Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:46 PM GMT

PDB ID	:	1H4L
Title	:	STRUCTURE AND REGULATION OF THE CDK5-P25(NCK5A) COMPLEX
Authors	:	Tarricone, C.; Dhavan, R.; Peng, J.; Areces, L.B.; Tsai, L.-H.; Musacchio, A.
Deposited on	:	2001-05-11
Resolution	:	2.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

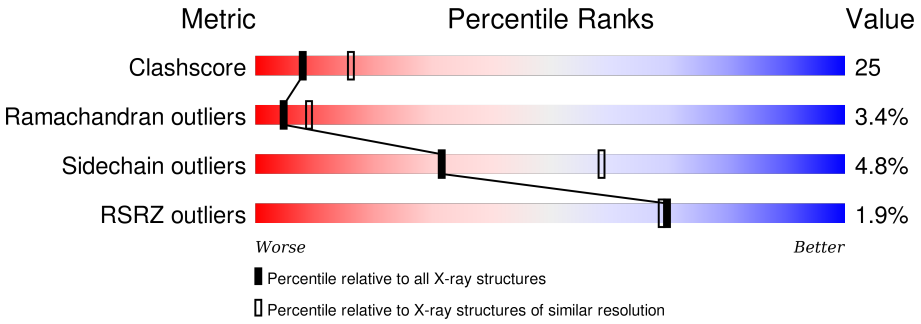
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.65 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	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 <=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	292	2% 54% 37% • 5%
1	B	292	2% 49% 41% 5% 5%
2	D	147	2% 51% 44% 5%
2	E	147	2% 56% 37% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6937 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 CELL DIVISION PROTEIN KINASE 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2243	1445	388	400	10			
1	B	278	Total	C	N	O	S	0	0	0
			2243	1445	388	400	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	GLY	CONFLICT	UNP Q00535
B	199	ALA	GLY	CONFLICT	UNP Q00535

- Molecule 2 is a protein called CYCLIN-DEPENDENT KINASE 5 ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	147	Total	C	N	O	S	0	0	0
			1191	765	196	219	11			
2	E	147	Total	C	N	O	S	0	0	0
			1191	765	196	219	11			

- Molecule 3 is water.

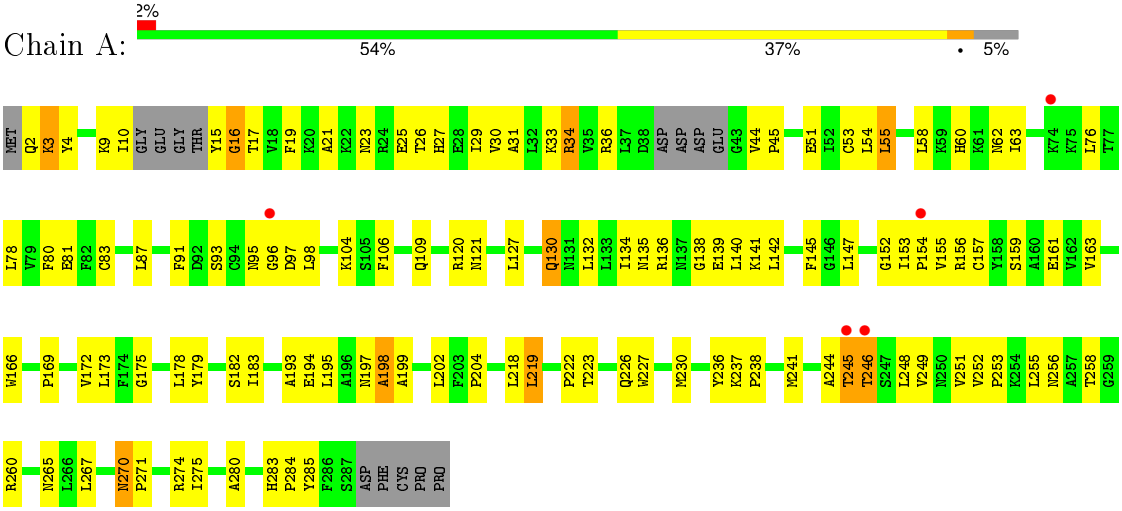
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	21	Total	O	0	0
			21	21		
3	D	9	Total	O	0	0
			9	9		
3	E	11	Total	O	0	0
			11	11		

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 errors 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.

