



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 03:59 am GMT

PDB ID : 2VQ1
Title : anti trimeric Lewis X Fab54-5C10-A
Authors : de Geus, D.C.; van Roon, A.M.M.; Thomassen, E.A.J.; Hokke, C.H.; Deelder, A.M.; Abrahams, J.P.
Deposited on : 2008-03-10
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

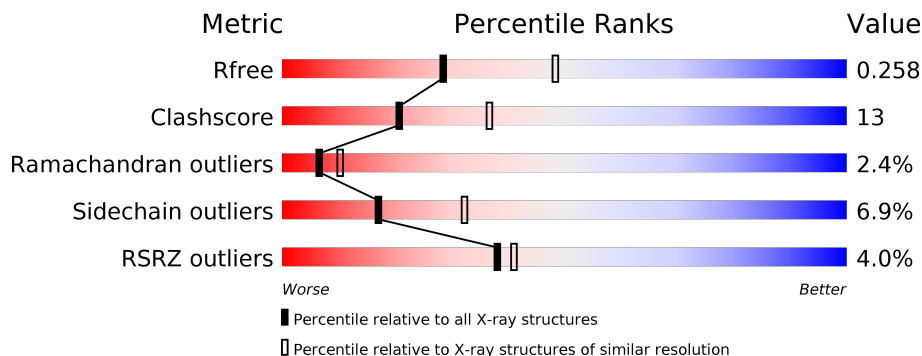
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	217	<div> <div>4%</div> <div>75%</div> <div>23%</div> <div>•</div> </div>
1	E	217	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>•</div> </div>
2	B	218	<div> <div>4%</div> <div>70%</div> <div>21%</div> <div>6%</div> <div>•</div> </div>
2	F	218	<div> <div>6%</div> <div>67%</div> <div>18%</div> <div>6%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6868 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.

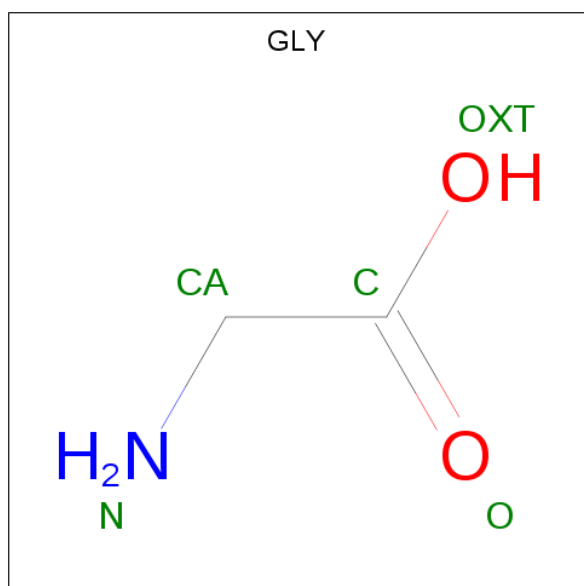
- Molecule 1 is a protein called IGKV1-117 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	1
			1676	1047	286	336	7			
1	E	217	Total	C	N	O	S	0	1	1
			1681	1050	286	338	7			

- Molecule 2 is a protein called ANTI-HUMAN FC GAMMA RECEPTOR III 3G8 GAMMA HEAVY CHAIN VARIABLE REGION.

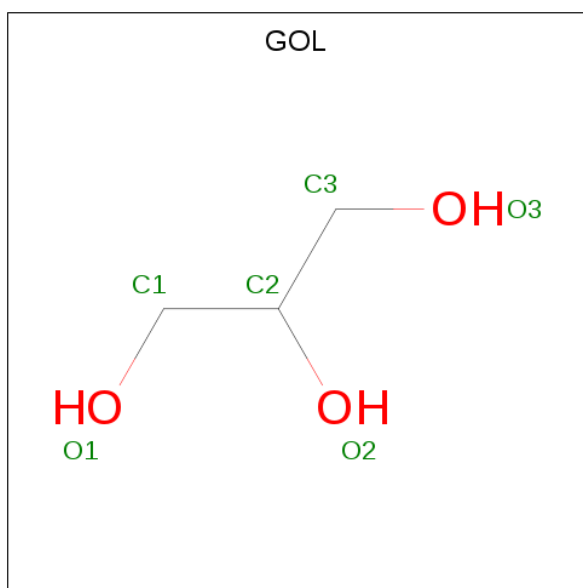
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1619	1036	264	313	6			
2	F	211	Total	C	N	O	S	0	2	0
			1617	1038	262	312	5			

