Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 12:55 AM EST

PDB ID	:	1GRI
Title	:	GRB2
Authors	:	Maignan, S.; Arnoux, B.; Ducruix, A.
Deposited on	:	1995-02-28
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 (i) 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 (i)) were used in the production of this report:

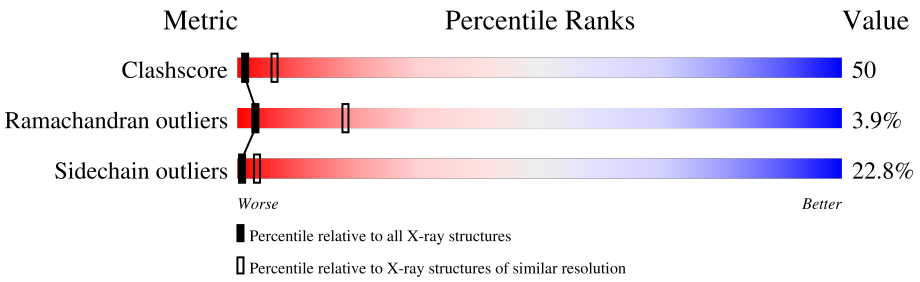
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	36% 47% 11% • •
1	B	217	26% 49% 19% • •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3468 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 GROWTH FACTOR BOUND PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1734	1110	303	315	6	0	0	0
			Total	C	N	O	S			
1	B	211	1734	1110	303	315	6	0	0	0

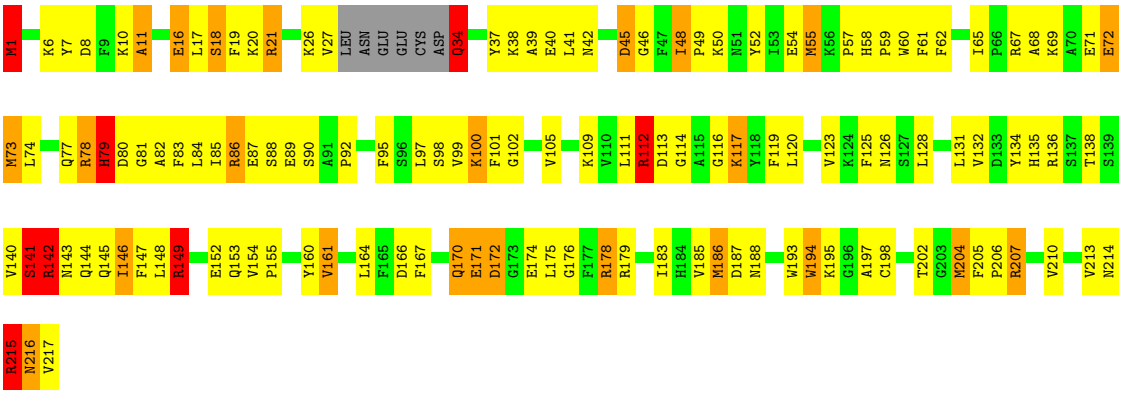
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

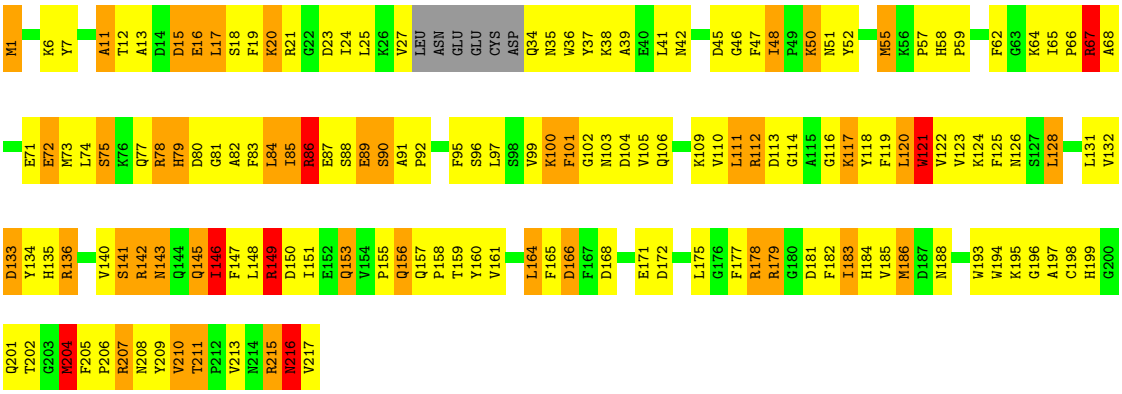
• Molecule 1: GROWTH FACTOR BOUND PROTEIN 2

Chain A: 36% 47% 11%



• Molecule 1: GROWTH FACTOR BOUND PROTEIN 2

Chain B: 26% 49% 19%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	88.87Å 88.87Å 97.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10	Depositor
% Data completeness (in resolution range)	82.2 (8.00-3.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3468	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

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	1.15	7/1783 (0.4%)	1.50	27/2405 (1.1%)
1	B	1.05	1/1783 (0.1%)	1.44	24/2405 (1.0%)
All	All	1.10	8/3566 (0.2%)	1.47	51/4810 (1.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	ARG	N-CA	8.70	1.63	1.46
1	A	34	GLN	C-O	-7.78	1.08	1.23
1	A	34	GLN	C-N	6.07	1.48	1.34
1	A	216	ASN	C-N	-6.01	1.20	1.34
1	A	170	GLN	N-CA	5.30	1.56	1.46
1	B	216	ASN	C-N	-5.25	1.22	1.34
1	A	170	GLN	C-N	-5.07	1.22	1.34
1	A	194	TRP	NE1-CE2	-5.07	1.30	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ASP	O-C-N	16.27	150.86	123.20
1	A	172	ASP	CA-C-N	-12.27	91.67	116.20
1	A	34	GLN	CA-C-N	-10.53	94.05	117.20
1	A	149	ARG	NE-CZ-NH2	9.61	125.11	120.30
1	A	172	ASP	C-N-CA	9.06	141.32	122.30
1	B	179	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	B	149	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	B	136	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	B	18	SER	O-C-N	-7.74	110.31	122.70
1	B	142	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	A	112	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	A	207	ARG	NE-CZ-NH2	7.57	124.09	120.30