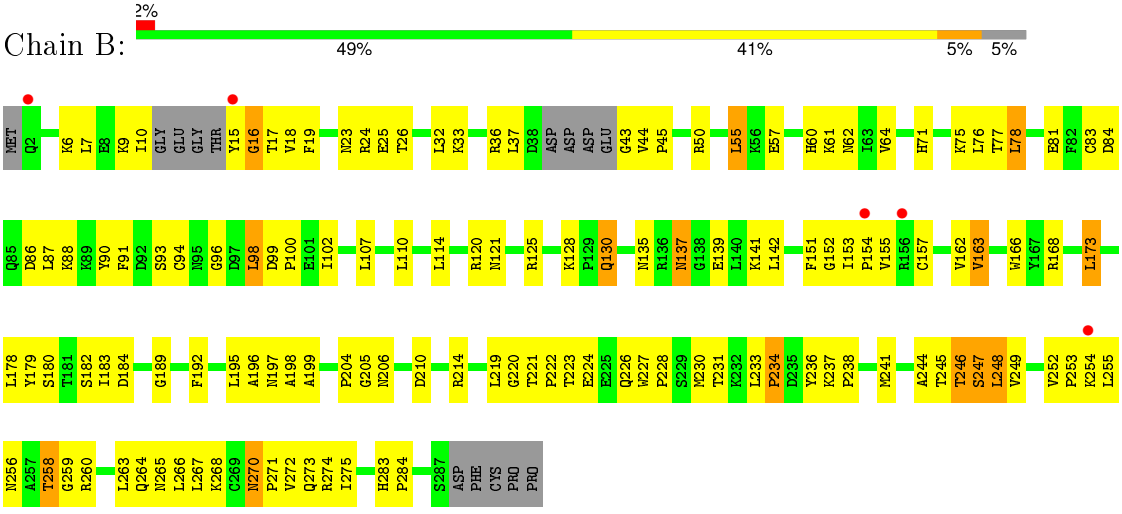
- Molecule 1: CELL DIVISION PROTEIN KINASE 5

Chain A:



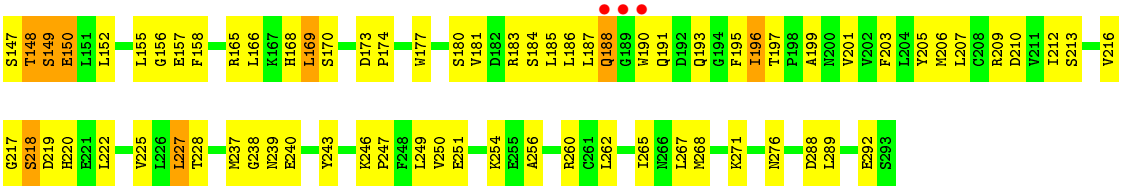
- Molecule 1: CELL DIVISION PROTEIN KINASE 5

Chain B:



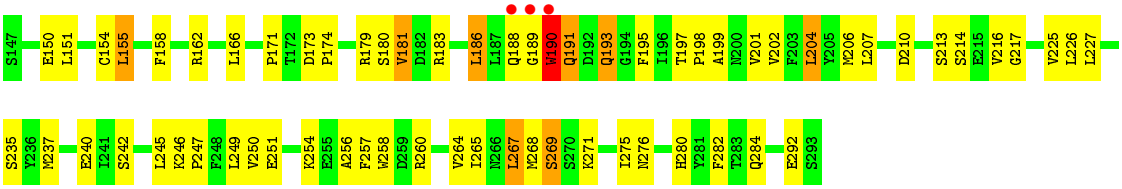
- Molecule 2: CYCLIN-DEPENDENT KINASE 5 ACTIVATOR

Chain D:



- Molecule 2: CYCLIN-DEPENDENT KINASE 5 ACTIVATOR

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.09Å 89.76Å 82.57Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	19.22 – 2.65 19.22 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.22-2.65) 95.5 (19.22-2.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.06 (at 2.67Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.287 0.250 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 30223 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6937	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/2294	0.62	0/3101
1	B	0.40	0/2294	0.65	1/3101 (0.0%)
2	D	0.38	0/1219	0.61	0/1652
2	E	0.39	0/1219	0.66	1/1652 (0.1%)
All	All	0.39	0/7026	0.64	2/9506 (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})
2	E	189	GLY	N-CA-C	-7.78	93.64	113.10
1	B	94	CYS	N-CA-C	-5.65	95.75	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	2243	0	2282	115	0
1	B	2243	0	2282	127	0
2	D	1191	0	1177	72	0
2	E	1191	0	1177	50	0
3	A	28	0	0	1	0
3	B	21	0	0	0	0
3	D	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	11	0	0	0	0
All	All	6937	0	6918	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 25.

