Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 10:03 AM BST

PDB ID	:	1F5Q
Title	:	CRYSTAL STRUCTURE OF MURINE GAMMA HERPESVIRUS CYCLIN COMPLEXED TO HUMAN CYCLIN DEPENDENT KINASE 2
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Deposited on	:	2000-06-15
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:

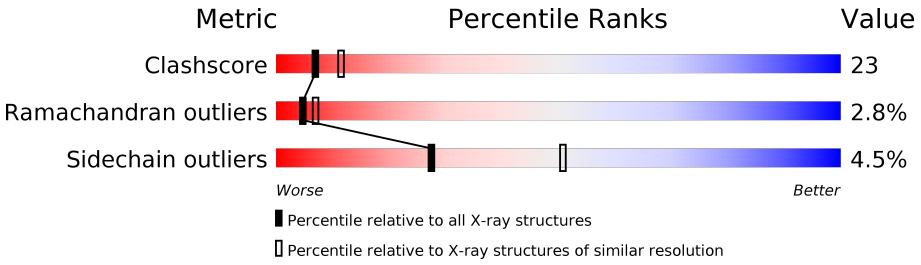
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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	298	57% 36% 5% ••
1	C	298	44% 47% 6% •
2	B	252	71% 25% • •
2	D	252	67% 29% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8723 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 CYCLIN DEPENDENT KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2346	1528	397	413	8			
1	C	288	Total	C	N	O	S	0	0	0
			2248	1462	378	400	8			

- Molecule 2 is a protein called GAMMA HERPESVIRUS CYCLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	1	0
			1986	1256	340	368	22			
2	D	248	Total	C	N	O	S	0	1	0
			1976	1247	340	368	21			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	57	Total	O	0	0
			57	57		
4	C	23	Total	O	0	0
			23	23		
4	D	32	Total	O	0	0
			32	32		

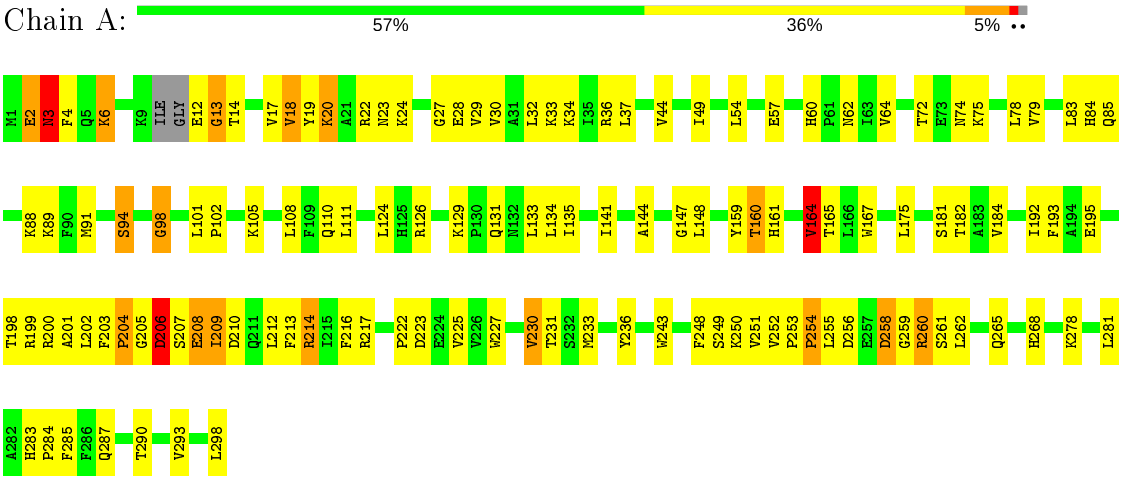
3 Residue-property plots (i)

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.

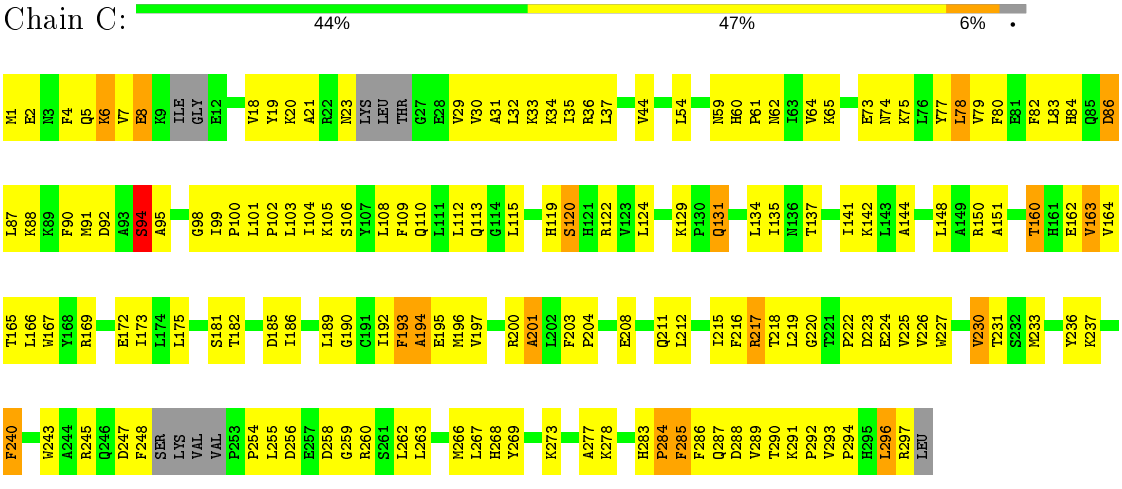
- Molecule 1: CYCLIN DEPENDENT KINASE 2

Chain A:



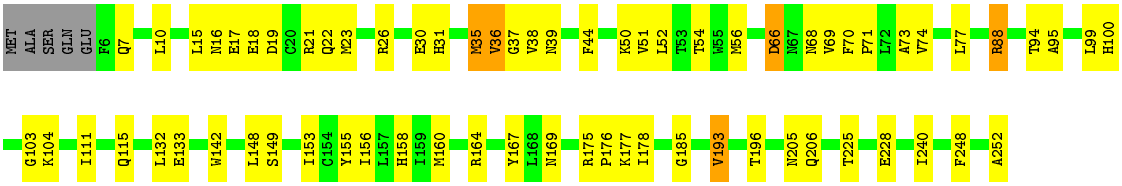
- Molecule 1: CYCLIN DEPENDENT KINASE 2

Chain C:



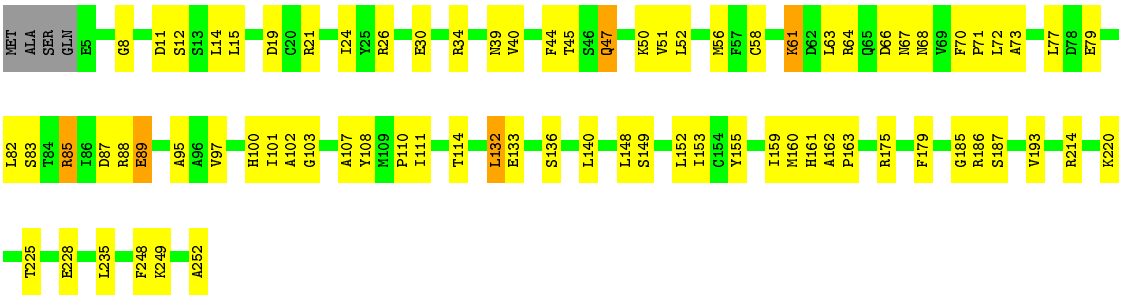
- Molecule 2: GAMMA HERPESVIRUS CYCLIN

Chain B:



- Molecule 2: GAMMA HERPESVIRUS CYCLIN

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.59Å 73.45Å 107.67Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8723	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.42	0/2407	0.70	2/3273 (0.1%)
1	C	0.47	0/2304	0.70	0/3131
2	B	0.44	0/2022	0.61	0/2737
2	D	0.44	0/2011	0.62	0/2723
All	All	0.44	0/8744	0.66	2/11864 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	ASN	N-CA-C	-5.74	95.51	111.00
1	A	20	LYS	N-CA-C	-5.28	96.75	111.00

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	2346	0	2364	113	0
1	C	2248	0	2231	152	0
2	B	1986	0	1970	58	0
2	D	1976	0	1951	79	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	54	0	0	0	0
4	B	57	0	0	5	0
4	C	23	0	0	2	0
4	D	32	0	0	2	0
All	All	8723	0	8516	392	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 23.