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



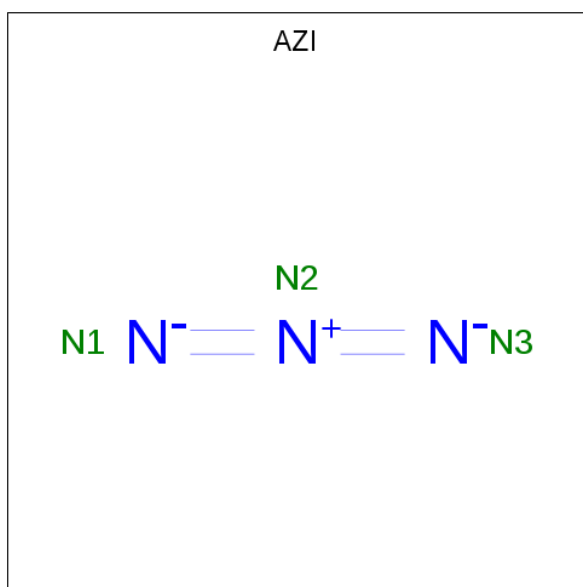
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 5 2 1 2	0	0
3	A	1	Total C N O 5 2 1 2	0	0
3	B	1	Total C N O 5 2 1 2	0	0
3	E	1	Total C N O 5 2 1 2	0	0
3	E	1	Total C N O 5 2 1 2	0	0
3	E	1	Total C N O 5 2 1 2	0	0
3	F	1	Total C N O 5 2 1 2	0	0
3	F	1	Total C N O 5 2 1 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 3 3	0	0

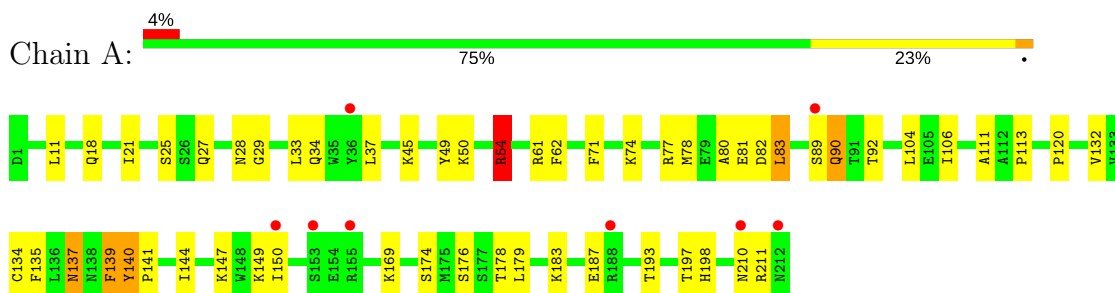
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	57	Total O 57 57	0	0
6	B	58	Total O 58 58	0	0
6	E	49	Total O 49 49	0	0
6	F	50	Total O 50 50	0	0

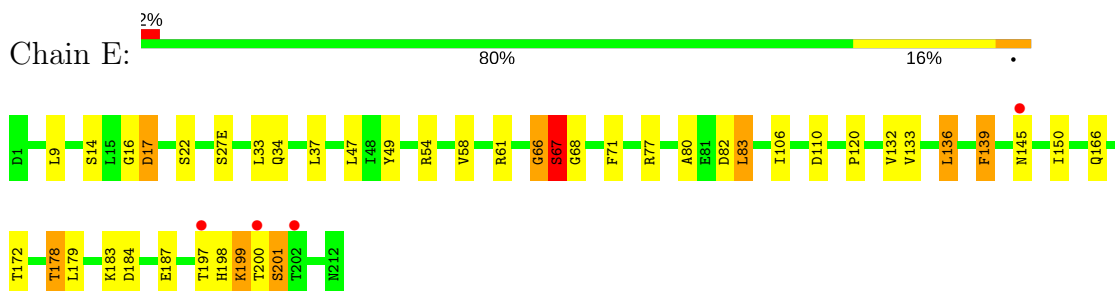
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