1	A	78	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	B	178	ARG	NE-CZ-NH2	7.57	124.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	67	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	B	78	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	142	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	178	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	215	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	179	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	67	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	A	141	SER	O-C-N	7.18	134.19	122.70
1	B	215	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	B	86	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	136	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	21	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	B	112	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	21	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	141	SER	C-N-CA	6.49	137.93	121.70
1	A	34	GLN	O-C-N	6.48	133.06	122.70
1	B	146	ILE	O-C-N	6.35	132.85	122.70
1	B	204	MET	CG-SD-CE	6.32	110.31	100.20
1	B	207	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	B	73	MET	CG-SD-CE	6.17	110.08	100.20
1	A	55	MET	CG-SD-CE	6.17	110.07	100.20
1	A	73	MET	CG-SD-CE	6.16	110.06	100.20
1	A	204	MET	CG-SD-CE	6.09	109.94	100.20
1	A	1	MET	CG-SD-CE	6.08	109.92	100.20
1	B	55	MET	CG-SD-CE	5.87	109.59	100.20
1	B	1	MET	CG-SD-CE	5.77	109.43	100.20
1	B	121	TRP	O-C-N	5.68	131.79	122.70
1	A	86	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	186	MET	CG-SD-CE	5.50	109.00	100.20
1	A	34	GLN	CA-C-O	5.42	131.49	120.10
1	A	172	ASP	N-CA-CB	5.42	120.35	110.60
1	B	34	GLN	O-C-N	5.34	131.24	122.70
1	B	186	MET	CG-SD-CE	5.33	108.73	100.20
1	B	34	GLN	N-CA-C	-5.32	96.62	111.00
1	B	18	SER	N-CA-CB	-5.22	102.67	110.50
1	B	89	GLU	O-C-N	5.17	130.97	122.70
1	A	149	ARG	NH1-CZ-NH2	-5.03	113.87	119.40

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	1734	0	1662	184	0
1	B	1734	0	1662	180	0
All	All	3468	0	3324	340	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 50.

All (340) 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:40:GLU:HB3	1:A:45:ASP:HB3	1.31	1.11
1:A:17:LEU:HD23	1:A:48:ILE:HD11	1.27	1.10
1:B:195:LYS:HG3	1:B:204:MET:SD	1.92	1.08
1:B:71:GLU:HA	1:B:105:VAL:HG11	1.34	1.06
1:A:16:GLU:OE1	1:A:16:GLU:N	1.90	1.04
1:B:117:LYS:HD2	1:B:126:ASN:HA	1.34	1.04
1:B:55:MET:HE1	1:B:185:VAL:HG12	1.41	1.00
1:B:149:ARG:HD3	1:B:150:ASP:H	1.27	0.99
1:A:71:GLU:HA	1:A:105:VAL:HG21	1.45	0.97
1:B:11:ALA:HB1	1:B:16:GLU:HG2	1.45	0.96
1:A:16:GLU:OE1	1:A:16:GLU:C	2.04	0.95
1:A:215:ARG:HD2	1:B:156:GLN:HG2	1.48	0.94
1:B:37:TYR:HE1	1:B:50:LYS:HG3	1.32	0.94
1:B:71:GLU:HG2	1:B:105:VAL:HG21	1.49	0.92
1:B:55:MET:CE	1:B:185:VAL:HG12	2.00	0.92
1:B:149:ARG:HD3	1:B:150:ASP:N	1.86	0.91