All (392) 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:4:PHE:HA	1:A:22:ARG:O	1.59	1.02
1:C:101:LEU:HD21	1:C:105:LYS:HE3	1.39	1.02
1:A:44:VAL:HG23	4:B:253:HOH:O	1.68	0.92
1:A:214:ARG:HH11	1:A:214:ARG:HG2	1.36	0.91
1:A:3:ASN:HA	1:A:24:LYS:CB	2.02	0.89
1:A:60:HIS:CD2	1:A:62:ASN:H	1.90	0.89
2:D:24:ILE:HG23	2:D:193:VAL:HG11	1.54	0.88
1:C:108:LEU:O	1:C:112:LEU:HD13	1.77	0.85
1:A:227:TRP:O	1:A:230:VAL:HG22	1.80	0.82
1:A:23:ASN:O	1:A:27:GLY:HA2	1.80	0.81
1:A:60:HIS:HD2	1:A:62:ASN:H	1.28	0.81
2:D:220:LYS:HB2	2:D:220:LYS:NZ	1.97	0.80
1:A:14:THR:HB	1:A:33:LYS:HE3	1.65	0.79
1:C:119:HIS:HB3	2:D:14:LEU:HD12	1.66	0.78
1:A:37:LEU:HD22	1:A:44:VAL:HG22	1.66	0.78
1:C:286:PHE:O	1:C:289:VAL:HG23	1.84	0.78
1:C:231:THR:HG22	1:C:236:TYR:CE2	2.18	0.77
2:D:111:ILE:H	2:D:111:ILE:HD12	1.48	0.77
1:C:290:THR:OG1	1:C:292:PRO:HD3	1.86	0.76
1:C:60:HIS:HD2	1:C:62:ASN:H	1.29	0.75
2:D:56:MET:HE2	2:D:73:ALA:HB1	1.68	0.75
1:C:30:VAL:HG23	1:C:80:PHE:O	1.87	0.75
1:A:3:ASN:O	1:A:23:ASN:HA	1.88	0.74
2:D:40:VAL:HG12	2:D:82:LEU:HD22	1.68	0.74
1:A:13:GLY:HA3	1:A:18:VAL:HG23	1.68	0.74
1:A:131:GLN:NE2	1:A:131:GLN:H	1.86	0.74
2:D:152:LEU:HD13	2:D:193:VAL:HG12	1.70	0.73
2:D:71:PRO:HB2	2:D:148:LEU:HD13	1.68	0.73
2:B:193:VAL:HG22	4:B:261:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HE3	1:A:75:LYS:HD3	1.70	0.73
1:C:103:LEU:HD12	1:C:292:PRO:HG2	1.69	0.72
1:A:217:ARG:HG2	1:A:243:TRP:CD1	2.24	0.72
2:D:220:LYS:HB2	2:D:220:LYS:HZ2	1.55	0.71
2:B:153:ILE:HD11	2:B:178:ILE:HD11	1.71	0.71
2:D:97:VAL:HG21	2:D:132:LEU:HB3	1.72	0.70
2:D:85:ARG:HG2	2:D:85:ARG:HH11	1.56	0.70
1:C:255:LEU:HB3	1:C:260:ARG:HG3	1.72	0.70
1:A:23:ASN:HB3	1:A:27:GLY:N	2.06	0.70
1:C:223:ASP:H	1:C:226:VAL:HG22	1.57	0.69
1:C:165:THR:HG23	1:C:165:THR:O	1.90	0.69
1:C:131:GLN:HE21	1:C:131:GLN:H	1.37	0.69
2:B:35:MET:CE	2:B:35:MET:HA	2.23	0.69
1:C:60:HIS:CD2	1:C:62:ASN:H	2.10	0.69
1:C:33:LYS:HB3	1:C:78:LEU:HB2	1.73	0.69
1:A:251:VAL:HG12	1:A:252:VAL:HG13	1.73	0.68
1:C:122:ARG:HD3	2:D:12:SER:HB2	1.76	0.68
1:C:122:ARG:CD	2:D:12:SER:HB2	2.24	0.68
2:D:64:ARG:HG2	2:D:64:ARG:HH11	1.59	0.68
1:A:135:ILE:HG22	1:A:141:ILE:HG13	1.76	0.68
2:D:58:CYS:HG	2:D:248:PHE:HE2	1.43	0.68
1:A:124:LEU:CD2	1:A:182:THR:HA	2.24	0.67
1:C:109:PHE:O	1:C:113:GLN:HG3	1.94	0.67
1:A:207:SER:O	1:A:209:ILE:N	2.28	0.67
2:B:36:VAL:HG12	2:B:36:VAL:O	1.96	0.66
1:A:36:ARG:HH11	1:A:74:ASN:ND2	1.93	0.66
2:B:225:THR:OG1	2:B:228:GLU:HG3	1.95	0.66
1:C:131:GLN:H	1:C:131:GLN:NE2	1.93	0.65
1:A:252:VAL:HG23	1:A:252:VAL:O	1.96	0.65
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.78	0.65
1:A:223:ASP:OD2	1:A:225:VAL:HB	1.96	0.65
1:C:6:LYS:HB2	1:C:21:ALA:HA	1.76	0.65
1:A:34:LYS:HE3	1:A:75:LYS:CD	2.27	0.65
2:B:26:ARG:O	2:B:30:GLU:HG3	1.96	0.65
1:C:223:ASP:H	1:C:226:VAL:CG2	2.10	0.65
2:D:79:GLU:O	2:D:83:SER:HB3	1.96	0.64
1:A:14:THR:CB	1:A:33:LYS:HE3	2.26	0.64
2:B:158:HIS:ND1	4:B:287:HOH:O	2.30	0.64
2:D:85:ARG:HG2	2:D:85:ARG:NH1	2.11	0.64
2:B:164:ARG:HH11	2:B:164:ARG:HG3	1.63	0.64
1:C:135:ILE:HG22	1:C:141:ILE:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.79	0.64
1:C:122:ARG:NH1	2:D:8:GLY:C	2.51	0.64
2:B:56:MET:HE2	2:B:73:ALA:HB1	1.80	0.63
2:D:61:LYS:HB3	2:D:61:LYS:NZ	2.14	0.63
1:A:214:ARG:HG2	1:A:214:ARG:NH1	2.08	0.62
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.34	0.62
2:D:45:THR:HG22	2:D:186:ARG:NH1	2.15	0.62
2:B:164:ARG:HG2	4:B:288:HOH:O	1.99	0.62
2:B:44:PHE:O	2:B:185:GLY:HA3	1.99	0.62
1:C:200:ARG:HH11	1:C:200:ARG:HG3	1.63	0.62
1:C:61:PRO:O	1:C:142:LYS:HE2	2.00	0.62