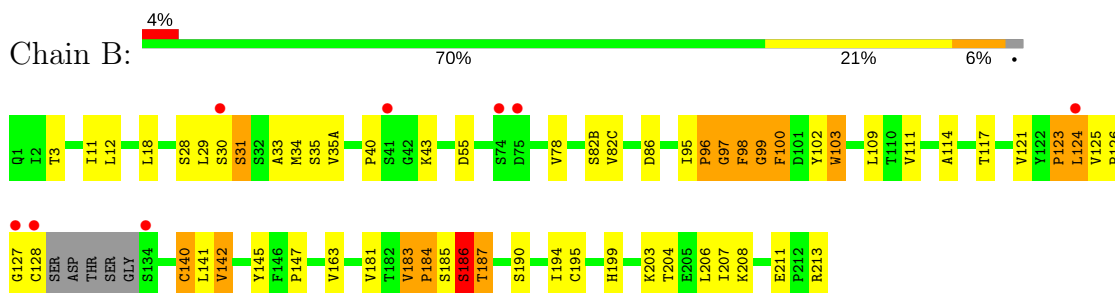
- Molecule 1: IGKV1-117 PROTEIN



- Molecule 1: IGKV1-117 PROTEIN

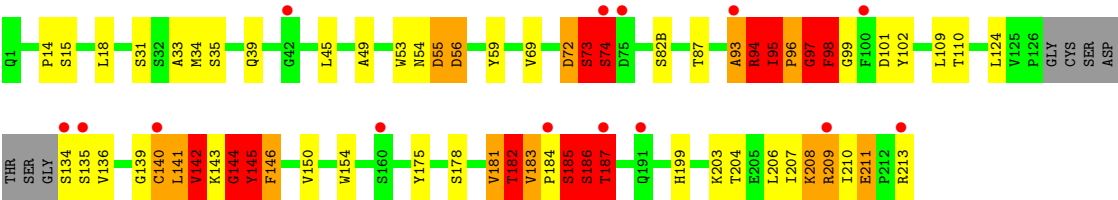


- Molecule 2: ANTI-HUMAN FC GAMMA RECEPTOR III 3G8 GAMMA HEAVY CHAIN VARIABLE REGION



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.38Å 161.01Å 53.48Å 90.00° 103.07° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 28.73 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.50) 95.9 (28.73-2.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.260 0.202 , 0.258	Depositor DCC
R_{free} test set	2064 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6868	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL

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	0.56	0/1714	0.72	6/2325 (0.3%)
1	E	0.57	0/1722	0.64	0/2336
2	B	0.70	3/1663 (0.2%)	0.78	5/2273 (0.2%)
2	F	0.68	0/1667	0.85	7/2280 (0.3%)
All	All	0.63	3/6766 (0.0%)	0.75	18/9214 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	E	0	4
2	B	3	10
2	F	3	13
All	All	7	31

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	140	CYS	CB-SG	7.70	1.95	1.82
2	B	145	TYR	CD1-CE1	-6.93	1.28	1.39
2	B	145	TYR	CD2-CE2	-5.36	1.31	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	CYS	CA-CB-SG	9.13	130.44	114.00
2	F	144	GLY	N-CA-C	-8.62	91.54	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	95	ILE	N-CA-C	8.08	132.82	111.00
2	F	74	SER	CB-CA-C	7.86	125.04	110.10
1	A	90	GLN	N-CA-C	7.79	132.03	111.00
1	A	135	PHE	N-CA-CB	7.75	124.54	110.60
2	F	56	ASP	N-CA-C	-7.68	90.25	111.00
2	F	145	TYR	CB-CA-C	7.20	124.81	110.40
2	F	142	VAL	N-CA-C	-7.05	91.97	111.00
2	F	146	PHE	N-CA-CB	-6.64	98.64	110.60
1	A	54	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	54	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	142	VAL	N-CA-C	-5.84	95.23	111.00
2	B	97	GLY	N-CA-C	-5.53	99.29	113.10
2	B	103	TRP	N-CA-C	5.50	125.86	111.00
1	A	140	TYR	N-CA-CB	-5.40	100.88	110.60
2	B	98	PHE	N-CA-C	-5.06	97.33	111.00
1	A	198	HIS	N-CA-C	-5.04	97.39	111.00

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	197	THR	CB
2	B	103	TRP	CA
2	B	187	THR	CB,CA
2	F	33	ALA	CA
2	F	183	VAL	CA
2	F	187	THR	CA

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	CYS	Peptide
1	A	139	PHE	Peptide
1	A	54	ARG	Peptide
1	A	89	SER	Peptide
2	B	102	TYR	Peptide
2	B	123	PRO	Peptide
2	B	141	LEU	Peptide
2	B	183	VAL	Peptide
2	B	185	SER	Peptide
2	B	186	SER	Peptide
2	B	31	SER	Peptide
2	B	33	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	B	97	GLY	Peptide
2	B	99	GLY	Peptide
1	E	139	PHE	Peptide
1	E	200	THR	Peptide
1	E	27(E)	SER	Peptide
1	E	66	GLY	Peptide
2	F	141	LEU	Peptide
2	F	143	LYS	Peptide
2	F	144	GLY	Peptide
2	F	145	TYR	Peptide
2	F	181	VAL	Peptide
2	F	182	THR	Peptide
2	F	185	SER	Peptide
2	F	186	SER	Peptide
2	F	72	ASP	Peptide
2	F	93	ALA	Peptide
2	F	94	ARG	Peptide
2	F	96	PRO	Peptide
2	F	97	GLY	Peptide