1:A:120:LEU:HD11	1:A:131:LEU:HD11	1.53	0.91
1:A:161:VAL:HG22	1:A:183:ILE:CD1	2.00	0.91
1:A:74:LEU:HD23	1:A:105:VAL:HG13	1.53	0.89
1:B:113:ASP:OD2	1:B:124:LYS:HE2	1.73	0.89
1:B:141:SER:HB2	1:B:146:ILE:HD11	1.55	0.88
1:A:161:VAL:CG2	1:A:183:ILE:HD11	2.04	0.87
1:A:37:TYR:HE2	1:A:50:LYS:HG3	1.40	0.87
1:A:161:VAL:HG22	1:A:183:ILE:HD11	1.55	0.86
1:B:116:GLY:O	1:B:117:LYS:HD3	1.75	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLN:HB2	1:A:100:LYS:HD2	1.58	0.86
1:A:1:MET:HG3	1:A:187:ASP:HB2	1.55	0.86
1:A:215:ARG:CD	1:B:156:GLN:HG2	2.06	0.85
1:A:214:ASN:HD21	1:B:188:ASN:HD21	1.24	0.85
1:A:16:GLU:OE1	1:A:16:GLU:CA	2.24	0.85
1:A:50:LYS:HD3	1:A:202:THR:HG21	1.57	0.85
1:A:109:LYS:HB3	1:A:111:LEU:HD21	1.59	0.85
1:A:58:HIS:ND1	1:A:59:PRO:HD2	1.94	0.83
1:A:11:ALA:HB1	1:A:16:GLU:CG	2.09	0.82
1:B:117:LYS:CD	1:B:126:ASN:HA	2.10	0.82
1:A:1:MET:HE1	1:A:186:MET:HG2	1.60	0.82
1:B:75:SER:HA	1:B:100:LYS:HE3	1.60	0.82
1:B:90:SER:O	1:B:92:PRO:HD3	1.78	0.82
1:A:17:LEU:CD2	1:A:48:ILE:HD11	2.09	0.81
1:B:216:ASN:N	1:B:216:ASN:HD22	1.78	0.81
1:B:101:PHE:CE1	1:B:146:ILE:HG21	2.16	0.80
1:A:213:VAL:HG13	1:B:58:HIS:HD2	1.46	0.80
1:A:17:LEU:HD23	1:A:48:ILE:CD1	2.11	0.80
1:B:16:GLU:O	1:B:46:GLY:HA3	1.83	0.79
1:A:39:ALA:HB3	1:A:48:ILE:HD13	1.64	0.79
1:A:40:GLU:CB	1:A:45:ASP:HB3	2.10	0.79
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.47	0.79
1:A:113:ASP:O	1:A:113:ASP:OD1	2.01	0.79
1:A:49:PRO:HG2	1:A:52:TYR:CD1	2.17	0.79
1:A:161:VAL:CG2	1:A:210:VAL:HG11	2.13	0.78
1:A:69:LYS:HE2	1:A:73:MET:HE2	1.66	0.77
1:A:161:VAL:HG21	1:A:210:VAL:HG11	1.66	0.77
1:A:120:LEU:HD22	1:A:135:HIS:CE1	2.20	0.77
1:B:132:VAL:HG12	1:B:136:ARG:NH1	1.98	0.77
1:B:164:LEU:O	1:B:179:ARG:HD2	1.84	0.76
1:A:16:GLU:OE1	1:A:16:GLU:O	2.02	0.76
1:B:112:ARG:HD2	1:B:118:TYR:CE1	2.20	0.76
1:A:11:ALA:HB1	1:A:16:GLU:HG3	1.66	0.76
1:A:90:SER:O	1:A:92:PRO:HD3	1.87	0.75
1:A:11:ALA:CB	1:A:16:GLU:HG2	2.17	0.75
1:A:37:TYR:CE2	1:A:50:LYS:HG3	2.20	0.75
1:B:74:LEU:HD21	1:B:83:PHE:HA	1.67	0.75
1:B:55:MET:HE1	1:B:185:VAL:CG1	2.16	0.75
1:A:109:LYS:HE2	1:A:111:LEU:CD2	2.17	0.75
1:B:25:LEU:HD13	1:B:48:ILE:HD11	1.67	0.74
1:A:68:ALA:O	1:A:72:GLU:HG3	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:OE1	1:B:153:GLN:HA	1.87	0.74
1:B:11:ALA:CB	1:B:16:GLU:HG2	2.16	0.74
1:A:217:VAL:HG11	1:B:65:ILE:HD13	1.69	0.73
1:B:133:ASP:HA	1:B:136:ARG:HD2	1.70	0.73
1:A:58:HIS:CE1	1:A:59:PRO:HD2	2.23	0.73
1:A:161:VAL:HG13	1:A:185:VAL:HG23	1.71	0.73
1:A:1:MET:CE	1:A:186:MET:HG2	2.19	0.72
1:A:55:MET:HG3	1:A:186:MET:O	1.89	0.72
1:A:161:VAL:HG22	1:A:183:ILE:CG1	2.19	0.72
1:A:154:VAL:CG2	1:A:155:PRO:HD2	2.20	0.72
1:B:58:HIS:ND1	1:B:59:PRO:HD2	2.05	0.71