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)
2:E:158:PHE:HB2	2:E:292:GLU:HG2	1.29	1.14
2:D:158:PHE:HB2	2:D:292:GLU:HG2	1.40	1.02
2:D:251:GLU:OE2	2:D:256:ALA:HB3	1.71	0.90
2:D:147:SER:O	2:D:150:GLU:HG3	1.71	0.88
1:A:60:HIS:HE1	1:A:62:ASN:HD22	1.16	0.88
2:E:210:ASP:HB2	2:E:268:MET:HE1	1.59	0.84
2:E:158:PHE:HB2	2:E:292:GLU:CG	2.09	0.81
1:A:15:TYR:CD1	1:A:33:LYS:HD3	2.16	0.81
1:B:249:VAL:HG22	1:B:260:ARG:NE	1.97	0.79
1:B:219:LEU:HA	1:B:246:THR:HG22	1.63	0.78
1:A:156:ARG:HH11	2:D:193:GLN:HE21	1.30	0.78
2:D:249:LEU:HD21	2:D:254:LYS:HG2	1.67	0.77
1:B:91:PHE:CG	1:B:199:ALA:HB1	2.21	0.75
1:B:178:LEU:HD23	1:B:179:TYR:N	2.02	0.74
1:B:227:TRP:HB3	1:B:230:MET:HE2	1.68	0.74
1:A:265:ASN:HB3	1:A:275:ILE:HG23	1.70	0.74
2:D:149:SER:HA	2:D:152:LEU:HD12	1.69	0.73
1:A:153:ILE:HD12	2:D:237:MET:CE	2.19	0.73
2:E:186:LEU:C	2:E:188:GLN:H	1.91	0.73
1:B:153:ILE:HD12	2:E:237:MET:CE	2.18	0.72
1:A:223:THR:OG1	1:A:226:GLN:HG3	1.90	0.70
2:E:191:GLN:OE1	2:E:195:PHE:HB2	1.93	0.69
1:A:91:PHE:CG	1:A:199:ALA:HB1	2.28	0.69
2:D:195:PHE:O	2:D:197:THR:HG23	1.92	0.69
2:D:173:ASP:HB2	2:D:174:PRO:HD3	1.74	0.69
1:A:153:ILE:HD12	2:D:237:MET:HE1	1.76	0.68
1:B:153:ILE:HD12	2:E:237:MET:HE2	1.73	0.68
1:B:210:ASP:O	1:B:214:ARG:HG3	1.93	0.68
1:B:244:ALA:C	1:B:246:THR:H	1.98	0.67
2:E:179:ARG:HG2	2:E:179:ARG:HH11	1.61	0.66
1:B:60:HIS:HE1	1:B:62:ASN:HD22	1.43	0.66
2:E:188:GLN:C	2:E:190:TRP:H	1.86	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:249:LEU:HD21	2:E:254:LYS:HG2	1.78	0.66
1:B:256:ASN:O	1:B:260:ARG:HG3	1.94	0.66
1:A:104:LYS:HE2	1:A:285:TYR:O	1.96	0.65
1:B:44:VAL:HB	1:B:45:PRO:HD3	1.78	0.65
1:A:265:ASN:HB3	1:A:275:ILE:CG2	2.26	0.65
1:B:253:PRO:C	1:B:255:LEU:H	2.00	0.65
2:E:166:LEU:HD21	2:E:217:GLY:O	1.96	0.65
1:B:270:ASN:HD21	1:B:272:VAL:HG23	1.62	0.65
1:B:283:HIS:CE1	1:B:284:PRO:HG2	2.32	0.65
2:D:187:LEU:O	2:D:188:GLN:O	2.15	0.64
2:D:205:TYR:CG	2:D:289:LEU:HD13	2.34	0.63
1:B:125:ARG:O	1:B:163:VAL:HG22	1.98	0.63
1:B:155:VAL:HG12	1:B:157:CYS:N	2.14	0.63
1:A:223:THR:HG22	1:A:241:MET:CE	2.29	0.62
1:B:155:VAL:HG12	1:B:157:CYS:H	1.63	0.62
1:A:156:ARG:HH11	2:D:193:GLN:NE2	1.96	0.62
1:A:249:VAL:HG22	1:A:260:ARG:NE	2.15	0.62
1:B:15:TYR:HD1	1:B:33:LYS:HE2	1.63	0.62
1:B:36:ARG:HD3	1:B:75:LYS:HE3	1.82	0.62
2:D:186:LEU:HD22	2:D:188:GLN:HE22	1.63	0.61
1:B:268:LYS:HG3	1:B:273:GLN:HG2	1.82	0.61
1:B:260:ARG:O	1:B:264:GLN:HG3	1.99	0.61
1:A:197:ASN:CG	1:A:198:ALA:H	2.02	0.61
1:B:206:ASN:N	1:B:206:ASN:HD22	1.98	0.61
2:D:169:LEU:HD23	2:D:170:SER:N	2.15	0.61
2:E:206:MET:HE2	2:E:207:LEU:HD23	1.83	0.61
1:B:43:GLY:HA3	2:E:242:SER:HB2	1.83	0.61
1:B:270:ASN:HD22	1:B:271:PRO:CD	2.14	0.60
2:D:209:ARG:NH2	2:D:288:ASP:OD2	2.34	0.60
1:B:107:LEU:HD22	1:B:192:PHE:CD1	2.36	0.60
1:B:120:ARG:O	1:B:121:ASN:HB2	2.01	0.60
1:A:252:VAL:O	1:A:252:VAL:HG13	2.01	0.60
1:B:98:LEU:N	1:B:98:LEU:HD12	2.16	0.60
1:A:21:ALA:O	1:A:29:ILE:HA	2.02	0.60
1:B:23:ASN:O	1:B:25:GLU:N	2.31	0.60
2:E:267:LEU:HD13	2:E:268:MET:SD	2.41	0.60
1:A:244:ALA:C	1:A:246:THR:H	2.05	0.59
2:E:155:LEU:HD11	2:E:204:LEU:HD13	1.84	0.59
1:A:270:ASN:HD22	1:A:271:PRO:CD	2.14	0.59
2:E:186:LEU:C	2:E:188:GLN:N	2.53	0.59
1:B:168:ARG:HB3	1:B:173:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:179:ARG:NH1	2:E:179:ARG:HG2	2.16	0.59
1:B:37:LEU:HD21	1:B:76:LEU:HG	1.84	0.59
1:B:236:TYR:HE1	1:B:238:PRO:HG3	1.68	0.59
2:D:149:SER:O	2:D:152:LEU:HB2	2.03	0.59
1:A:270:ASN:HD22	1:A:270:ASN:C	2.05	0.59
1:B:168:ARG:HG2	1:B:173:LEU:HD13	1.84	0.58
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.68	0.58
2:D:186:LEU:C	2:D:188:GLN:H	2.05	0.58
1:B:227:TRP:HB3	1:B:230:MET:CE	2.34	0.58
1:A:140:LEU:HD23	1:A:140:LEU:C	2.24	0.58
1:B:6:LYS:O	1:B:7:LEU:HD23	2.03	0.58