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	1676	0	1622	28	0
1	E	1681	0	1626	23	0
2	B	1619	0	1596	47	0
2	F	1617	0	1604	76	0
3	A	10	0	4	3	0
3	B	5	0	2	2	0
3	E	15	0	6	0	0
3	F	10	0	4	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	F	6	0	8	0	0
5	A	3	0	0	0	0
6	A	57	0	0	1	0
6	B	58	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	49	0	0	2	0
6	F	50	0	0	1	0
All	All	6868	0	6488	174	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 13.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:VAL:CG2	2:B:187:THR:HG22	1.54	1.36
2:B:183:VAL:CG2	2:B:187:THR:CG2	2.05	1.34
2:B:183:VAL:HG21	2:B:187:THR:CG2	1.61	1.27
2:F:72:ASP:CA	2:F:73:SER:HB2	1.66	1.26
2:B:140:CYS:SG	2:B:195:CYS:CB	2.25	1.22
2:F:72:ASP:HA	2:F:73:SER:CB	1.71	1.16
1:E:198:HIS:O	1:E:201:SER:HB2	1.47	1.14
2:B:184:PRO:HD3	6:B:2048:HOH:O	1.49	1.12
2:F:182:THR:O	2:F:183:VAL:HG23	1.53	1.08
2:B:183:VAL:HG22	2:B:187:THR:HG22	1.17	1.07
2:F:183:VAL:HG13	2:F:184:PRO:HD2	1.33	1.06
2:F:184:PRO:O	2:F:185:SER:HB2	1.56	1.02
2:F:184:PRO:HG2	2:F:187:THR:CG2	1.90	1.01
2:B:31:SER:O	2:B:34:MET:HB2	1.61	0.99
2:F:184:PRO:CG	2:F:187:THR:HG22	1.93	0.98
2:B:128:CYS:SG	2:B:213:ARG:HB3	2.04	0.96
2:B:183:VAL:HG21	2:B:187:THR:HG23	1.51	0.93
2:F:134:SER:O	2:F:185:SER:HB2	1.69	0.92
2:F:72:ASP:OD1	2:F:73:SER:HB3	1.71	0.90
2:F:183:VAL:HG13	2:F:184:PRO:CD	2.04	0.88
2:F:184:PRO:HG2	2:F:187:THR:HG22	1.50	0.88
2:B:140:CYS:CB	2:B:195:CYS:SG	2.62	0.88
2:F:183:VAL:HG22	2:F:184:PRO:HD3	1.57	0.85
1:A:18:GLN:NE2	1:A:74:LYS:HE3	1.92	0.84
2:B:183:VAL:CG2	2:B:187:THR:HG21	2.06	0.82
2:F:184:PRO:CG	2:F:187:THR:CG2	2.54	0.81
2:F:134:SER:N	2:F:185:SER:OG	2.15	0.80
1:A:210:ASN:O	1:A:211:ARG:HG2	1.82	0.80
2:B:140:CYS:SG	2:B:195:CYS:SG	0.80	0.80
2:F:182:THR:C	2:F:183:VAL:HG23	2.00	0.80
2:F:184:PRO:HG2	2:F:187:THR:HG21	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:PRO:HD2	2:F:187:THR:CG2	2.13	0.79
1:E:110:ASP:OD2	1:E:199:LYS:HE3	1.84	0.78
2:B:186:SER:O	2:B:190:SER:OG	2.02	0.78
1:A:34:GLN:HE21	1:A:50:LYS:H	1.28	0.77
2:F:144:GLY:HA3	2:F:175:TYR:O	1.87	0.74
2:F:184:PRO:CB	2:F:187:THR:HG22	2.17	0.74
2:F:35:SER:HB3	2:F:95:ILE:HB	1.70	0.73
2:F:135:SER:HA	2:F:184:PRO:O	1.89	0.73
2:B:40:PRO:HB2	2:B:43:LYS:HD2	1.71	0.71
2:F:184:PRO:CD	2:F:187:THR:CG2	2.70	0.70
2:F:184:PRO:HD2	2:F:187:THR:HG23	1.74	0.69
2:F:184:PRO:HB2	2:F:187:THR:HG22	1.74	0.68
2:B:29:LEU:O	2:B:30:SER:CB	2.39	0.68
2:B:183:VAL:HG23	2:B:187:THR:CG2	2.21	0.68
1:A:28:ASN:N	1:A:29:GLY:HA2	2.09	0.67
1:A:61:ARG:HD3	1:A:77:ARG:HH21	1.60	0.67
2:F:134:SER:C	2:F:185:SER:OG	2.34	0.66
2:F:144:GLY:CA	2:F:175:TYR:O	2.44	0.66
2:B:183:VAL:HG21	2:B:187:THR:HG21	1.70	0.66
1:E:136:LEU:CD1	1:E:136:LEU:N	2.57	0.66
2:F:183:VAL:CG1	2:F:184:PRO:HD2	2.19	0.65
2:F:94:ARG:HB3	2:F:101:ASP:OD1	1.98	0.63