1:A:154:VAL:HG23	1:A:155:PRO:HD2	1.71	0.71
1:A:134:TYR:CZ	1:A:138:THR:HG21	2.24	0.71
1:A:160:TYR:O	1:A:213:VAL:HB	1.89	0.71
1:A:1:MET:HE3	1:A:195:LYS:HD3	1.72	0.70
1:A:1:MET:O	1:A:27:VAL:HG12	1.90	0.70
1:A:69:LYS:HE2	1:A:73:MET:CE	2.21	0.70
1:A:134:TYR:OH	1:A:138:THR:HG21	1.92	0.70
1:B:13:ALA:O	1:B:16:GLU:HG3	1.92	0.69
1:B:85:ILE:HG21	1:B:128:LEU:HD22	1.75	0.69
1:A:87:GLU:HB2	1:A:95:PHE:HE1	1.58	0.68
1:B:145:GLN:OE1	1:B:145:GLN:O	2.12	0.68
1:A:175:LEU:HD23	1:A:176:GLY:N	2.07	0.68
1:B:74:LEU:O	1:B:100:LYS:HD3	1.93	0.68
1:B:67:ARG:HD3	1:B:71:GLU:HG3	1.74	0.68
1:B:88:SER:HB2	1:B:91:ALA:O	1.92	0.67
1:B:78:ARG:HH11	1:B:78:ARG:HB3	1.60	0.67
1:B:119:PHE:HB3	1:B:124:LYS:HA	1.77	0.67
1:B:128:LEU:O	1:B:132:VAL:HG23	1.93	0.67
1:A:57:PRO:HB3	1:B:215:ARG:O	1.95	0.67
1:A:161:VAL:CG2	1:A:210:VAL:CG1	2.73	0.67
1:B:37:TYR:HE1	1:B:50:LYS:CG	2.07	0.67
1:A:161:VAL:HG22	1:A:183:ILE:HG13	1.76	0.67
1:A:213:VAL:HG13	1:B:58:HIS:CD2	2.28	0.67
1:A:7:TYR:HB2	1:A:52:TYR:CD2	2.31	0.66
1:B:216:ASN:N	1:B:216:ASN:ND2	2.41	0.66
1:B:182:PHE:CE1	1:B:213:VAL:HG21	2.31	0.66
1:B:25:LEU:HD13	1:B:48:ILE:CD1	2.26	0.66
1:A:175:LEU:HD21	1:A:198:CYS:HB3	1.79	0.65
1:B:171:GLU:HG2	1:B:172:ASP:H	1.61	0.65
1:A:142:ARG:HG3	1:A:142:ARG:NH1	2.08	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:CE1	1:B:50:LYS:HG3	2.23	0.65
1:B:132:VAL:HG12	1:B:136:ARG:HH11	1.59	0.65
1:A:65:ILE:CD1	1:B:217:VAL:HG11	2.26	0.65
1:A:97:LEU:HD23	1:A:98:SER:H	1.62	0.65
1:A:140:VAL:HG22	1:A:140:VAL:O	1.95	0.65
1:B:101:PHE:HE1	1:B:146:ILE:HG21	1.58	0.65
1:A:58:HIS:CG	1:A:59:PRO:HD2	2.32	0.65
1:A:97:LEU:HD23	1:A:98:SER:N	2.11	0.65
1:A:120:LEU:HD11	1:A:131:LEU:CD1	2.26	0.65
1:B:81:GLY:HA3	1:B:147:PHE:O	1.97	0.64
1:B:145:GLN:CD	1:B:145:GLN:C	2.56	0.64
1:B:164:LEU:HD21	1:B:211:THR:HB	1.80	0.64
1:B:216:ASN:HD22	1:B:216:ASN:H	1.45	0.64
1:A:34:GLN:CG	1:A:34:GLN:O	2.45	0.64
1:B:65:ILE:O	1:B:65:ILE:CG2	2.45	0.63
1:A:112:ARG:HA	1:A:117:LYS:O	1.98	0.63
1:B:182:PHE:HE1	1:B:213:VAL:HG21	1.63	0.63
1:A:183:ILE:HD13	1:A:205:PHE:CZ	2.34	0.62
1:A:11:ALA:CB	1:A:16:GLU:CG	2.74	0.62
1:A:161:VAL:HG13	1:A:185:VAL:CG2	2.30	0.62
1:B:160:TYR:O	1:B:213:VAL:HB	1.99	0.62
1:A:62:PHE:HD1	1:B:217:VAL:HG23	1.65	0.62
1:A:217:VAL:HG11	1:B:65:ILE:CD1	2.29	0.61
1:A:161:VAL:HG21	1:A:183:ILE:HD11	1.82	0.61
1:A:131:LEU:C	1:A:131:LEU:HD23	2.20	0.61
1:A:161:VAL:CG1	1:A:185:VAL:CG2	2.78	0.61
1:A:214:ASN:ND2	1:B:188:ASN:HD21	1.96	0.61
1:A:68:ALA:O	1:A:71:GLU:HB2	2.00	0.61
1:B:20:LYS:HE2	1:B:23:ASP:OD1	1.99	0.61
1:A:109:LYS:HE2	1:A:111:LEU:HD21	1.83	0.61
1:A:79:HIS:HB3	1:A:149:ARG:NH2	2.16	0.61
1:A:34:GLN:O	1:A:34:GLN:HG2	2.01	0.61