2:E:198:PRO:O	2:E:202:VAL:HG23	2.04	0.58
2:D:213:SER:O	2:D:216:VAL:HG23	2.04	0.58
1:A:60:HIS:CE1	1:A:62:ASN:HD22	2.08	0.57
1:A:197:ASN:C	1:A:199:ALA:H	2.06	0.57
1:A:161:GLU:O	1:A:161:GLU:HG3	2.04	0.57
1:A:87:LEU:HD13	1:A:134:ILE:HD11	1.85	0.57
1:A:60:HIS:HE1	1:A:62:ASN:ND2	1.95	0.57
1:A:230:MET:HG3	1:A:236:TYR:CE2	2.40	0.57
1:B:205:GLY:HA2	1:B:214:ARG:HD2	1.86	0.57
1:A:15:TYR:HD1	1:A:33:LYS:HD3	1.70	0.57
2:D:181:VAL:HB	2:D:247:PRO:HB2	1.85	0.57
1:B:283:HIS:CG	1:B:284:PRO:HD2	2.40	0.57
1:B:252:VAL:HG13	1:B:252:VAL:O	2.05	0.57
1:A:23:ASN:ND2	1:A:26:THR:HG23	2.19	0.57
1:B:270:ASN:HD22	1:B:271:PRO:HD2	1.70	0.56
1:A:169:PRO:HG2	1:A:172:VAL:HG23	1.87	0.56
1:A:153:ILE:HD12	2:D:237:MET:HE2	1.87	0.56
2:D:267:LEU:HD13	2:D:268:MET:SD	2.46	0.56
1:B:268:LYS:HD2	1:B:273:GLN:OE1	2.04	0.56
1:A:275:ILE:HD12	1:A:280:ALA:HB2	1.87	0.56
1:A:270:ASN:HD22	1:A:271:PRO:N	2.04	0.56
1:A:10:ILE:HG22	1:A:10:ILE:O	2.06	0.56
2:D:219:ASP:OD1	2:D:220:HIS:N	2.39	0.56
1:B:252:VAL:N	1:B:253:PRO:HD3	2.21	0.55
1:B:15:TYR:HD2	1:B:44:VAL:HG13	1.71	0.55
1:A:106:PHE:CZ	1:A:134:ILE:HD13	2.41	0.55
1:B:128:LYS:HG3	1:B:130:GLN:HG2	1.89	0.55
1:B:248:LEU:HD23	1:B:263:LEU:HD23	1.89	0.55
1:B:153:ILE:HG21	2:E:199:ALA:HB1	1.88	0.54
1:B:152:GLY:HA3	2:E:276:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD21	1:A:267:LEU:HB3	1.89	0.54
1:B:36:ARG:CD	1:B:75:LYS:HE3	2.37	0.54
2:D:206:MET:HE2	2:D:207:LEU:HD23	1.88	0.54
1:A:182:SER:HB2	1:A:274:ARG:HD2	1.89	0.54
1:A:223:THR:HG22	1:A:241:MET:HE2	1.89	0.54
2:D:197:THR:O	2:D:201:VAL:HG23	2.08	0.54
1:A:2:GLN:C	1:A:4:TYR:H	2.10	0.54
2:E:213:SER:O	2:E:216:VAL:HG23	2.07	0.54
1:A:95:ASN:O	1:A:97:ASP:N	2.41	0.54
2:E:210:ASP:OD1	2:E:271:LYS:NZ	2.39	0.54
1:A:237:LYS:HE3	3:A:2021:HOH:O	2.09	0.53
1:B:246:THR:C	1:B:248:LEU:H	2.12	0.53
1:A:197:ASN:O	1:A:199:ALA:N	2.42	0.53
1:B:253:PRO:O	1:B:255:LEU:N	2.39	0.53
1:B:96:GLY:O	1:B:98:LEU:HD12	2.09	0.53
2:E:245:LEU:HD11	2:E:257:PHE:CE2	2.44	0.53
1:B:86:ASP:OD1	1:B:88:LYS:HB3	2.08	0.53
1:B:15:TYR:O	1:B:16:GLY:O	2.26	0.53
2:E:251:GLU:OE2	2:E:256:ALA:HB3	2.08	0.53
1:B:198:ALA:O	1:B:199:ALA:HB3	2.09	0.53
1:B:224:GLU:O	1:B:228:PRO:HA	2.08	0.53
1:B:166:TRP:CD1	1:B:204:PRO:HA	2.43	0.52
1:A:256:ASN:O	1:A:260:ARG:HG3	2.08	0.52
2:D:185:LEU:HD12	2:D:190:TRP:CE3	2.44	0.52
1:B:18:VAL:HA	1:B:32:LEU:O	2.09	0.52
1:B:244:ALA:O	1:B:246:THR:N	2.42	0.52
1:B:168:ARG:HB3	1:B:173:LEU:CD1	2.40	0.51
2:E:173:ASP:HB2	2:E:174:PRO:HD3	1.92	0.51
1:A:9:LYS:HG3	1:A:9:LYS:O	2.10	0.51
1:A:153:ILE:O	1:A:155:VAL:HG23	2.11	0.51
1:A:26:THR:O	1:A:27:HIS:ND1	2.43	0.51
1:A:166:TRP:CD1	1:A:204:PRO:HA	2.45	0.51
2:E:188:GLN:C	2:E:190:TRP:N	2.52	0.51
1:A:81:GLU:OE1	1:A:141:LYS:HE2	2.10	0.51
2:D:158:PHE:HB2	2:D:292:GLU:CG	2.25	0.51
2:D:187:LEU:HD12	2:D:190:TRP:CZ3	2.46	0.51
1:A:78:LEU:N	1:A:78:LEU:HD23	2.26	0.51
1:A:152:GLY:HA3	2:D:276:ASN:O	2.11	0.51
1:A:83:CYS:HA	1:A:135:ASN:HD21	1.75	0.51
1:A:222:PRO:HB2	1:A:230:MET:HE3	1.93	0.51
1:A:44:VAL:HB	1:A:45:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASN:ND2	1:B:26:THR:HG23	2.26	0.50
1:B:270:ASN:C	1:B:270:ASN:HD22	2.14	0.50
2:E:245:LEU:HD22	2:E:258:TRP:CZ2	2.47	0.50
1:A:249:VAL:HG22	1:A:260:ARG:CZ	2.40	0.50
1:A:248:LEU:O	1:A:251:VAL:N	2.45	0.50
1:B:162:VAL:C	1:B:163:VAL:HG23	2.32	0.50
1:B:231:THR:HG22	1:B:236:TYR:CZ	2.47	0.50
1:A:155:VAL:HG12	1:A:157:CYS:H	1.76	0.50
1:B:223:THR:HG22	1:B:241:MET:CE	2.42	0.50
1:A:198:ALA:O	1:A:199:ALA:HB3	2.12	0.50
1:B:230:MET:SD	1:B:236:TYR:HE2	2.35	0.49
1:B:78:LEU:CD2	1:B:78:LEU:N	2.75	0.49
1:B:244:ALA:HB1	1:B:246:THR:HG23	1.94	0.49
1:B:206:ASN:ND2	1:B:206:ASN:N	2.57	0.49
1:A:270:ASN:HD22	1:A:271:PRO:HD2	1.76	0.49
1:A:136:ARG:C	1:A:138:GLY:H	2.15	0.49
1:A:218:LEU:HD23	1:A:219:LEU:HD13	1.93	0.49