2:F:72:ASP:HA	2:F:73:SER:HB2	0.78	0.63
1:E:14:SER:O	1:E:17:ASP:HB2	1.99	0.63
2:F:182:THR:HG22	2:F:183:VAL:N	2.14	0.62
2:B:125:VAL:O	2:B:127:GLY:HA2	2.00	0.62
2:B:82(C):VAL:HB	6:B:2003:HOH:O	1.99	0.61
1:A:111:ALA:HB3	1:A:140:TYR:H	1.66	0.61
2:F:134:SER:O	2:F:185:SER:CB	2.45	0.61
2:F:72:ASP:CA	2:F:73:SER:CB	2.47	0.60
2:F:136:VAL:O	2:F:183:VAL:HA	2.02	0.60
2:F:183:VAL:HG22	2:F:184:PRO:CD	2.29	0.60
2:F:184:PRO:O	2:F:185:SER:CB	2.35	0.59
1:A:183:LYS:O	1:A:187:GLU:HG2	2.03	0.59
2:F:95:ILE:HG22	2:F:97:GLY:HA2	1.87	0.57
2:B:124:LEU:N	2:B:124:LEU:HD13	2.20	0.56
2:F:33:ALA:HB2	2:F:53:TRP:CZ3	2.40	0.56
2:B:35(A):VAL:HB	2:B:78:VAL:HG21	1.87	0.56
1:E:83:LEU:HD12	1:E:166:GLN:HB3	1.87	0.56
2:F:49:ALA:HB1	2:F:69[A]:VAL:HG21	1.87	0.55
1:E:66:GLY:HA2	1:E:67:SER:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:PRO:CD	2:F:187:THR:HG22	2.34	0.55
2:B:123:PRO:HB2	2:B:125:VAL:HG23	1.89	0.55
2:B:35:SER:HB3	2:B:95:ILE:HB	1.89	0.55
2:B:117:THR:HG1	3:B:1214:GLY:N	2.06	0.54
1:A:80:ALA:HA	1:A:106:ILE:HD13	1.90	0.54
2:B:121:VAL:HB	2:B:206:LEU:HD11	1.90	0.53
1:E:183:LYS:O	1:E:187:GLU:HG3	2.07	0.53
2:F:96:PRO:O	2:F:97:GLY:O	2.27	0.53
1:A:137:ASN:ND2	1:A:174:SER:OG	2.41	0.53
1:A:34:GLN:NE2	1:A:50:LYS:H	2.02	0.53
2:B:183:VAL:HG23	2:B:187:THR:HG21	1.84	0.52
2:F:183:VAL:CG1	2:F:184:PRO:CD	2.85	0.52
2:F:73:SER:C	2:F:74:SER:OG	2.48	0.52
2:B:29:LEU:O	2:B:30:SER:OG	2.26	0.52
2:F:97:GLY:O	2:F:98:PHE:CB	2.53	0.52
2:F:134:SER:CA	2:F:185:SER:OG	2.58	0.52
1:E:110:ASP:OD2	1:E:199:LYS:CE	2.56	0.52
2:B:163:VAL:HG22	2:B:181:VAL:HG22	1.92	0.52
1:E:61:ARG:NH1	1:E:82:ASP:OD2	2.37	0.51
1:A:178:THR:HG1	3:A:1213:GLY:N	2.09	0.51
2:B:96:PRO:HD2	2:B:99:GLY:O	2.11	0.51
2:F:54:ASN:OD1	2:F:54:ASN:C	2.43	0.51
2:F:183:VAL:HG13	2:F:187:THR:HG23	1.93	0.51
2:F:95:ILE:HG23	2:F:99:GLY:H	1.75	0.51
1:A:149:LYS:HB2	1:A:193:THR:HB	1.93	0.50
2:F:59:TYR:CE1	2:F:69[A]:VAL:HG23	2.45	0.50
2:F:142:VAL:HG11	2:F:150:VAL:HG11	1.93	0.50
1:A:21:ILE:HD11	1:A:104:LEU:HD13	1.94	0.50
1:E:150:ILE:HD11	1:E:179:LEU:HD21	1.94	0.50
2:F:134:SER:O	2:F:184:PRO:O	2.31	0.49
2:F:134:SER:C	2:F:185:SER:CB	2.81	0.49
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.95	0.48
2:F:186:SER:OG	2:F:187:THR:N	2.46	0.48
2:B:29:LEU:C	2:B:31:SER:H	2.16	0.48
1:E:198:HIS:O	1:E:201:SER:CB	2.39	0.48
1:E:80:ALA:HA	1:E:106:ILE:HD13	1.95	0.48
1:E:136:LEU:HD12	1:E:136:LEU:N	2.27	0.47
1:A:54:ARG:HD3	1:A:62:PHE:O	2.15	0.47
2:F:187:THR:O	2:F:187:THR:OG1	2.31	0.47
1:E:133:VAL:HG22	1:E:178:THR:HB	1.97	0.47
1:A:78:MET:HE1	1:A:104:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:ALA:HA	2:F:102:TYR:O	2.14	0.47
2:B:98:PHE:CD1	2:B:99:GLY:N	2.83	0.47
1:E:136:LEU:N	1:E:136:LEU:HD13	2.29	0.46
2:F:209:ARG:HD2	2:F:211:GLU:OE1	2.15	0.46
2:F:208:LYS:HE3	2:F:208:LYS:HA	1.97	0.46