1:A:117:LYS:HZ2	1:A:117:LYS:HA	1.65	0.61
1:A:16:GLU:C	1:A:16:GLU:CD	2.59	0.60
1:B:188:ASN:HA	1:B:194:TRP:CD1	2.36	0.60
1:B:206:PRO:HG2	1:B:209:TYR:CD2	2.36	0.60
1:B:120:LEU:HD12	1:B:120:LEU:H	1.64	0.60
1:B:161:VAL:HG22	1:B:185:VAL:HG23	1.84	0.60
1:A:16:GLU:O	1:A:46:GLY:HA3	2.02	0.60
1:A:109:LYS:CB	1:A:111:LEU:HD21	2.30	0.60
1:A:62:PHE:CD1	1:B:217:VAL:HG23	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:O	1:B:71:GLU:HG3	2.03	0.59
1:B:145:GLN:OE1	1:B:145:GLN:C	2.41	0.59
1:A:120:LEU:CD1	1:A:131:LEU:HD11	2.31	0.59
1:B:19:PHE:CE1	1:B:48:ILE:HG13	2.38	0.59
1:B:71:GLU:O	1:B:75:SER:HB3	2.02	0.59
1:B:161:VAL:HG22	1:B:185:VAL:CG2	2.33	0.58
1:A:40:GLU:HB3	1:A:45:ASP:CB	2.21	0.58
1:A:83:PHE:CE1	1:A:148:LEU:HB3	2.37	0.58
1:A:161:VAL:HG21	1:A:210:VAL:CG1	2.34	0.58
1:B:55:MET:O	1:B:57:PRO:HD3	2.03	0.58
1:B:206:PRO:HG2	1:B:209:TYR:CE2	2.39	0.58
1:A:6:LYS:HD3	1:A:7:TYR:CZ	2.39	0.58
1:A:161:VAL:HG23	1:A:210:VAL:CG1	2.34	0.58
1:A:65:ILE:CG2	1:A:65:ILE:O	2.52	0.58
1:A:215:ARG:HD2	1:B:156:GLN:CG	2.29	0.57
1:A:69:LYS:HG3	1:A:73:MET:HE2	1.87	0.57
1:B:146:ILE:HG13	1:B:146:ILE:O	2.04	0.57
1:A:188:ASN:HB2	1:A:194:TRP:CE2	2.40	0.57
1:B:134:TYR:CD2	1:B:135:HIS:CD2	2.93	0.57
1:B:205:PHE:HE2	1:B:210:VAL:HG21	1.70	0.56
1:A:65:ILE:HD13	1:B:217:VAL:HG11	1.87	0.56
1:A:193:TRP:CZ3	1:A:206:PRO:HD3	2.40	0.56
1:B:193:TRP:HE3	1:B:204:MET:HB3	1.70	0.56
1:A:109:LYS:HB3	1:A:111:LEU:CD2	2.33	0.56
1:A:19:PHE:HE2	1:A:48:ILE:HG13	1.72	0.55
1:A:65:ILE:O	1:A:65:ILE:HG23	2.06	0.55
1:A:170:GLN:HB3	1:A:174:GLU:OE2	2.07	0.55
1:B:64:LYS:HG2	1:B:87:GLU:HB3	1.89	0.55
1:B:77:GLN:NE2	1:B:151:ILE:HG23	2.22	0.55
1:B:181:ASP:OD2	1:B:199:HIS:HE1	1.89	0.55
1:B:75:SER:HA	1:B:100:LYS:CE	2.33	0.55
1:B:131:LEU:HD23	1:B:131:LEU:C	2.27	0.55
1:B:171:GLU:CG	1:B:172:ASP:H	2.20	0.55
1:B:117:LYS:HB2	1:B:124:LYS:NZ	2.22	0.54
1:A:183:ILE:CD1	1:A:205:PHE:CZ	2.91	0.54
1:B:112:ARG:HA	1:B:117:LYS:O	2.07	0.54
1:B:120:LEU:HD11	1:B:135:HIS:HE1	1.72	0.54
1:A:41:LEU:HG	1:A:42:ASN:N	2.23	0.54
1:A:113:ASP:HB3	1:A:119:PHE:CE1	2.42	0.54
1:B:111:LEU:O	1:B:118:TYR:HA	2.06	0.54
1:B:132:VAL:CG1	1:B:136:ARG:NH1	2.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLU:HG3	1:A:55:MET:N	2.23	0.53
1:A:62:PHE:CE1	1:B:216:ASN:HB2	2.42	0.53
1:B:116:GLY:C	1:B:117:LYS:HD3	2.29	0.53
1:B:153:GLN:OE1	1:B:153:GLN:CA	2.54	0.53
1:B:64:LYS:O	1:B:66:PRO:HD3	2.09	0.53
1:A:61:PHE:HE2	1:B:160:TYR:CD2	2.27	0.52
1:B:158:PRO:HB2	1:B:160:TYR:HE1	1.74	0.52
1:A:183:ILE:HG22	1:A:198:CYS:SG	2.49	0.52
1:B:1:MET:O	1:B:27:VAL:HG12	2.10	0.52
1:A:113:ASP:HB3	1:A:119:PHE:HE1	1.75	0.52
1:B:11:ALA:HB1	1:B:16:GLU:CG	2.29	0.52
1:B:38:LYS:HE2	1:B:47:PHE:CE1	2.45	0.52