2:D:152:LEU:HD13	2:D:193:VAL:CG1	2.30	0.62
1:A:111:LEU:HD11	1:A:141:ILE:HD13	1.81	0.62
1:A:6:LYS:HD3	1:A:19:TYR:CD1	2.35	0.62
1:C:36:ARG:NH1	1:C:74:ASN:ND2	2.48	0.61
2:B:7:GLN:CB	2:B:10:LEU:HD21	2.30	0.61
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.16	0.61
1:C:224:GLU:OE2	1:C:230:VAL:HG23	2.01	0.61
2:B:164:ARG:NH1	2:B:164:ARG:HG3	2.15	0.61
2:B:103:GLY:HA3	2:B:111:ILE:HD12	1.83	0.60
1:A:23:ASN:HB3	1:A:28:GLU:H	1.66	0.60
2:B:35:MET:C	2:B:37:GLY:H	2.05	0.60
1:C:200:ARG:HB2	1:C:200:ARG:CZ	2.31	0.60
2:D:15:LEU:HD22	2:D:19:ASP:HB3	1.82	0.60
1:C:190:GLY:HA2	1:C:266:MET:CE	2.31	0.60
1:A:44:VAL:HG11	1:A:49:ILE:HD11	1.82	0.60
2:B:71:PRO:HB2	2:B:148:LEU:HD13	1.83	0.60
2:D:64:ARG:NH1	2:D:64:ARG:HG2	2.17	0.60
1:A:88:LYS:HA	1:A:91:MET:HE2	1.84	0.59
2:D:44:PHE:O	2:D:185:GLY:HA3	2.02	0.59
2:B:66:ASP:OD1	2:B:68:ASN:N	2.26	0.59
2:B:88:ARG:HB3	2:B:88:ARG:NH1	2.16	0.59
1:C:258:ASP:HB2	1:C:285:PHE:HD1	1.67	0.59
4:C:303:HOH:O	2:D:114:THR:HG23	2.02	0.59
1:C:99:ILE:CG2	1:C:104:ILE:HG13	2.32	0.59
1:C:105:LYS:HG2	1:C:285:PHE:CE2	2.37	0.59
2:D:26:ARG:O	2:D:30:GLU:HG3	2.02	0.59
1:A:124:LEU:HD22	1:A:182:THR:HA	1.83	0.59
1:C:162:GLU:O	1:C:164:VAL:N	2.36	0.58
2:B:153:ILE:HD11	2:B:178:ILE:CD1	2.33	0.58
1:C:87:LEU:HG	1:C:87:LEU:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG12	1:C:169:ARG:HH12	1.69	0.58
1:C:247:ASP:OD1	1:C:248:PHE:N	2.37	0.58
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.39	0.58
2:B:50:LYS:O	2:B:54:THR:HG23	2.04	0.57
1:A:202:LEU:C	1:A:204:PRO:HD3	2.25	0.57
1:A:208:GLU:HA	1:A:208:GLU:OE1	2.04	0.57
1:C:290:THR:HG1	1:C:292:PRO:HD3	1.69	0.57
2:D:67:ASN:CG	2:D:175:ARG:CZ	2.72	0.57
1:C:65:LYS:NZ	1:C:65:LYS:HB2	2.19	0.57
1:C:284:PRO:C	1:C:286:PHE:H	2.08	0.57
2:B:35:MET:HE2	2:B:35:MET:HA	1.86	0.57
2:D:72:LEU:HD23	2:D:102:ALA:HA	1.85	0.57
2:D:88:ARG:HB3	2:D:88:ARG:HH11	1.70	0.57
1:C:124:LEU:HD22	1:C:182:THR:HA	1.86	0.57
1:C:212:LEU:HD22	1:C:216:PHE:CZ	2.40	0.57
1:C:112:LEU:HD12	1:C:189:LEU:HD13	1.87	0.56
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.87	0.56
2:B:149:SER:O	2:B:153:ILE:HG13	2.06	0.56
2:D:15:LEU:HD22	2:D:19:ASP:CB	2.34	0.56
2:D:51:VAL:HG13	2:D:248:PHE:CB	2.35	0.56
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.40	0.56
1:C:101:LEU:CD2	1:C:105:LYS:HE3	2.26	0.56
1:C:217:ARG:HG3	1:C:243:TRP:CZ3	2.41	0.56
1:A:284:PRO:O	1:A:287:GLN:HG3	2.06	0.55
1:C:237:LYS:HB2	1:C:240:PHE:CD1	2.41	0.55
1:A:284:PRO:HA	1:A:287:GLN:HG3	1.87	0.55
1:C:90:PHE:O	1:C:94:SER:HB3	2.06	0.55
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.86	0.55
1:A:204:PRO:HD2	1:A:214:ARG:HE	1.70	0.55
1:C:164:VAL:CG1	1:C:169:ARG:HH12	2.20	0.55
1:A:94:SER:O	1:A:98:GLY:N	2.39	0.55
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.89	0.55
1:C:110:GLN:O	1:C:113:GLN:HB2	2.07	0.54
1:C:83:LEU:HD22	1:C:134:LEU:HB2	1.89	0.54
1:C:34:LYS:HD2	1:C:75:LYS:HD2	1.89	0.54
1:C:190:GLY:HA2	1:C:266:MET:HE2	1.89	0.54
2:B:38:VAL:HG12	2:B:39:ASN:OD1	2.07	0.54
1:A:175:LEU:HB3	1:A:233:MET:HG2	1.89	0.54
1:C:129:LYS:HD3	1:C:165:THR:HG21	1.89	0.54
1:C:255:LEU:HB3	1:C:260:ARG:CG	2.38	0.53
2:D:77:LEU:HD13	2:D:95:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:O	1:A:184:VAL:HG22	2.08	0.53
2:B:248:PHE:O	2:B:252:ALA:HB3	2.08	0.53
1:C:226:VAL:HG23	1:C:227:TRP:N	2.22	0.53
1:A:209:ILE:O	1:A:213:PHE:HD1	1.91	0.53
1:C:84:HIS:CE1	1:C:137:THR:HG23	2.44	0.53
2:D:58:CYS:SG	2:D:248:PHE:HE2	2.31	0.53
2:B:56:MET:HE2	2:B:99:LEU:HD13	1.91	0.53
1:C:86:ASP:HA	1:C:134:LEU:HA	1.89	0.52
