Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:36 AM GMT

PDB ID	:	3PCS
Title	:	Structure of EspG-PAK2 autoinhibitory Ialpha3 helix complex
Authors	:	Tomchick, D.R.; Alto, N.M.; Selyunin, A.S.
Deposited on	:	2010-10-21
Resolution	:	2.86 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:

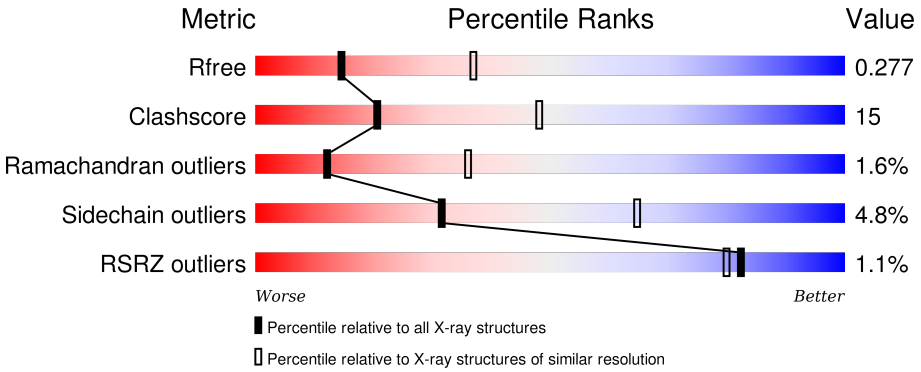
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.86 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	357	65% 30%
1	B	357	67% 30%
1	C	357	67% 28%
1	D	357	67% 31%
2	E	16	63% 25% 13%

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Mol	Chain	Length	Quality of chain
2	F	16	63% 13% 25%
2	G	16	25% 31% 6% 38%
2	H	16	38% 38% 6% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11254 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 EspG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2719	1688	478	539	14			
1	B	355	Total	C	N	O	S	0	0	0
			2757	1709	482	551	15			
1	C	345	Total	C	N	O	S	0	0	0
			2678	1666	468	530	14			
1	D	348	Total	C	N	O	S	0	0	0
			2704	1680	474	536	14			

- Molecule 2 is a protein called Serine/threonine-protein kinase PAK 2.

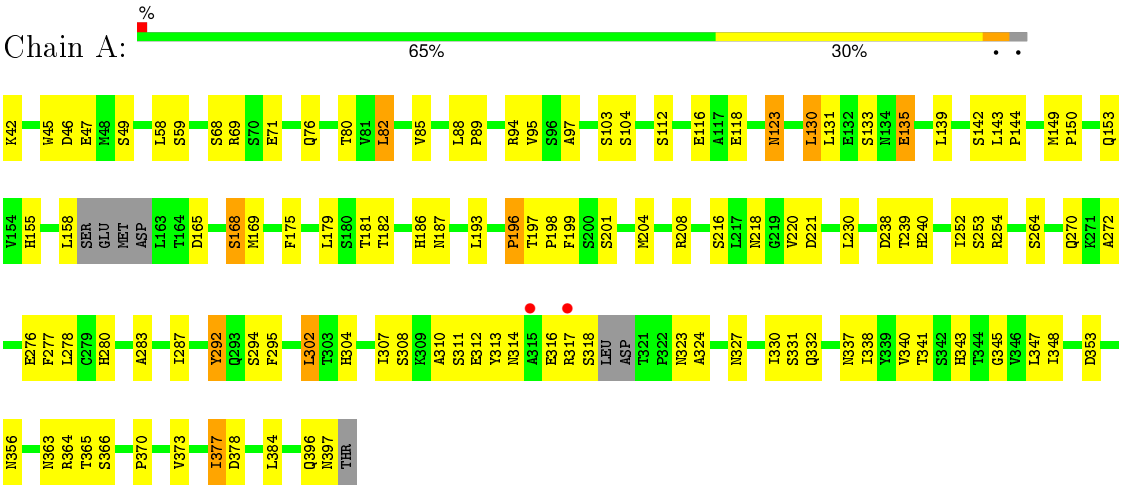
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	0	0	0
			111	73	16	22			
2	F	12	Total	C	N	O	0	0	0
			97	64	14	19			
2	G	10	Total	C	N	O	0	0	0
			84	57	11	16			
2	H	13	Total	C	N	O	0	0	0
			104	68	15	21			

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.