1:A:69:LYS:HA	1:A:72:GLU:OE1	2.10	0.51
1:A:87:GLU:HB2	1:A:95:PHE:CE1	2.44	0.51
1:A:62:PHE:HD1	1:B:217:VAL:CG2	2.23	0.51
1:B:145:GLN:OE1	1:B:146:ILE:HA	2.10	0.51
1:A:171:GLU:O	1:A:174:GLU:HB2	2.10	0.51
1:B:71:GLU:CG	1:B:105:VAL:HG21	2.32	0.51
1:A:120:LEU:N	1:A:120:LEU:HD12	2.25	0.51
1:B:1:MET:HG2	1:B:27:VAL:HG12	1.92	0.51
1:B:27:VAL:HG23	1:B:39:ALA:HB2	1.92	0.51
1:A:77:GLN:HB2	1:A:100:LYS:CD	2.38	0.51
1:A:80:ASP:HA	1:A:100:LYS:HG2	1.92	0.51
1:A:215:ARG:NH1	1:B:157:GLN:HB2	2.26	0.51
1:B:117:LYS:HD2	1:B:126:ASN:CA	2.23	0.51
1:B:81:GLY:HA2	1:B:99:VAL:CG1	2.41	0.50
1:A:97:LEU:HD22	1:A:99:VAL:HG23	1.94	0.50
1:B:38:LYS:HE2	1:B:47:PHE:CZ	2.47	0.50
1:B:84:LEU:HD13	1:B:86:ARG:HG2	1.94	0.50
1:B:158:PRO:HB2	1:B:160:TYR:CE1	2.46	0.50
1:A:135:HIS:HD2	1:A:138:THR:O	1.95	0.50
1:A:113:ASP:OD1	1:A:113:ASP:C	2.50	0.50
1:B:13:ALA:O	1:B:16:GLU:CG	2.59	0.49
1:B:113:ASP:HB3	1:B:119:PHE:HE1	1.78	0.49
1:A:59:PRO:HA	1:A:153:GLN:OE1	2.11	0.49
1:A:145:GLN:O	1:A:147:PHE:CD2	2.65	0.49
1:B:182:PHE:HE1	1:B:213:VAL:CG2	2.24	0.49
1:B:83:PHE:CE1	1:B:148:LEU:HB3	2.48	0.49
1:A:1:MET:CE	1:A:195:LYS:HD3	2.42	0.49
1:B:35:ASN:HB3	1:B:36:TRP:HD1	1.77	0.48
1:B:114:GLY:C	1:B:116:GLY:H	2.17	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:HA	1:A:202:THR:HA	1.94	0.48
1:A:141:SER:HB3	1:A:143:ASN:H	1.78	0.48
1:A:50:LYS:CD	1:A:202:THR:HG21	2.35	0.48
1:A:82:ALA:HA	1:A:149:ARG:O	2.13	0.48
1:B:20:LYS:HG3	1:B:23:ASP:OD2	2.13	0.47
1:B:188:ASN:HB2	1:B:194:TRP:CE2	2.49	0.47
1:A:109:LYS:HE2	1:A:111:LEU:HD22	1.96	0.47
1:B:145:GLN:O	1:B:145:GLN:CD	2.53	0.47
1:A:126:ASN:HD22	1:B:178:ARG:NH2	2.13	0.47
1:A:61:PHE:CE2	1:B:160:TYR:CD2	3.03	0.47
1:A:207:ARG:HE	1:B:207:ARG:HH21	1.62	0.47
1:B:141:SER:HB2	1:B:146:ILE:CD1	2.37	0.47
1:B:120:LEU:HD13	1:B:121:TRP:CD2	2.49	0.47
1:B:183:ILE:HD11	1:B:205:PHE:CE1	2.49	0.47
1:A:131:LEU:HD23	1:A:131:LEU:O	2.15	0.47
1:A:161:VAL:CG2	1:A:210:VAL:CB	2.92	0.47
1:B:117:LYS:HB2	1:B:124:LYS:HZ3	1.78	0.47
1:A:81:GLY:HA3	1:A:147:PHE:O	2.15	0.46
1:B:140:VAL:O	1:B:140:VAL:HG13	2.14	0.46
1:B:197:ALA:HA	1:B:202:THR:HA	1.97	0.46
1:B:6:LYS:HA	1:B:155:PRO:HG3	1.96	0.46
1:B:64:LYS:HD2	1:B:89:GLU:HA	1.98	0.46
1:B:134:TYR:HD2	1:B:135:HIS:CD2	2.32	0.46
1:A:11:ALA:CA	1:A:16:GLU:HG2	2.46	0.46
1:B:68:ALA:O	1:B:71:GLU:HB2	2.15	0.46
1:A:215:ARG:O	1:B:57:PRO:HB3	2.15	0.46
1:B:175:LEU:HD21	1:B:198:CYS:HB3	1.98	0.46
1:A:61:PHE:HE2	1:B:160:TYR:CE2	2.34	0.46
1:B:65:ILE:O	1:B:65:ILE:HG22	2.14	0.46
1:A:79:HIS:CD2	1:A:149:ARG:CZ	2.99	0.46
1:B:95:PHE:HB2	1:B:110:VAL:HG13	1.97	0.46
1:A:54:GLU:HG3	1:A:55:MET:H	1.80	0.46
1:A:167:PHE:O	1:A:167:PHE:CD2	2.69	0.46