2:B:31:SER:O	2:B:34:MET:CB	2.48	0.46
1:A:25:SER:OG	1:A:27:GLN:O	2.23	0.46
2:F:34:MET:CE	2:F:94:ARG:HD2	2.44	0.46
2:F:97:GLY:O	2:F:98:PHE:HB3	2.15	0.46
1:E:33:LEU:HD22	1:E:71:PHE:CG	2.51	0.46
2:B:28:SER:O	2:B:31:SER:HB3	2.16	0.46
2:F:49:ALA:CB	2:F:69[A]:VAL:HG21	2.46	0.46
2:B:11:ILE:HB	2:B:147:PRO:HG3	1.97	0.45
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.42	0.45
2:B:95:ILE:HA	2:B:99:GLY:O	2.15	0.45
1:A:81:GLU:HG2	6:A:2021:HOH:O	2.16	0.45
2:F:73:SER:O	2:F:74:SER:OG	2.33	0.45
2:B:203:LYS:HD3	6:E:2004:HOH:O	2.16	0.45
2:F:18:LEU:HD22	2:F:109:LEU:HD22	1.99	0.44
2:F:73:SER:O	2:F:74:SER:CB	2.64	0.44
1:A:113:PRO:HG3	1:A:144:ILE:HD11	2.00	0.44
2:B:194:ILE:HG23	2:B:207:ILE:HG23	1.99	0.44
2:B:18:LEU:HD22	2:B:109:LEU:HD22	1.99	0.44
1:E:16:GLY:HA2	1:E:77:ARG:HG2	1.98	0.44
2:B:114:ALA:HB1	3:B:1214:GLY:HA2	1.99	0.43
2:B:124:LEU:CD1	2:B:124:LEU:N	2.80	0.43
1:E:145:ASN:HB3	1:E:197:THR:HB	1.99	0.43
2:F:139:GLY:HA2	2:F:154:TRP:CH2	2.53	0.43
1:A:176:SER:HG	3:A:1213:GLY:N	2.17	0.43
2:B:123:PRO:HD3	2:B:208:LYS:HD2	2.01	0.43
1:E:83:LEU:HD23	6:E:2025:HOH:O	2.18	0.43
2:B:98:PHE:CD1	2:B:98:PHE:C	2.92	0.43
1:A:120:PRO:HD3	1:A:132:VAL:HG22	2.00	0.43
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.54	0.43
2:F:72:ASP:OD1	2:F:73:SER:CB	2.54	0.42
1:A:45:LYS:NZ	3:A:1214:GLY:OXT	2.50	0.42
1:E:34:GLN:HG3	1:E:49:TYR:HA	2.01	0.42
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.99	0.42
1:E:120:PRO:HD3	1:E:132:VAL:HG22	1.99	0.42
1:E:83:LEU:HD11	1:E:166:GLN:O	2.20	0.42
2:F:96:PRO:C	2:F:97:GLY:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:209:ARG:NH2	6:F:2046:HOH:O	2.52	0.42
2:B:199:HIS:HB3	2:B:204:THR:HB	2.01	0.42
2:F:181:VAL:HG22	2:F:182:THR:O	2.20	0.42
1:E:47:LEU:HA	1:E:58:VAL:HG21	2.01	0.42
2:F:199:HIS:HB3	2:F:204:THR:HB	2.01	0.42
2:F:59:TYR:CZ	2:F:69[B]:VAL:HG22	2.55	0.42
1:A:77:ARG:HE	1:A:77:ARG:HB2	1.75	0.42
2:F:144:GLY:HA2	2:F:175:TYR:O	2.20	0.42
1:A:139:PHE:HD1	1:A:141:PRO:O	2.03	0.41
2:F:146:PHE:CG	3:F:1215:GLY:OXT	2.74	0.41
2:F:34:MET:HE3	2:F:94:ARG:HD2	2.02	0.41
2:B:183:VAL:HA	2:B:184:PRO:HD2	1.76	0.41
2:B:82(C):VAL:HG13	2:B:86:ASP:HB2	2.02	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD12	1.91	0.41
2:B:82(C):VAL:CG1	2:B:111:VAL:HG21	2.51	0.41
2:F:140:CYS:SG	2:F:210:ILE:HD11	2.61	0.41
2:F:14:PRO:O	2:F:15:SER:HB2	2.21	0.41
1:A:34:GLN:HG3	1:A:49:TYR:HA	2.02	0.40
2:B:12:LEU:O	2:B:111:VAL:HA	2.21	0.40
2:F:87:THR:HG23	2:F:110:THR:HA	2.02	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	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
1	E	216/217 (100%)	206 (95%)	8 (4%)	2 (1%)	19	34
2	B	209/218 (96%)	192 (92%)	11 (5%)	6 (3%)	5	7
2	F	209/218 (96%)	189 (90%)	8 (4%)	12 (6%)	2	2
All	All	849/870 (98%)	794 (94%)	35 (4%)	20 (2%)	6	10

