 (1%) 73 65	48, 71, 112, 123	0
3	F	216/233 (92%)	-0.04	0 100 100	49, 81, 116, 133	0
All	All	1076/1128 (95%)	-0.06	8 (0%) 84 79	36, 72, 114, 133	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	170	ALA	3.9
2	C	151	VAL	3.4
2	C	166	GLU	3.3
2	E	122	ILE	2.9
3	D	225	PRO	2.2
3	D	196	VAL	2.1
1	A	393	TYR	2.0
2	E	125	PRO	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.