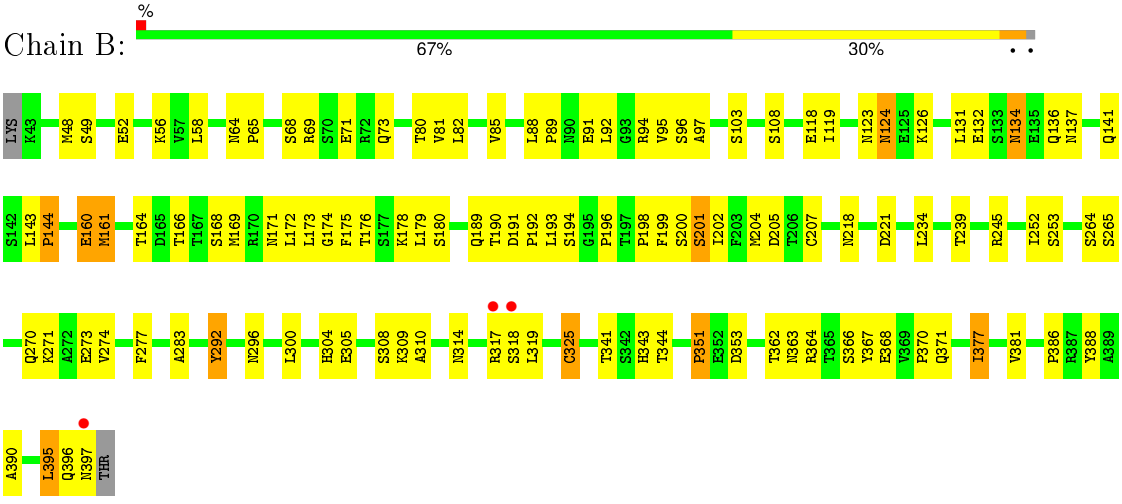
- Molecule 1: EspG

Chain A:



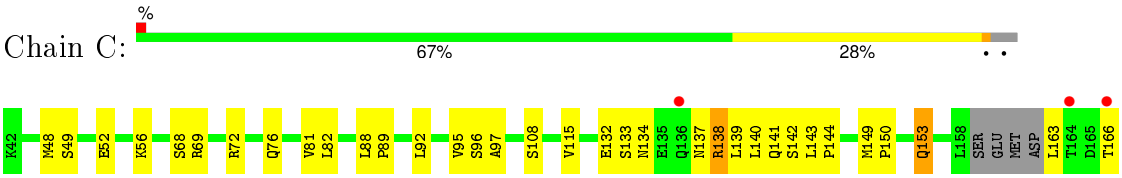
- Molecule 1: EspG

Chain B:

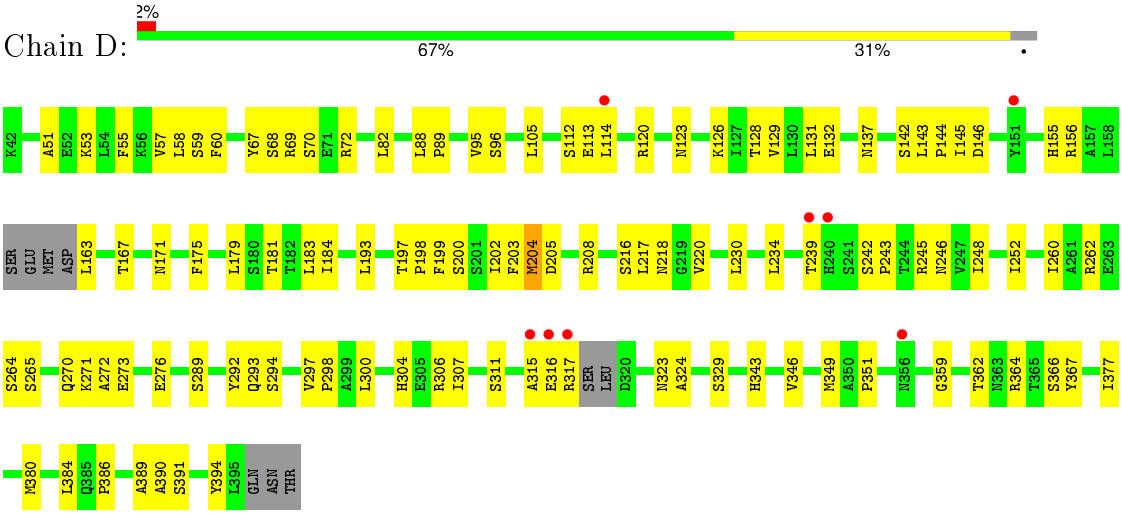


- Molecule 1: EspG

Chain C:



• Molecule 1: EspG



• Molecule 2: Serine/threonine-protein kinase PAK 2

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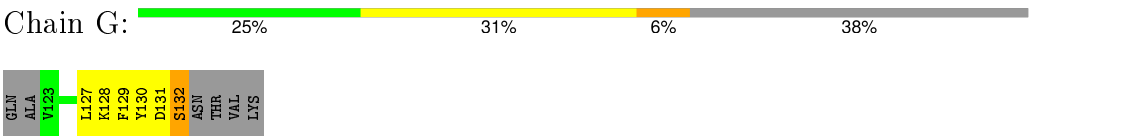
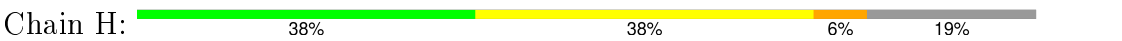


• Molecule 2: Serine/threonine-protein kinase PAK 2




GLN
A122
V123
V126
L127
K128
D131
S132
N133
T134
VAL
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.72Å 104.60Å 191.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.50 – 2.86 40.50 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.50-2.86) 99.1 (40.50-2.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.191 , 0.281 0.183 , 0.277	Depositor DCC
R_{free} test set	2033 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 44193 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11254	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.45	0/2767	0.66	0/3753
1	B	0.42	0/2807	0.63	0/3811
1	C	0.37	0/2726	0.58	0/3697
1	D	0.40	0/2752	0.58	0/3733
2	E	0.51	0/112	0.65	0/152
2	F	0.35	0/98	0.63	0/132
2	G	0.45	0/85	0.54	0/114
2	H	0.34	0/105	0.63	0/142
All	All	0.41	0/11452	0.61	0/15534

There are no bond length outliers.

There are no bond angle outliers.

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	2719	0	2686	89	0
1	B	2757	0	2714	90	0
1	C	2678	0	2648	78	0
1	D	2704	0	2671	78	0
2	E	111	0	110	3	0
2	F	97	0	94	1	0
2	G	84	0	83	7	0
2	H	104	0	101	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11254	0	11107	325	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 15.