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	184	PRO
1	E	67	SER
2	F	97	GLY
2	F	98	PHE
2	F	185	SER
2	F	187	THR
2	B	100	PHE
2	B	142	VAL
2	F	74	SER
2	F	82(B)	SER
2	F	94	ARG
2	F	145	TYR
2	B	82(B)	SER
2	F	55	ASP
2	B	96	PRO
1	E	68	GLY
2	F	73	SER
2	F	142	VAL
2	B	126	PRO
2	F	183	VAL

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	194/195 (100%)	185 (95%)	9 (5%)	29	53
1	E	195/195 (100%)	181 (93%)	14 (7%)	16	30
2	B	185/189 (98%)	178 (96%)	7 (4%)	36	62
2	F	186/189 (98%)	164 (88%)	22 (12%)	6	11
All	All	760/768 (99%)	708 (93%)	52 (7%)	17	33

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	37	LEU
1	A	83	LEU
1	A	90	GLN
1	A	92	THR
1	A	137	ASN
1	A	147	LYS
1	A	169	LYS
1	A	197	THR
2	B	3	THR
2	B	55	ASP
2	B	100	PHE
2	B	103	TRP
2	B	124	LEU
2	B	186	SER
2	B	211	GLU
1	E	9	LEU
1	E	17	ASP
1	E	22	SER
1	E	37	LEU
1	E	54	ARG
1	E	67	SER
1	E	83	LEU
1	E	136	LEU
1	E	139	PHE
1	E	172	THR
1	E	178	THR
1	E	184	ASP
1	E	199	LYS
1	E	201	SER
2	F	31	SER
2	F	55	ASP
2	F	56	ASP
2	F	73	SER
2	F	74	SER
2	F	95	ILE
2	F	98	PHE
2	F	124	LEU
2	F	140	CYS
2	F	141	LEU
2	F	145	TYR
2	F	178	SER
2	F	182	THR