1:A:252:VAL:N	1:A:253:PRO:HD3	2.26	0.49
1:B:247:SER:O	1:B:249:VAL:N	2.45	0.49
2:E:251:GLU:OE1	2:E:260:ARG:NH2	2.40	0.49
1:B:99:ASP:O	1:B:102:ILE:N	2.44	0.49
1:B:71:HIS:CE1	2:E:258:TRP:HB2	2.48	0.49
1:B:50:ARG:HD3	2:E:235:SER:O	2.13	0.49
1:B:270:ASN:ND2	1:B:272:VAL:HG23	2.27	0.49
1:B:64:VAL:HG23	1:B:81:GLU:HG2	1.95	0.48
2:D:190:TRP:O	2:D:240:GLU:HG3	2.13	0.48
1:B:10:ILE:O	1:B:10:ILE:HG22	2.13	0.48
1:A:222:PRO:HB2	1:A:230:MET:CE	2.44	0.48
1:A:218:LEU:HA	1:A:245:THR:OG1	2.14	0.48
2:E:191:GLN:HG2	2:E:193:GLN:O	2.12	0.48
1:B:57:GLU:HB3	1:B:120:ARG:HH21	1.78	0.48
1:B:249:VAL:HG22	1:B:260:ARG:CZ	2.42	0.48
1:B:270:ASN:HD22	1:B:271:PRO:N	2.11	0.48
2:D:217:GLY:O	2:D:218:SER:CB	2.61	0.48
1:A:251:VAL:HG22	1:A:251:VAL:O	2.14	0.48
1:B:61:LYS:O	1:B:141:LYS:HE2	2.14	0.48
1:B:43:GLY:CA	2:E:242:SER:HB2	2.44	0.48
1:B:23:ASN:HD22	1:B:26:THR:N	2.11	0.48
2:E:197:THR:O	2:E:201:VAL:HG23	2.12	0.47
1:B:253:PRO:C	1:B:255:LEU:N	2.67	0.47
1:B:258:THR:HG23	1:B:259:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:CE1	1:A:284:PRO:HG2	2.49	0.47
1:A:156:ARG:HD3	2:D:193:GLN:HE22	1.80	0.47
1:A:178:LEU:HD23	1:A:179:TYR:N	2.30	0.47
2:D:205:TYR:CD1	2:D:289:LEU:HD13	2.49	0.47
2:D:267:LEU:CD1	2:D:268:MET:SD	3.03	0.47
1:A:51:GLU:HG3	1:A:145:PHE:HB2	1.95	0.47
1:A:156:ARG:CD	2:D:193:GLN:HE22	2.27	0.47
1:B:114:LEU:HD11	1:B:184:ASP:HB3	1.96	0.47
2:D:148:THR:O	2:D:149:SER:C	2.51	0.47
1:A:197:ASN:C	1:A:199:ALA:N	2.68	0.47
1:A:270:ASN:ND2	1:A:270:ASN:C	2.68	0.47
1:B:32:LEU:HG	1:B:77:THR:CG2	2.44	0.47
2:E:250:VAL:HG22	2:E:250:VAL:O	2.13	0.47
1:B:87:LEU:HD12	1:B:90:TYR:HB3	1.97	0.47
2:D:205:TYR:O	2:D:209:ARG:HB2	2.15	0.47
1:A:23:ASN:C	1:A:25:GLU:H	2.17	0.47
1:B:182:SER:HB2	1:B:274:ARG:HD2	1.96	0.47
1:B:189:GLY:HA2	1:B:266:LEU:HD13	1.96	0.47
1:B:244:ALA:C	1:B:246:THR:N	2.67	0.47
1:B:55:LEU:HD12	1:B:55:LEU:HA	1.79	0.46
1:A:3:LYS:O	1:A:23:ASN:O	2.33	0.46
1:B:121:ASN:HA	1:B:151:PHE:CE1	2.51	0.46
2:D:249:LEU:CD2	2:D:254:LYS:HG2	2.42	0.46
2:E:275:ILE:HG12	2:E:282:PHE:HD1	1.80	0.46
1:A:159:SER:HB2	2:D:239:ASN:O	2.16	0.46
2:E:186:LEU:O	2:E:188:GLN:N	2.36	0.46
1:B:135:ASN:HB3	1:B:137:ASN:OD1	2.15	0.46
1:B:196:ALA:HB3	1:B:252:VAL:CG2	2.46	0.46
1:A:17:THR:HG23	1:A:19:PHE:CE1	2.51	0.46
1:B:231:THR:HA	1:B:236:TYR:CG	2.51	0.46
2:D:148:THR:HG22	2:D:152:LEU:HD11	1.97	0.46
2:D:148:THR:HG23	2:D:196:ILE:HG22	1.98	0.45
2:D:185:LEU:C	2:D:187:LEU:H	2.20	0.45
1:A:87:LEU:HD13	1:A:134:ILE:CD1	2.46	0.45
1:B:130:GLN:H	1:B:130:GLN:CD	2.16	0.45
1:B:153:ILE:HD12	2:E:237:MET:HE1	1.95	0.45
1:A:197:ASN:ND2	1:A:198:ALA:H	2.15	0.45
2:D:169:LEU:HD23	2:D:170:SER:O	2.16	0.45
2:D:246:LYS:HB2	2:D:247:PRO:HD3	1.99	0.45
2:D:212:ILE:CD1	2:D:225:VAL:HG13	2.46	0.45
1:B:168:ARG:HG2	1:B:173:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:LEU:HG	2:E:245:LEU:O	2.17	0.45
1:B:44:VAL:N	1:B:45:PRO:CD	2.79	0.45
2:D:210:ASP:OD1	2:D:271:LYS:NZ	2.46	0.45
1:A:97:ASP:C	1:A:98:LEU:HD12	2.36	0.45
1:B:23:ASN:C	1:B:25:GLU:H	2.17	0.45
1:A:19:PHE:O	1:A:31:ALA:HA	2.16	0.45
1:A:109:GLN:HE22	1:A:139:GLU:HA	1.81	0.45
1:A:155:VAL:HG12	1:A:156:ARG:N	2.32	0.45
1:B:153:ILE:HG13	2:E:276:ASN:HA	1.99	0.45
2:D:185:LEU:HD13	2:D:247:PRO:HG3	1.98	0.45
1:B:223:THR:OG1	1:B:226:GLN:HG3	2.17	0.44
1:B:23:ASN:ND2	1:B:26:THR:OG1	2.51	0.44
1:A:120:ARG:O	1:A:121:ASN:HB2	2.18	0.44
1:A:197:ASN:CG	1:A:198:ALA:N	2.70	0.44
2:D:184:SER:C	2:D:186:LEU:N	2.69	0.44
2:D:186:LEU:HA	2:D:186:LEU:HD23	1.76	0.44
2:E:280:HIS:O	2:E:284:GLN:HG3	2.17	0.44
1:B:236:TYR:C	1:B:236:TYR:CD1	2.91	0.44
1:B:107:LEU:HD22	1:B:192:PHE:CG	2.52	0.44
2:D:174:PRO:HA	2:D:177:TRP:CE3	2.52	0.44
2:E:151:LEU:O	2:E:154:CYS:HB2	2.18	0.44
1:A:202:LEU:HD11	1:A:251:VAL:HG21	2.00	0.44
1:B:219:LEU:CA	1:B:246:THR:HG22	2.43	0.44