All (325) 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:B:204:MET:HG3	1:B:239:THR:CG2	1.98	0.93
1:C:153:GLN:HE21	1:C:153:GLN:HA	1.35	0.90
1:D:82:LEU:HG	1:D:95:VAL:HG11	1.57	0.86
1:C:367:TYR:HB3	1:C:386:PRO:HA	1.61	0.82
1:B:189:GLN:HE22	1:C:305:GLU:HB2	1.46	0.79
1:A:88:LEU:HB3	1:A:89:PRO:HD2	1.64	0.77
1:A:150:PRO:HB2	1:D:262:ARG:HD2	1.66	0.76
1:B:82:LEU:HD12	1:B:97:ALA:HB2	1.68	0.76
1:B:396:GLN:O	1:B:397:ASN:HB2	1.85	0.76
1:C:197:THR:HB	1:C:200:SER:HB3	1.69	0.75
1:D:204:MET:HG3	1:D:239:THR:CG2	2.18	0.74
1:A:356:ASN:HD22	1:D:123:ASN:HA	1.53	0.73
1:A:330:ILE:HG12	1:A:340:VAL:HG22	1.71	0.73
1:D:264:SER:O	1:D:271:LYS:HE2	1.88	0.73
1:A:155:HIS:CE1	1:A:179:LEU:HB3	2.24	0.72
1:A:343:HIS:CD2	1:A:364:ARG:HG3	2.25	0.72
1:B:204:MET:HG3	1:B:239:THR:HG21	1.71	0.72
1:B:221:ASP:O	1:B:264:SER:HB3	1.90	0.71
1:C:144:PRO:HG3	1:C:178:LYS:HA	1.73	0.71
1:A:343:HIS:NE2	1:A:364:ARG:HG3	2.06	0.71
1:B:204:MET:HG3	1:B:239:THR:HG22	1.72	0.70
1:A:150:PRO:CB	1:D:262:ARG:HD2	2.22	0.70
1:B:189:GLN:HE22	1:C:305:GLU:CB	2.03	0.70
1:A:82:LEU:HG	1:A:95:VAL:HG11	1.73	0.70
1:C:343:HIS:CD2	1:C:364:ARG:HG3	2.27	0.69
1:A:68:SER:O	1:A:69:ARG:HB3	1.92	0.69
1:C:82:LEU:HG	1:C:95:VAL:HG11	1.74	0.68
1:B:68:SER:O	1:B:69:ARG:HB3	1.93	0.68
1:D:82:LEU:HG	1:D:95:VAL:CG1	2.24	0.68
1:B:192:PRO:HG2	1:B:388:TYR:OH	1.94	0.67
2:H:123:VAL:O	2:H:126:VAL:HG22	1.95	0.66
1:C:212:ASN:HB3	2:G:130:TYR:CD2	2.32	0.65
1:B:88:LEU:HB3	1:B:89:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:TYR:HB3	1:B:386:PRO:HA	1.77	0.65
1:B:314:ASN:O	1:B:319:LEU:HB2	1.96	0.65
1:A:196:PRO:C	1:A:198:PRO:HD3	2.18	0.64
1:B:198:PRO:O	1:B:199:PHE:HB2	1.97	0.64
1:D:292:TYR:CE2	1:D:294:SER:HB2	2.33	0.63
1:A:198:PRO:O	1:A:199:PHE:HB2	1.97	0.63
1:A:197:THR:O	1:A:197:THR:HG23	1.98	0.63
1:B:343:HIS:CD2	1:B:364:ARG:HG3	2.35	0.62
1:C:177:SER:HB2	1:C:343:HIS:CE1	2.35	0.62
1:A:82:LEU:HG	1:A:95:VAL:CG1	2.29	0.62
1:D:69:ARG:HA	1:D:72:ARG:HB2	1.81	0.62
1:D:300:LEU:O	1:D:304:HIS:HB3	2.00	0.62
1:C:82:LEU:HG	1:C:95:VAL:CG1	2.30	0.61
1:C:153:GLN:NE2	1:C:153:GLN:HA	2.13	0.61
1:D:88:LEU:HB3	1:D:89:PRO:CD	2.31	0.61
1:A:341:THR:HG22	1:A:343:HIS:CE1	2.36	0.61
1:A:142:SER:O	1:A:143:LEU:HD23	2.01	0.60
1:A:356:ASN:ND2	1:D:123:ASN:HA	2.15	0.60
1:A:68:SER:OG	1:A:71:GLU:HG3	2.01	0.60
1:A:45:TRP:CZ3	1:A:46:ASP:HB3	2.38	0.59
1:D:95:VAL:HG21	1:D:144:PRO:HD2	1.85	0.59