1:A:20:LYS:HE3	1:A:29:VAL:CG1	2.39	0.52
1:A:84:HIS:HB3	1:A:298:LEU:HD21	1.91	0.52
1:C:122:ARG:HH12	2:D:8:GLY:C	2.11	0.52
2:B:70:PHE:HB3	2:B:71:PRO:HD3	1.90	0.52
1:A:2:GLU:O	1:A:3:ASN:ND2	2.42	0.52
1:C:30:VAL:HG22	1:C:31:ALA:N	2.24	0.52
1:C:167:TRP:CD1	1:C:167:TRP:N	2.76	0.52
1:C:36:ARG:NH1	1:C:74:ASN:HD21	2.08	0.52
1:A:129:LYS:NZ	1:A:164:VAL:CG1	2.73	0.51
1:C:217:ARG:HG3	1:C:243:TRP:CE3	2.44	0.51
2:D:70:PHE:HB3	2:D:71:PRO:HD3	1.91	0.51
1:C:122:ARG:NH1	2:D:8:GLY:O	2.44	0.51
1:C:218:THR:HG22	1:C:219:LEU:HD23	1.91	0.51
1:C:186:ILE:HD11	1:C:277:ALA:HB2	1.91	0.51
2:D:12:SER:OG	2:D:15:LEU:HD12	2.11	0.51
1:A:159:TYR:O	1:A:161:HIS:N	2.43	0.51
2:B:100:HIS:ND1	2:B:133:GLU:OE2	2.38	0.51
1:C:226:VAL:HG23	1:C:227:TRP:H	1.76	0.51
2:B:56:MET:CE	2:B:73:ALA:HB1	2.40	0.51
1:C:99:ILE:O	1:C:100:PRO:C	2.49	0.51
1:A:258:ASP:O	1:A:261:SER:HB3	2.11	0.51
2:D:52:LEU:O	2:D:56:MET:HG3	2.11	0.50
2:B:177:LYS:HG2	2:B:240:ILE:HD11	1.93	0.50
1:A:129:LYS:NZ	1:A:164:VAL:HG12	2.26	0.50
2:D:160:MET:O	2:D:161:HIS:C	2.50	0.50
1:A:36:ARG:NH1	1:A:74:ASN:ND2	2.59	0.50
1:C:256:ASP:OD1	1:C:256:ASP:N	2.44	0.50
1:C:35:ILE:HD12	1:C:78:LEU:HD21	1.94	0.50
1:A:253:PRO:HG2	1:A:254:PRO:CD	2.42	0.50
2:D:214:ARG:HD3	4:D:270:HOH:O	2.12	0.50
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.94	0.50
1:A:23:ASN:CB	1:A:28:GLU:H	2.25	0.50
1:C:215:ILE:HG22	1:C:269:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HZ3	1:A:164:VAL:CG1	2.25	0.49
1:A:202:LEU:O	1:A:204:PRO:HD3	2.11	0.49
1:C:172:GLU:HG2	1:C:173:ILE:N	2.27	0.49
1:C:60:HIS:CD2	1:C:62:ASN:HB2	2.47	0.49
1:A:209:ILE:O	1:A:210:ASP:C	2.51	0.49
1:C:268:HIS:CD2	1:C:273:LYS:HB3	2.47	0.49
1:C:104:ILE:HD13	1:C:197:VAL:HG23	1.94	0.49
1:C:263:LEU:HG	1:C:267:LEU:HD12	1.95	0.49
1:A:108:LEU:HD22	1:A:193:PHE:CD1	2.48	0.49
1:A:201:ALA:O	1:A:204:PRO:HG3	2.13	0.49
1:A:60:HIS:HD2	1:A:62:ASN:N	2.04	0.49
2:D:51:VAL:HG13	2:D:248:PHE:HB2	1.93	0.49
1:A:210:ASP:O	1:A:213:PHE:N	2.45	0.49
2:B:156:ILE:O	2:B:160:MET:HG3	2.13	0.49
1:C:222:PRO:HA	1:C:226:VAL:HG21	1.93	0.49
2:D:136:SER:O	2:D:140:LEU:HG	2.13	0.49
1:A:214:ARG:CG	1:A:214:ARG:NH1	2.73	0.48
1:C:262:LEU:HD13	1:C:283:HIS:CD2	2.48	0.48
1:A:83:LEU:HD22	1:A:134:LEU:HB2	1.95	0.48
2:D:67:ASN:HA	2:D:175:ARG:NH2	2.27	0.48
1:C:5:GLN:O	1:C:6:LYS:CB	2.61	0.48
2:D:47:GLN:HE21	2:D:47:GLN:C	2.17	0.48
1:C:216:PHE:O	1:C:220:GLY:N	2.46	0.48
1:C:36:ARG:HH11	1:C:74:ASN:ND2	2.10	0.48
1:A:129:LYS:O	1:A:133:LEU:HG	2.14	0.48
1:C:30:VAL:HA	1:C:82:PHE:HB2	1.95	0.48
2:D:12:SER:C	2:D:14:LEU:H	2.17	0.48
1:A:62:ASN:OD1	1:A:110:GLN:HB3	2.13	0.48
1:C:101:LEU:O	1:C:103:LEU:N	2.47	0.48
2:D:47:GLN:HA	2:D:50:LYS:HE2	1.96	0.48
1:A:262:LEU:HD13	1:A:283:HIS:CG	2.49	0.48
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.44	0.48
1:C:103:LEU:HD12	1:C:292:PRO:CG	2.41	0.48
1:A:12:GLU:O	1:A:13:GLY:O	2.32	0.47
2:D:111:ILE:HD12	2:D:111:ILE:N	2.22	0.47
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.95	0.47
2:B:77:LEU:HD13	2:B:95:ALA:HA	1.96	0.47
1:C:193:PHE:O	1:C:194:ALA:C	2.52	0.47
1:C:99:ILE:HD12	1:C:196:MET:HB3	1.97	0.47
2:D:63:LEU:O	2:D:64:ARG:C	2.53	0.47
1:C:129:LYS:CA	1:C:192:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:HIS:O	2:B:35:MET:HB2	2.15	0.47
1:C:19:TYR:HB2	1:C:32:LEU:HB2	1.95	0.47
1:C:223:ASP:OD2	1:C:225:VAL:HB	2.15	0.47
1:C:4:PHE:HA	1:C:23:ASN:HA	1.96	0.47
1:C:95:ALA:O	1:C:98:GLY:N	2.48	0.47
2:D:249:LYS:O	2:D:252:ALA:HB2	2.15	0.47
1:A:213:PHE:O	1:A:217:ARG:HG3	2.15	0.47
1:C:212:LEU:HD22	1:C:216:PHE:CE2	2.49	0.47