1:B:82:ALA:HA	1:B:149:ARG:O	2.16	0.45
1:A:123:VAL:HG23	1:A:125:PHE:CZ	2.51	0.45
1:A:161:VAL:CG2	1:A:210:VAL:HB	2.46	0.45
1:A:161:VAL:HG21	1:A:210:VAL:CB	2.46	0.45
1:A:55:MET:O	1:A:57:PRO:HD3	2.16	0.45
1:A:62:PHE:O	1:A:65:ILE:HB	2.17	0.45
1:A:65:ILE:HD11	1:A:69:LYS:HG2	1.98	0.45
1:B:16:GLU:C	1:B:16:GLU:CD	2.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:C	1:B:143:ASN:H	2.21	0.45
1:B:171:GLU:CG	1:B:172:ASP:N	2.80	0.45
1:A:145:GLN:O	1:A:147:PHE:CG	2.70	0.45
1:A:11:ALA:HA	1:A:16:GLU:HG2	1.97	0.44
1:A:65:ILE:HD13	1:B:217:VAL:HG21	1.98	0.44
1:A:69:LYS:CE	1:A:73:MET:HE2	2.43	0.44
1:B:132:VAL:CG1	1:B:136:ARG:HH12	2.28	0.44
1:A:58:HIS:ND1	1:A:59:PRO:CD	2.75	0.44
1:A:140:VAL:O	1:A:140:VAL:HG13	2.16	0.44
1:B:121:TRP:HB2	1:B:122:VAL:H	1.29	0.44
1:A:17:LEU:CG	1:A:48:ILE:HD11	2.47	0.44
1:B:193:TRP:CE3	1:B:204:MET:HB3	2.51	0.44
1:A:8:ASP:OD2	1:A:20:LYS:HG3	2.18	0.44
1:B:120:LEU:HD13	1:B:121:TRP:CE3	2.52	0.44
1:B:177:PHE:HE2	1:B:205:PHE:HB2	1.82	0.44
1:B:161:VAL:HG13	1:B:185:VAL:HG21	2.00	0.44
1:A:99:VAL:O	1:A:105:VAL:HA	2.16	0.44
1:A:205:PHE:HE2	1:A:210:VAL:HG21	1.82	0.44
1:B:101:PHE:CD1	1:B:146:ILE:HG21	2.53	0.44
1:A:11:ALA:HB2	1:A:18:SER:OG	2.18	0.43
1:A:116:GLY:C	1:A:117:LYS:HZ3	2.21	0.43
1:A:1:MET:SD	1:A:186:MET:HG2	2.58	0.43
1:A:58:HIS:HE1	1:A:60:TRP:CD2	2.36	0.43
1:B:78:ARG:O	1:B:78:ARG:HG2	2.19	0.43
1:B:75:SER:HA	1:B:100:LYS:CD	2.48	0.43
1:B:183:ILE:CD1	1:B:196:GLY:HA3	2.49	0.43
1:A:20:LYS:HG2	1:A:21:ARG:N	2.34	0.43
1:A:71:GLU:CA	1:A:105:VAL:HG21	2.32	0.43
1:B:48:ILE:O	1:B:48:ILE:CG2	2.66	0.43
1:A:128:LEU:O	1:A:131:LEU:HB3	2.19	0.42
1:B:25:LEU:CD2	1:B:41:LEU:HD12	2.49	0.42
1:B:164:LEU:CD2	1:B:211:THR:HB	2.48	0.42
1:B:7:TYR:HB2	1:B:52:TYR:CD2	2.54	0.42
1:B:67:ARG:HD3	1:B:71:GLU:CG	2.45	0.42
1:B:117:LYS:HD3	1:B:117:LYS:HA	1.45	0.42
1:A:69:LYS:HE2	1:A:73:MET:HE1	2.01	0.42
1:A:100:LYS:O	1:A:100:LYS:CG	2.67	0.42
1:A:128:LEU:O	1:A:132:VAL:HG23	2.20	0.42
1:B:113:ASP:HB3	1:B:119:PHE:CE1	2.54	0.42
1:A:142:ARG:HD2	1:A:143:ASN:OD1	2.19	0.42
1:A:161:VAL:HG21	1:A:210:VAL:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD23	1:B:41:LEU:C	2.39	0.42
1:B:65:ILE:O	1:B:65:ILE:HG23	2.19	0.42
1:A:117:LYS:HA	1:A:117:LYS:NZ	2.34	0.42
1:B:15:ASP:HB2	1:B:47:PHE:CD1	2.55	0.42
1:B:62:PHE:O	1:B:65:ILE:HB	2.20	0.42
1:A:146:ILE:HD13	1:A:146:ILE:HG21	1.76	0.41
1:B:19:PHE:CE1	1:B:48:ILE:CD1	3.03	0.41
1:B:25:LEU:HD23	1:B:41:LEU:HD12	2.02	0.41
1:B:183:ILE:HD11	1:B:205:PHE:CZ	2.55	0.41
1:A:58:HIS:CG	1:A:59:PRO:CD	3.01	0.41
1:B:35:ASN:HA	1:B:50:LYS:HE2	2.02	0.41
1:A:19:PHE:HE2	1:A:48:ILE:CG1	2.34	0.41
1:A:88:SER:O	1:A:90:SER:N	2.54	0.41
1:A:154:VAL:HG22	1:A:155:PRO:HD2	2.00	0.41