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Mol	Chain	Res	Type
2	F	186	SER
2	F	187	THR
2	F	203	LYS
2	F	206	LEU
2	F	207	ILE
2	F	208	LYS
2	F	209	ARG
2	F	211	GLU
2	F	213	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	27(D)	HIS
1	A	34	GLN
1	A	137	ASN
2	B	16	GLN
1	E	53	ASN
2	F	105	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLY	A	1213	-	1,4,4	0.07	0	0,4,4	0.00	-
3	GLY	A	1214	-	1,4,4	0.06	0	0,4,4	0.00	-
4	GOL	A	1215	-	5,5,5	0.37	0	5,5,5	0.19	0
5	AZI	A	1216	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GLY	B	1214	-	1,4,4	0.08	0	0,4,4	0.00	-
4	GOL	B	1215	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GLY	E	1213	-	1,4,4	0.07	0	0,4,4	0.00	-
3	GLY	E	1214	-	1,4,4	0.06	0	0,4,4	0.00	-
3	GLY	E	1215	-	1,4,4	0.08	0	0,4,4	0.00	-
3	GLY	F	1214	-	1,4,4	0.11	0	0,4,4	0.00	-
3	GLY	F	1215	-	1,4,4	0.09	0	0,4,4	0.00	-
4	GOL	F	1216	-	5,5,5	0.36	0	5,5,5	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	A	1213	-	-	0/0/2/2	0/0/0/0
3	GLY	A	1214	-	-	0/0/2/2	0/0/0/0
4	GOL	A	1215	-	-	0/4/4/4	0/0/0/0
5	AZI	A	1216	-	-	0/0/0/0	0/0/0/0
3	GLY	B	1214	-	-	0/0/2/2	0/0/0/0
4	GOL	B	1215	-	-	0/4/4/4	0/0/0/0
3	GLY	E	1213	-	-	0/0/2/2	0/0/0/0
3	GLY	E	1214	-	-	0/0/2/2	0/0/0/0
3	GLY	E	1215	-	-	0/0/2/2	0/0/0/0
3	GLY	F	1214	-	-	0/0/2/2	0/0/0/0
3	GLY	F	1215	-	-	0/0/2/2	0/0/0/0
4	GOL	F	1216	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1213	GLY	2	0
3	A	1214	GLY	1	0
3	B	1214	GLY	2	0
3	F	1215	GLY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/217 (100%)	0.06	8 (3%) 41 44	25, 42, 61, 70	0
1	E	217/217 (100%)	0.04	4 (1%) 68 71	24, 43, 68, 89	0
2	B	213/218 (97%)	0.08	8 (3%) 40 43	23, 41, 61, 93	0
2	F	211/218 (96%)	0.17	14 (6%) 18 19	19, 37, 72, 93	1 (0%)
All	All	858/870 (98%)	0.09	34 (3%) 38 41	19, 41, 66, 93	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	42	GLY	5.0
2	F	74	SER	4.3
2	B	128	CYS	3.9
2	F	75	ASP	3.9
1	E	202	THR	3.7
2	F	191	GLN	3.7
2	F	140	CYS	3.6
2	F	184	PRO	3.0
2	B	127	GLY	3.0
1	A	150	ILE	2.9
2	B	30	SER	2.9
2	F	135	SER	2.6
1	E	197	THR	2.6
1	A	210	ASN	2.5
2	B	74	SER	2.4
2	B	134	SER	2.4
2	F	209	ARG	2.4
2	B	41	SER	2.4
2	B	75	ASP	2.4
2	F	100	PHE	2.3
2	F	187	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	145	ASN	2.3
2	F	213	ARG	2.3
2	F	134	SER	2.3
1	A	188	ARG	2.2
1	A	153	SER	2.2
2	F	93	ALA	2.2
1	E	200	THR	2.1
2	F	160	SER	2.1
1	A	155	ARG	2.1
1	A	212	ASN	2.1
1	A	89	SER	2.0
2	B	124	LEU	2.0
1	A	36	TYR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLY	F	1215	5/5	0.72	0.26	49,49,49,49	0
3	GLY	B	1214	5/5	0.73	0.22	50,50,51,51	0
4	GOL	F	1216	6/6	0.82	0.31	41,43,44,44	0
3	GLY	F	1214	5/5	0.84	0.18	49,49,50,50	0
4	GOL	B	1215	6/6	0.85	0.24	62,62,63,63	0
4	GOL	A	1215	6/6	0.85	0.23	45,48,49,49	0
3	GLY	E	1214	5/5	0.88	0.14	51,51,51,51	0
5	AZI	A	1216	3/3	0.89	0.15	45,45,45,46	0
3	GLY	A	1214	5/5	0.91	0.10	42,42,43,43	0
3	GLY	A	1213	5/5	0.93	0.24	41,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLY	E	1213	5/5	0.94	0.27	43,43,43,43	0
3	GLY	E	1215	5/5	0.94	0.11	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.