2:D:85:ARG:CG	2:D:85:ARG:HH11	2.27	0.47
2:D:103:GLY:O	2:D:107:ALA:HB3	2.15	0.47
2:B:68:ASN:C	2:B:71:PRO:HD2	2.36	0.47
1:A:164:VAL:HB	1:A:165:THR:H	1.46	0.46
1:C:141:ILE:O	1:C:141:ILE:HG23	2.15	0.46
1:C:237:LYS:HB2	1:C:240:PHE:CE1	2.50	0.46
1:A:217:ARG:HG2	1:A:243:TRP:NE1	2.30	0.46
1:C:200:ARG:CG	1:C:200:ARG:HH11	2.24	0.46
1:A:135:ILE:CG2	1:A:141:ILE:HG13	2.44	0.46
1:A:20:LYS:HE3	1:A:29:VAL:HG11	1.97	0.46
1:C:109:PHE:HB2	1:C:286:PHE:CE1	2.51	0.46
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.97	0.46
1:C:284:PRO:C	1:C:286:PHE:N	2.69	0.46
1:A:253:PRO:O	1:A:255:LEU:N	2.48	0.46
1:A:44:VAL:HG21	2:B:142:TRP:HZ3	1.78	0.46
1:C:88:LYS:HE3	1:C:92:ASP:OD1	2.16	0.46
2:D:67:ASN:O	2:D:179:PHE:HZ	1.99	0.46
1:A:265:GLN:HA	1:A:268:HIS:HD2	1.80	0.46
2:B:23:MET:HG2	2:B:155:TYR:CZ	2.51	0.46
1:C:175:LEU:HB3	1:C:233:MET:HG2	1.97	0.46
1:A:85:GLN:HB2	1:A:89:LYS:HD2	1.98	0.45
2:B:51:VAL:HG13	2:B:248:PHE:HB2	1.97	0.45
1:C:203:PHE:N	1:C:204:PRO:HD3	2.30	0.45
1:A:206:ASP:OD2	1:A:206:ASP:N	2.49	0.45
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.98	0.45
1:A:74:ASN:OD1	1:A:75:LYS:HG3	2.16	0.45
2:B:35:MET:C	2:B:37:GLY:N	2.70	0.45
1:C:200:ARG:CG	1:C:200:ARG:NH1	2.80	0.45
2:D:100:HIS:ND1	2:D:133:GLU:OE2	2.50	0.45
1:C:91:MET:HE3	1:C:196:MET:HA	1.99	0.45
2:D:225:THR:HG23	2:D:228:GLU:OE2	2.17	0.45
1:C:5:GLN:O	1:C:6:LYS:HB2	2.16	0.45
1:C:124:LEU:HD11	2:D:11:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:HD3	1:A:148:LEU:O	2.16	0.45
1:A:250:LYS:HG2	1:A:250:LYS:O	2.16	0.45
1:A:253:PRO:HG2	1:A:254:PRO:HD3	1.98	0.45
1:A:54:LEU:C	1:A:54:LEU:HD23	2.37	0.45
2:B:18:GLU:OE2	2:B:22:GLN:NE2	2.50	0.45
1:A:260:ARG:HG3	1:A:260:ARG:NH1	2.32	0.44
1:C:59:ASN:ND2	1:C:65:LYS:HE3	2.32	0.44
1:A:13:GLY:HA3	1:A:18:VAL:CG2	2.43	0.44
1:A:203:PHE:O	1:A:205:GLY:N	2.43	0.44
1:C:227:TRP:O	1:C:230:VAL:HG22	2.17	0.44
2:D:155:TYR:O	2:D:159:ILE:HG13	2.17	0.44
2:D:66:ASP:OD1	2:D:107:ALA:HA	2.17	0.44
2:D:67:ASN:CG	2:D:175:ARG:NH1	2.70	0.44
2:B:156:ILE:HD12	2:B:196:THR:HG21	2.00	0.44
2:B:77:LEU:HD12	2:B:94:THR:HG22	1.98	0.44
1:C:268:HIS:NE2	1:C:273:LYS:HB3	2.33	0.44
2:D:220:LYS:NZ	2:D:220:LYS:CB	2.76	0.44
1:A:17:VAL:O	1:A:18:VAL:HG23	2.18	0.44
1:A:223:ASP:OD2	1:A:225:VAL:N	2.43	0.44
1:C:268:HIS:CD2	1:C:273:LYS:CB	3.00	0.44
1:C:291:LYS:N	1:C:292:PRO:CD	2.80	0.44
1:C:99:ILE:HG22	1:C:104:ILE:HG13	1.98	0.44
1:A:231:THR:HA	1:A:236:TYR:CD2	2.53	0.44
2:B:167:TYR:H	2:B:167:TYR:HD1	1.64	0.44
2:B:77:LEU:CD1	2:B:94:THR:HG22	2.48	0.44
1:A:260:ARG:H	1:A:260:ARG:HG2	1.60	0.43
1:C:99:ILE:HG21	1:C:104:ILE:HG13	2.00	0.43
1:C:30:VAL:CG2	1:C:31:ALA:N	2.80	0.43
2:D:187:SER:HB3	2:D:235:LEU:HB3	2.00	0.43
2:B:16:ASN:O	2:B:17:GLU:C	2.56	0.43
1:C:112:LEU:CD1	1:C:189:LEU:HD13	2.47	0.43
1:C:217:ARG:NE	1:C:243:TRP:CH2	2.87	0.43
2:D:186:ARG:HG3	2:D:186:ARG:HH11	1.82	0.43
1:C:115:LEU:HG	1:C:119:HIS:CE1	2.54	0.43
1:C:6:LYS:HE3	1:C:20:LYS:HG2	2.00	0.43
2:D:149:SER:O	2:D:153:ILE:HG13	2.18	0.43
1:A:101:LEU:HB3	1:A:102:PRO:HD3	2.01	0.43
1:A:124:LEU:HD21	1:A:182:THR:HA	1.98	0.43
1:C:189:LEU:O	1:C:190:GLY:C	2.56	0.43
1:C:1:MET:HG3	1:C:77:TYR:CE1	2.53	0.43
2:D:61:LYS:HZ3	2:D:61:LYS:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:MET:CE	2:D:73:ALA:HB1	2.43	0.43
1:C:29:VAL:HG12	1:C:30:VAL:N	2.34	0.43
1:C:148:LEU:CD2	1:C:162:GLU:HG3	2.48	0.43
1:C:162:GLU:O	1:C:163:VAL:C	2.56	0.43
2:D:47:GLN:O	2:D:50:LYS:HB2	2.18	0.43
1:C:166:LEU:HD11	1:C:208:GLU:HG2	2.01	0.42
1:C:30:VAL:HG21	1:C:79:VAL:CG1	2.49	0.42