2:E:123:VAL:O	2:E:126:VAL:HG22	2.03	0.59
1:B:305:GLU:HB2	1:C:189:GLN:HE22	1.68	0.59
1:D:205:ASP:CG	1:D:293:GLN:HG3	2.23	0.59
1:D:146:ASP:HB3	1:D:183:LEU:HD21	1.85	0.59
1:B:48:MET:CE	1:B:56:LYS:HD3	2.33	0.59
1:D:58:LEU:CD2	1:D:142:SER:HB3	2.33	0.58
1:C:115:VAL:HG11	1:C:139:LEU:HD21	1.84	0.58
1:B:134:ASN:HB2	1:B:136:GLN:H	1.68	0.58
1:A:186:HIS:CD2	1:B:69:ARG:HB2	2.39	0.58
1:B:193:LEU:HD21	1:B:199:PHE:CE2	2.38	0.58
1:D:220:VAL:HG23	1:D:270:GLN:HB3	1.86	0.58
1:B:308:SER:C	1:B:310:ALA:H	2.07	0.58
1:D:198:PRO:O	1:D:199:PHE:HB2	2.04	0.57
1:B:161:MET:O	1:B:161:MET:CG	2.52	0.57
1:B:85:VAL:CG2	1:B:94:ARG:HG2	2.34	0.57
1:D:218:ASN:HD22	1:D:273:GLU:HB3	1.69	0.57
1:B:201:SER:HB2	1:B:205:ASP:OD2	2.05	0.57
1:B:161:MET:HB2	1:B:395:LEU:HD22	1.84	0.57
1:B:218:ASN:HD22	1:B:273:GLU:HB3	1.70	0.57
1:A:133:SER:HA	1:D:246:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ALA:C	1:D:317:ARG:H	2.07	0.56
1:C:69:ARG:HA	1:C:72:ARG:HB2	1.86	0.56
1:C:193:LEU:HD21	1:C:199:PHE:CE2	2.41	0.56
1:A:58:LEU:HB3	1:A:139:LEU:CD1	2.35	0.55
1:B:234:LEU:HD23	1:B:252:ILE:HD11	1.88	0.55
1:B:48:MET:HE1	1:B:56:LYS:HD3	1.88	0.55
1:B:161:MET:CB	1:B:395:LEU:HD22	2.36	0.55
1:D:343:HIS:NE2	1:D:364:ARG:HG3	2.21	0.55
1:B:137:ASN:OD1	1:B:137:ASN:O	2.25	0.55
1:C:300:LEU:O	1:C:304:HIS:HB3	2.07	0.55
1:D:68:SER:C	1:D:70:SER:H	2.10	0.55
1:A:58:LEU:HB3	1:A:139:LEU:HD12	1.87	0.55
1:B:296:ASN:O	1:B:300:LEU:HG	2.07	0.55
1:B:179:LEU:O	1:B:364:ARG:NH2	2.26	0.55
1:C:324:ALA:O	2:G:129:PHE:HA	2.06	0.55
1:A:165:ASP:OD1	1:A:168:SER:HB2	2.07	0.55
1:B:173:LEU:HD23	1:B:325:CYS:HB2	1.88	0.54
1:C:212:ASN:HB3	2:G:130:TYR:HD2	1.69	0.54
1:A:153:GLN:CG	1:A:155:HIS:HE2	2.21	0.54
1:D:179:LEU:O	1:D:364:ARG:NH2	2.33	0.54
2:F:123:VAL:O	2:F:126:VAL:HG22	2.07	0.54
1:A:116:GLU:HG3	1:A:130:LEU:CD1	2.37	0.54
1:A:116:GLU:HG3	1:A:130:LEU:HD11	1.88	0.54
1:C:307:ILE:O	1:C:310:ALA:HB3	2.08	0.54
1:B:80:THR:HA	1:B:178:LYS:HD2	1.89	0.54
1:B:118:GLU:OE1	1:B:126:LYS:HE2	2.07	0.54
1:C:192:PRO:HG2	1:C:388:TYR:OH	2.08	0.53
1:D:362:THR:O	1:D:390:ALA:HA	2.07	0.53
1:A:272:ALA:O	1:A:276:GLU:HG2	2.09	0.53
1:B:377:ILE:O	1:B:381:VAL:HG23	2.08	0.53
1:B:308:SER:C	1:B:310:ALA:N	2.62	0.53
1:C:88:LEU:HB3	1:C:89:PRO:CD	2.39	0.53
1:B:252:ILE:HG22	1:B:253:SER:O	2.08	0.52
1:C:197:THR:HB	1:C:200:SER:CB	2.38	0.52
1:C:82:LEU:HD12	1:C:97:ALA:HB2	1.92	0.52