2:E:265:ILE:O	2:E:269:SER:HB3	2.18	0.43
2:E:162:ARG:HD3	2:E:214:SER:HB3	2.00	0.43
1:A:16:GLY:HA3	1:A:34:ARG:O	2.18	0.43
1:A:15:TYR:N	1:A:15:TYR:CD1	2.86	0.43
1:B:227:TRP:N	1:B:228:PRO:HD3	2.33	0.43
1:B:237:LYS:HA	1:B:238:PRO:HD3	1.85	0.43
2:E:180:SER:O	2:E:183:ARG:HB3	2.17	0.43
1:B:221:THR:HA	1:B:222:PRO:HD3	1.82	0.43
2:D:169:LEU:HD21	2:D:174:PRO:HD3	2.01	0.43
1:B:57:GLU:OE2	2:E:269:SER:OG	2.37	0.43
1:A:91:PHE:CD1	1:A:199:ALA:HB1	2.53	0.43
1:A:253:PRO:C	1:A:255:LEU:H	2.22	0.43
1:A:23:ASN:HD22	1:A:26:THR:CG2	2.32	0.43
2:D:210:ASP:HB2	2:D:268:MET:HE1	2.00	0.43
1:B:231:THR:HG22	1:B:236:TYR:CE1	2.54	0.43
1:A:23:ASN:HD22	1:A:26:THR:CB	2.32	0.43
2:E:260:ARG:O	2:E:264:VAL:HG23	2.19	0.43
1:A:194:GLU:O	1:A:199:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PRO:HG3	1:A:183:ILE:HG13	2.01	0.43
1:B:83:CYS:HA	1:B:135:ASN:HD21	1.84	0.43
2:D:250:VAL:HG12	2:D:250:VAL:O	2.19	0.43
2:D:228:THR:HG21	2:D:260:ARG:HB3	2.01	0.42
1:A:244:ALA:C	1:A:246:THR:N	2.72	0.42
2:E:171:PRO:O	2:E:174:PRO:HD2	2.19	0.42
1:A:237:LYS:HA	1:A:238:PRO:HD3	1.87	0.42
1:A:202:LEU:CD1	1:A:251:VAL:HG21	2.49	0.42
1:A:63:ILE:HG12	1:A:142:LEU:HD12	2.01	0.42
1:B:258:THR:HG23	1:B:259:GLY:N	2.34	0.42
1:B:220:GLY:HA3	1:B:244:ALA:HA	2.00	0.42
2:D:156:GLY:O	2:D:157:GLU:C	2.57	0.42
1:B:180:SER:O	1:B:183:ILE:HG22	2.20	0.42
1:A:244:ALA:O	1:A:246:THR:HG22	2.20	0.42
2:D:206:MET:CE	2:D:268:MET:HE3	2.49	0.42
2:D:251:GLU:OE1	2:D:260:ARG:NH2	2.48	0.42
1:B:246:THR:C	1:B:248:LEU:N	2.73	0.42
1:A:178:LEU:C	1:A:178:LEU:HD23	2.40	0.42
1:A:21:ALA:O	1:A:29:ILE:HG23	2.20	0.42
2:D:165:ARG:HG2	2:D:165:ARG:O	2.20	0.42
2:D:262:LEU:HD23	2:D:262:LEU:HA	1.86	0.41
2:E:188:GLN:OE1	2:E:188:GLN:HA	2.20	0.41
1:A:26:THR:O	1:A:27:HIS:CG	2.72	0.41
2:D:166:LEU:C	2:D:168:HIS:H	2.22	0.41
1:B:9:LYS:HA	1:B:19:PHE:HA	2.01	0.41
1:B:78:LEU:HD23	1:B:78:LEU:N	2.35	0.41
2:D:238:GLY:HA3	2:D:243:TYR:HE1	1.84	0.41
1:B:223:THR:HG22	1:B:241:MET:HE3	2.02	0.41
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.83	0.41
1:B:249:VAL:HG22	1:B:260:ARG:CD	2.50	0.41
2:D:186:LEU:HD23	2:D:191:GLN:HG3	2.01	0.41
1:A:193:ALA:CB	1:A:202:LEU:HD22	2.50	0.41
1:A:30:VAL:HB	1:A:80:PHE:O	2.20	0.41
1:B:10:ILE:N	1:B:18:VAL:O	2.54	0.41
1:B:219:LEU:HD21	1:B:267:LEU:HB3	2.01	0.41
1:B:98:LEU:H	1:B:98:LEU:HD12	1.86	0.41
1:A:51:GLU:HG2	1:A:55:LEU:HD22	2.01	0.41
1:A:53:CYS:SG	2:D:265:ILE:HG12	2.61	0.41
1:B:270:ASN:C	1:B:270:ASN:ND2	2.74	0.41
1:A:23:ASN:O	1:A:25:GLU:N	2.43	0.41
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HD12	1:B:142:LEU:HD11	2.02	0.41
1:A:173:LEU:C	1:A:175:GLY:H	2.23	0.41
1:B:84:ASP:OD2	1:B:135:ASN:HA	2.20	0.41
1:A:54:LEU:O	1:A:58:LEU:HG	2.20	0.41
2:D:227:LEU:HD12	2:D:227:LEU:HA	1.80	0.41
2:D:180:SER:O	2:D:183:ARG:HB3	2.21	0.41
1:A:136:ARG:C	1:A:138:GLY:N	2.74	0.41
2:E:181:VAL:HB	2:E:247:PRO:HB2	2.02	0.41
1:A:156:ARG:HD2	2:D:193:GLN:NE2	2.37	0.40
1:B:230:MET:HG3	1:B:231:THR:N	2.36	0.40
2:D:222:LEU:O	2:D:225:VAL:HG12	2.21	0.40
1:A:130:GLN:N	1:A:130:GLN:OE1	2.45	0.40
1:A:153:ILE:HG21	2:D:199:ALA:HB1	2.03	0.40
1:A:156:ARG:CD	2:D:193:GLN:NE2	2.85	0.40
2:D:181:VAL:O	2:D:185:LEU:HB2	2.21	0.40
2:D:183:ARG:O	2:D:186:LEU:HB2	2.22	0.40
1:A:227:TRP:CE3	1:A:230:MET:HE3	2.56	0.40
2:D:203:PHE:O	2:D:206:MET:HB3	2.21	0.40
1:B:233:LEU:HA	1:B:234:PRO:HD3	1.90	0.40
1:B:265:ASN:HB3	1:B:275:ILE:HB	2.03	0.40
2:E:225:VAL:HG13	2:E:226:LEU:N	2.36	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	272/292 (93%)	228 (84%)	34 (12%)	10 (4%)	4 8
1	B	272/292 (93%)	236 (87%)	25 (9%)	11 (4%)	4 7
2	D	145/147 (99%)	124 (86%)	16 (11%)	5 (3%)	5 9
2	E	145/147 (99%)	132 (91%)	11 (8%)	2 (1%)	14 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	834/878 (95%)	720 (86%)	86 (10%)	28 (3%)	5 9