2:B:56:MET:CE	2:B:99:LEU:HD13	2.48	0.42
1:C:120:SER:O	2:D:15:LEU:CD2	2.67	0.42
1:C:112:LEU:HD12	1:C:189:LEU:CD1	2.49	0.42
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.00	0.42
1:A:227:TRP:CE3	1:A:230:VAL:CG1	3.02	0.42
2:B:15:LEU:HD22	2:B:19:ASP:CB	2.49	0.42
2:B:35:MET:HE3	2:B:35:MET:HA	2.01	0.42
1:C:193:PHE:O	1:C:195:GLU:N	2.53	0.42
1:A:278:LYS:O	1:A:281:LEU:HB2	2.20	0.42
1:C:181:SER:HB3	4:C:315:HOH:O	2.20	0.42
1:C:190:GLY:HA2	1:C:266:MET:HE3	2.02	0.42
2:D:40:VAL:HA	2:D:82:LEU:CD2	2.49	0.42
1:C:278:LYS:HB2	1:C:278:LYS:HE3	1.90	0.42
2:D:34:ARG:NH1	4:D:255:HOH:O	2.49	0.42
1:A:84:HIS:ND1	1:A:84:HIS:N	2.67	0.42
2:B:51:VAL:HG13	2:B:248:PHE:HA	2.00	0.42
1:C:284:PRO:O	1:C:286:PHE:N	2.53	0.42
2:D:108:TYR:O	2:D:110:PRO:HD3	2.19	0.42
2:D:97:VAL:O	2:D:101:ILE:HG13	2.20	0.42
2:B:36:VAL:O	2:B:36:VAL:CG1	2.67	0.42
1:C:124:LEU:HD11	1:C:150:ARG:NH2	2.35	0.42
1:C:18:VAL:O	1:C:19:TYR:CG	2.73	0.42
1:A:44:VAL:O	2:B:104:LYS:NZ	2.43	0.42
2:B:205:ASN:ND2	2:B:206:GLN:HG3	2.34	0.42
2:B:66:ASP:HB3	2:B:69:VAL:HG23	2.02	0.42
1:C:165:THR:CG2	1:C:165:THR:O	2.62	0.42
1:C:255:LEU:HD21	1:C:259:GLY:C	2.39	0.42
2:B:115:GLN:HB2	2:B:115:GLN:HE21	1.63	0.42
2:B:70:PHE:O	2:B:74:VAL:HG23	2.20	0.42
2:B:164:ARG:HH11	2:B:164:ARG:CG	2.29	0.41
1:A:147:GLY:C	1:A:148:LEU:HD12	2.40	0.41
1:A:198:THR:O	1:A:199:ARG:CB	2.68	0.41
1:A:167:TRP:HE1	1:A:205:GLY:N	2.18	0.41
2:B:51:VAL:HG13	2:B:248:PHE:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:VAL:O	1:C:197:VAL:CG1	2.68	0.41
2:D:45:THR:HG22	2:D:186:ARG:HH12	1.85	0.41
1:A:167:TRP:NE1	1:A:205:GLY:N	2.68	0.41
1:C:203:PHE:HB3	1:C:211:GLN:HE22	1.85	0.41
2:D:68:ASN:C	2:D:71:PRO:HD2	2.41	0.41
2:D:21:ARG:HA	2:D:24:ILE:HD12	2.03	0.41
1:A:195:GLU:HA	1:A:200:ARG:O	2.19	0.41
1:C:186:ILE:HD11	1:C:277:ALA:N	2.35	0.41
1:C:296:LEU:O	1:C:297:ARG:CB	2.68	0.41
2:D:220:LYS:HZ3	2:D:220:LYS:HB2	1.82	0.41
2:D:79:GLU:O	2:D:83:SER:CB	2.65	0.41
1:A:105:LYS:HD3	1:A:285:PHE:O	2.20	0.41
2:B:169:ASN:HB2	4:B:289:HOH:O	2.21	0.41
2:D:88:ARG:CG	2:D:88:ARG:HH11	2.32	0.41
1:A:167:TRP:CD1	1:A:203:PHE:O	2.74	0.41
1:A:6:LYS:HD3	1:A:19:TYR:CG	2.56	0.41
2:D:87:ASP:HB3	2:D:89:GLU:OE2	2.21	0.41
1:A:72:THR:HG23	1:A:72:THR:O	2.20	0.41
1:C:113:GLN:HB3	1:C:113:GLN:HE21	1.55	0.41
1:C:54:LEU:HD13	1:C:151:ALA:CB	2.51	0.41
1:A:255:LEU:HD23	1:A:260:ARG:HD3	2.03	0.41
2:D:12:SER:OG	2:D:12:SER:O	2.35	0.41
2:B:175:ARG:N	2:B:176:PRO:HD2	2.36	0.41
1:A:209:ILE:O	1:A:213:PHE:CD1	2.74	0.40
1:C:286:PHE:O	1:C:288:ASP:N	2.54	0.40
2:D:162:ALA:HA	2:D:163:PRO:HD3	1.97	0.40
1:A:216:PHE:CE2	1:A:222:PRO:HD2	2.56	0.40
1:C:255:LEU:HD23	1:C:260:ARG:CA	2.51	0.40
1:C:54:LEU:HD13	1:C:151:ALA:HB2	2.02	0.40
1:C:60:HIS:HD2	1:C:62:ASN:HB2	1.87	0.40
1:C:6:LYS:CE	1:C:20:LYS:HG2	2.52	0.40
1:A:84:HIS:HB3	1:A:298:LEU:CD2	2.50	0.40
2:B:21:ARG:HG2	2:B:21:ARG:HH11	1.86	0.40
1:C:200:ARG:O	1:C:201:ALA:O	2.39	0.40
1:C:258:ASP:HB3	1:C:285:PHE:HA	2.04	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	292/298 (98%)	257 (88%)	23 (8%)	12 (4%)	3	3
1	C	280/298 (94%)	219 (78%)	45 (16%)	16 (6%)	1	1
2	B	246/252 (98%)	235 (96%)	10 (4%)	1 (0%)	34	54
2	D	246/252 (98%)	235 (96%)	10 (4%)	1 (0%)	34	54
All	All	1064/1100 (97%)	946 (89%)	88 (8%)	30 (3%)	5	7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	13	GLY
1	A	94	SER
1	A	160	THR
1	A	164	VAL
1	A	208	GLU
1	C	6	LYS
1	C	8	GLU
1	C	94	SER
1	C	163	VAL
1	C	201	ALA
2	D	39	ASN
1	A	6	LYS
1	A	206	ASP
2	B	36	VAL
1	C	296	LEU
1	A	18	VAL
1	C	160	THR
1	C	194	ALA
1	C	217	ARG
1	C	285	PHE
1	C	287	GLN