1:C:68:SER:O	1:C:69:ARG:HB3	2.10	0.52
1:B:308:SER:O	1:B:310:ALA:N	2.42	0.52
1:C:177:SER:HB2	1:C:343:HIS:ND1	2.24	0.52
1:B:95:VAL:HG12	1:B:96:SER:N	2.25	0.52
1:B:192:PRO:HG2	1:B:388:TYR:CZ	2.45	0.52
1:D:204:MET:HG3	1:D:239:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TYR:CZ	1:D:294:SER:HB2	2.44	0.52
1:B:161:MET:HB2	1:B:395:LEU:HD13	1.91	0.52
1:B:190:THR:O	1:B:192:PRO:HD3	2.10	0.52
1:D:323:ASN:HB3	2:H:128:LYS:H	1.75	0.52
1:B:175:PHE:CE2	1:B:179:LEU:HD11	2.45	0.52
1:B:296:ASN:OD1	1:B:344:THR:HB	2.09	0.52
1:D:155:HIS:O	1:D:156:ARG:HD3	2.10	0.52
1:D:359:GLY:HA3	1:D:394:TYR:CD1	2.45	0.52
1:B:82:LEU:HG	1:B:95:VAL:CG1	2.40	0.51
1:A:238:ASP:OD2	1:A:240:HIS:NE2	2.43	0.51
1:C:209:GLY:HA3	1:C:291:PHE:CE1	2.45	0.51
1:C:166:THR:HG21	1:C:322:PRO:HG2	1.92	0.51
1:B:82:LEU:HG	1:B:95:VAL:HG11	1.92	0.51
1:A:204:MET:O	1:A:208:ARG:HG2	2.10	0.51
1:D:146:ASP:HB3	1:D:183:LEU:CD2	2.40	0.51
1:D:243:PRO:HB2	1:D:248:ILE:HG13	1.93	0.51
1:A:230:LEU:HD21	1:A:287:ILE:HD13	1.93	0.51
1:B:141:GLN:HA	1:B:180:SER:OG	2.11	0.51
1:A:149:MET:HB3	1:A:182:THR:HG23	1.92	0.51
1:D:343:HIS:CD2	1:D:364:ARG:HG3	2.46	0.51
2:E:124:LEU:H	2:E:124:LEU:HD12	1.75	0.51
1:C:307:ILE:HD13	1:C:346:VAL:HG11	1.92	0.51
1:A:196:PRO:O	1:A:198:PRO:HD3	2.12	0.50
1:C:306:ARG:HD2	1:C:349:MET:O	2.11	0.50
1:B:123:ASN:O	1:B:124:ASN:HB3	2.12	0.50
1:D:324:ALA:HB2	1:D:346:VAL:HG22	1.93	0.50
1:D:204:MET:O	1:D:208:ARG:HG2	2.12	0.50
1:D:181:THR:HG23	1:D:364:ARG:NH2	2.26	0.50
1:D:220:VAL:CG2	1:D:270:GLN:HB3	2.41	0.50
1:B:131:LEU:HD12	1:B:132:GLU:H	1.76	0.50
1:B:199:PHE:CE1	1:B:292:TYR:CD2	2.99	0.50
1:A:295:PHE:CG	1:A:365:THR:HG21	2.47	0.50
1:D:53:LYS:O	1:D:57:VAL:HG23	2.12	0.50
1:B:264:SER:O	1:B:271:LYS:HE2	2.12	0.50
1:A:169:MET:HG3	1:A:347:LEU:HD21	1.93	0.50
1:A:396:GLN:O	1:A:397:ASN:HB3	2.12	0.49
1:A:254:ARG:NH2	1:A:276:GLU:OE1	2.45	0.49
1:D:120:ARG:NH2	1:D:126:LYS:HD2	2.27	0.49
1:A:304:HIS:HA	1:A:307:ILE:HD12	1.94	0.49
1:B:381:VAL:O	1:B:381:VAL:HG12	2.12	0.49
1:B:368:GLU:O	1:B:370:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:HG3	1:C:239:THR:HG23	1.94	0.49
1:B:317:ARG:HB2	1:B:319:LEU:HG	1.94	0.49
1:C:297:VAL:HB	1:C:298:PRO:HD3	1.95	0.49
1:B:49:SER:HB2	1:B:103:SER:HB3	1.95	0.49
1:A:82:LEU:HD13	1:A:97:ALA:HB2	1.94	0.48
1:D:300:LEU:HD11	2:H:127:LEU:HG	1.95	0.48
1:D:175:PHE:CE2	1:D:179:LEU:HD11	2.48	0.48