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ARG
1	B	197	ASN
1	B	246	THR
1	B	248	LEU
2	D	148	THR
2	D	188	GLN
1	A	16	GLY
1	A	34	ARG
1	A	96	GLY
1	A	163	VAL
1	A	198	ALA
1	B	16	GLY
1	B	93	SER
1	B	163	VAL
2	D	149	SER
2	E	191	GLN
1	A	3	LYS
1	A	246	THR
1	B	245	THR
1	B	254	LYS
2	D	218	SER
1	A	245	THR
2	E	190	TRP
1	A	93	SER
1	B	154	PRO
1	A	154	PRO
2	D	196	ILE
1	B	234	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	248/260 (95%)	240 (97%)	8 (3%)	46 74
1	B	248/260 (95%)	235 (95%)	13 (5%)	29 54
2	D	137/138 (99%)	133 (97%)	4 (3%)	50 77
2	E	137/138 (99%)	125 (91%)	12 (9%)	12 25
All	All	770/796 (97%)	733 (95%)	37 (5%)	31 59

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	130	GLN
1	A	132	LEU
1	A	147	LEU
1	A	195	LEU
1	A	219	LEU
1	A	258	THR
1	A	270	ASN
1	B	17	THR
1	B	55	LEU
1	B	78	LEU
1	B	98	LEU
1	B	100	PRO
1	B	130	GLN
1	B	137	ASN
1	B	139	GLU
1	B	173	LEU
1	B	195	LEU
1	B	247	SER
1	B	258	THR
1	B	270	ASN
2	D	150	GLU
2	D	155	LEU
2	D	169	LEU
2	D	227	LEU
2	E	150	GLU
2	E	155	LEU
2	E	181	VAL
2	E	186	LEU
2	E	190	TRP
2	E	193	GLN
2	E	204	LEU
2	E	227	LEU