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Mol	Chain	Res	Type
1	A	254	PRO
1	C	73	GLU
1	C	245	ARG
1	C	106	SER
1	C	254	PRO
1	A	204	PRO
1	C	7	VAL
1	A	98	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/263 (96%)	236 (93%)	17 (7%)	16	31
1	C	237/263 (90%)	223 (94%)	14 (6%)	19	37
2	B	220/225 (98%)	214 (97%)	6 (3%)	44	71
2	D	217/225 (96%)	212 (98%)	5 (2%)	50	76
All	All	927/976 (95%)	885 (96%)	42 (4%)	27	51

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	30	VAL
1	A	57	GLU
1	A	160	THR
1	A	164	VAL
1	A	206	ASP
1	A	209	ILE
1	A	212	LEU
1	A	214	ARG
1	A	230	VAL
1	A	248	PHE
1	A	249	SER
1	A	256	ASP

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Mol	Chain	Res	Type
1	A	258	ASP
1	A	260	ARG
1	A	290	THR
1	A	293	VAL
2	B	35	MET
2	B	52	LEU
2	B	66	ASP
2	B	88	ARG
2	B	132	LEU
2	B	193	VAL
1	C	2	GLU
1	C	8	GLU
1	C	78	LEU
1	C	86	ASP
1	C	94	SER
1	C	120	SER
1	C	131	GLN
1	C	160	THR
1	C	193	PHE
1	C	230	VAL
1	C	240	PHE
1	C	284	PRO
1	C	293	VAL
1	C	294	PRO
2	D	47	GLN
2	D	61	LYS
2	D	85	ARG
2	D	89	GLU
2	D	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	60	HIS
1	A	62	ASN
1	A	131	GLN
1	A	268	HIS
1	A	272	ASN
2	B	47	GLN
2	B	115	GLN
2	B	169	ASN

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Mol	Chain	Res	Type
2	B	213	ASN
2	B	230	HIS
1	C	60	HIS
1	C	62	ASN
1	C	85	GLN
1	C	113	GLN
1	C	131	GLN
1	C	211	GLN
2	D	39	ASN
2	D	65	GLN
2	D	67	ASN
2	D	115	GLN
2	D	169	ASN
2	D	205	ASN
2	D	246	ASN
2	D	251	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.