1:B:78:ARG:HB3	1:B:78:ARG:NH1	2.31	0.41
1:A:131:LEU:C	1:A:131:LEU:CD2	2.87	0.40
1:B:145:GLN:HG3	1:B:146:ILE:N	2.37	0.40
1:B:210:VAL:O	1:B:210:VAL:CG1	2.69	0.40
1:A:114:GLY:C	1:A:116:GLY:H	2.24	0.40
1:A:81:GLY:HA2	1:A:99:VAL:HG13	2.02	0.40
1:B:17:LEU:CD2	1:B:45:ASP:HA	2.51	0.40
1:B:35:ASN:HB3	1:B:36:TRP:CD1	2.56	0.40
1:A:74:LEU:HD11	1:A:82:ALA:O	2.21	0.40
1:B:65:ILE:HD12	1:B:65:ILE:HA	1.83	0.40
1:A:50:LYS:HB2	1:A:50:LYS:HE2	1.87	0.40
1:B:119:PHE:HB2	1:B:123:VAL:O	2.21	0.40
1:B:166:ASP:OD1	1:B:166:ASP:N	2.54	0.40
1:B:193:TRP:CZ3	1:B:206:PRO:HD3	2.57	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	207/217 (95%)	168 (81%)	29 (14%)	10 (5%)	2 14
1	B	207/217 (95%)	165 (80%)	36 (17%)	6 (3%)	4 24
All	All	414/434 (95%)	333 (80%)	65 (16%)	16 (4%)	3 18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	89	GLU
1	A	11	ALA
1	A	79	HIS
1	A	144	GLN
1	A	146	ILE
1	B	72	GLU
1	B	79	HIS
1	B	11	ALA
1	A	102	GLY
1	A	141	SER
1	A	142	ARG
1	A	152	GLU
1	B	90	SER
1	B	102	GLY
1	B	146	ILE

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	184/190 (97%)	154 (84%)	30 (16%)	2 10
1	B	184/190 (97%)	130 (71%)	54 (29%)	0 1
All	All	368/380 (97%)	284 (77%)	84 (23%)	1 3

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	LYS
1	A	16	GLU
1	A	18	SER
1	A	26	LYS
1	A	34	GLN
1	A	38	LYS
1	A	45	ASP
1	A	48	ILE
1	A	78	ARG
1	A	79	HIS
1	A	84	LEU
1	A	85	ILE
1	A	86	ARG
1	A	100	LYS
1	A	101	PHE
1	A	112	ARG
1	A	117	LYS
1	A	141	SER
1	A	142	ARG
1	A	149	ARG
1	A	161	VAL
1	A	164	LEU
1	A	166	ASP
1	A	171	GLU
1	A	172	ASP
1	A	178	ARG
1	A	204	MET
1	A	215	ARG
1	A	216	ASN
1	B	12	THR
1	B	15	ASP
1	B	16	GLU
1	B	17	LEU
1	B	20	LYS
1	B	24	ILE
1	B	42	ASN
1	B	48	ILE
1	B	50	LYS
1	B	51	ASN
1	B	67	ARG
1	B	72	GLU
1	B	75	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	79	HIS
1	B	80	ASP
1	B	84	LEU
1	B	85	ILE
1	B	86	ARG
1	B	96	SER
1	B	97	LEU
1	B	100	LYS
1	B	101	PHE
1	B	103	ASN
1	B	104	ASP
1	B	106	GLN
1	B	109	LYS
1	B	111	LEU
1	B	117	LYS
1	B	120	LEU
1	B	121	TRP
1	B	125	PHE
1	B	128	LEU
1	B	133	ASP
1	B	141	SER
1	B	142	ARG
1	B	143	ASN
1	B	145	GLN
1	B	149	ARG
1	B	153	GLN
1	B	156	GLN
1	B	159	THR
1	B	164	LEU
1	B	165	PHE
1	B	166	ASP
1	B	168	ASP
1	B	183	ILE
1	B	184	HIS
1	B	186	MET
1	B	201	GLN
1	B	204	MET
1	B	208	ASN
1	B	210	VAL
1	B	211	THR
1	B	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	79	HIS
1	A	126	ASN
1	A	135	HIS
1	A	184	HIS
1	A	214	ASN
1	A	216	ASN
1	B	135	HIS
1	B	156	GLN
1	B	162	GLN
1	B	214	ASN
1	B	216	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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	216:ASN	C	217:VAL	N	1.20

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.