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Mol	Chain	Res	Type
2	E	240	GLU
2	E	246	LYS
2	E	267	LEU
2	E	269	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	62	ASN
1	A	67	HIS
1	A	71	HIS
1	A	121	ASN
1	A	131	ASN
1	A	135	ASN
1	A	250	ASN
1	A	270	ASN
1	A	282	GLN
1	B	23	ASN
1	B	62	ASN
1	B	71	HIS
1	B	121	ASN
1	B	131	ASN
1	B	135	ASN
1	B	206	ASN
1	B	226	GLN
1	B	270	ASN
1	B	282	GLN
2	D	188	GLN
2	D	193	GLN
2	D	200	ASN
2	D	223	GLN
2	E	200	ASN
2	E	223	GLN
2	E	274	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	278/292 (95%)	-0.30	5 (1%)	71	70	26, 48, 110, 174	0
1	B	278/292 (95%)	-0.26	5 (1%)	71	70	25, 50, 114, 169	0
2	D	147/147 (100%)	-0.17	3 (2%)	68	67	32, 59, 113, 175	0
2	E	147/147 (100%)	-0.24	3 (2%)	68	67	30, 50, 102, 164	0
All	All	850/878 (96%)	-0.25	16 (1%)	70	69	25, 51, 113, 175	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	189	GLY	5.2
2	E	189	GLY	3.6
2	E	188	GLN	3.3
1	A	96	GLY	3.0
2	D	188	GLN	2.9
2	D	190	TRP	2.9
1	B	15	TYR	2.8
1	A	245	THR	2.8
1	B	154	PRO	2.7
1	A	154	PRO	2.6
1	B	2	GLN	2.5
1	B	156	ARG	2.4
1	A	74	LYS	2.3
2	E	190	TRP	2.3
1	B	254	LYS	2.2
1	A	246	THR	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.