1:A:307:ILE:HG13	1:A:348:ILE:HD12	1.95	0.48
1:C:138:ARG:HD3	1:C:141:GLN:HE22	1.78	0.48
1:A:323:ASN:HB3	2:E:128:LYS:H	1.79	0.48
1:A:252:ILE:HG22	1:A:253:SER:O	2.13	0.48
1:A:295:PHE:CD1	1:A:365:THR:HG21	2.48	0.48
1:D:145:ILE:HG13	1:D:145:ILE:O	2.12	0.48
1:B:189:GLN:NE2	1:C:305:GLU:HB2	2.24	0.48
1:B:270:GLN:O	1:B:273:GLU:HB2	2.14	0.48
1:D:60:PHE:HD2	1:D:67:TYR:OH	1.96	0.48
1:A:49:SER:HB2	1:A:103:SER:HB3	1.95	0.48
1:A:131:LEU:HD22	1:A:135:GLU:HB2	1.95	0.48
1:A:82:LEU:CD1	1:A:97:ALA:HB2	2.43	0.48
1:B:343:HIS:HA	1:B:363:ASN:O	2.14	0.48
1:C:286:ALA:HB1	1:C:330:ILE:HD13	1.96	0.48
1:C:378:ASP:N	1:C:378:ASP:OD1	2.40	0.48
2:G:131:ASP:O	2:G:132:SER:C	2.52	0.48
1:A:181:THR:HG23	1:A:364:ARG:NH2	2.29	0.47
1:D:167:THR:O	1:D:171:ASN:ND2	2.47	0.47
1:A:197:THR:N	1:A:198:PRO:HD3	2.28	0.47
1:B:161:MET:O	1:B:161:MET:HG2	2.12	0.47
1:A:123:ASN:N	1:A:123:ASN:OD1	2.48	0.47
1:A:343:HIS:HA	1:A:363:ASN:O	2.15	0.47
1:C:324:ALA:HB2	2:G:127:LEU:HD22	1.96	0.47
1:B:52:GLU:HA	1:B:119:ILE:HD13	1.96	0.47
1:A:153:GLN:HG2	1:A:155:HIS:HE2	1.79	0.47
1:A:45:TRP:CE3	1:A:46:ASP:HB3	2.49	0.47
1:B:172:LEU:O	1:B:176:THR:HG23	2.14	0.47
1:C:202:ILE:HD11	1:C:289:SER:N	2.29	0.47
1:A:204:MET:HG3	1:A:239:THR:HG22	1.95	0.47
1:D:137:ASN:CG	1:D:137:ASN:O	2.53	0.47
1:D:193:LEU:HD21	1:D:199:PHE:CE2	2.49	0.47
1:A:317:ARG:O	1:A:318:SER:C	2.52	0.47
1:C:149:MET:HB3	1:C:150:PRO:HD2	1.97	0.46
1:D:306:ARG:HD2	1:D:349:MET:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:CE2	1:A:179:LEU:HD11	2.50	0.46
1:D:242:SER:HB2	1:D:243:PRO:HD2	1.97	0.46
1:A:370:PRO:O	1:A:373:VAL:HG23	2.15	0.46
1:B:351:PRO:HB2	1:B:353:ASP:OD1	2.15	0.46
1:A:221:ASP:O	1:A:264:SER:HB3	2.14	0.46
1:D:197:THR:HB	1:D:200:SER:HB3	1.98	0.46
1:A:308:SER:O	1:A:312:GLU:HG3	2.16	0.46
1:A:186:HIS:NE2	1:B:69:ARG:HG3	2.31	0.46
1:A:277:PHE:O	1:A:280:HIS:HB2	2.15	0.46
1:B:160:GLU:HG3	1:B:161:MET:N	2.30	0.46
1:C:366:SER:O	1:C:387:ARG:HG2	2.16	0.45
1:B:68:SER:H	1:B:71:GLU:HB2	1.80	0.45
1:C:115:VAL:HG11	1:C:139:LEU:CD2	2.45	0.45
1:C:169:MET:HG3	1:C:347:LEU:HD21	1.96	0.45
1:D:156:ARG:HA	1:D:394:TYR:O	2.17	0.45
1:A:85:VAL:CG2	1:A:94:ARG:HG2	2.46	0.45
1:C:48:MET:CE	1:C:56:LYS:HE2	2.46	0.45
1:D:51:ALA:HB1	1:D:105:LEU:HB2	1.99	0.45
1:A:88:LEU:HB3	1:A:89:PRO:CD	2.38	0.45
1:A:130:LEU:N	1:A:130:LEU:HD13	2.31	0.45
1:A:316:GLU:C	1:A:317:ARG:HG3	2.37	0.45
1:D:367:TYR:HB3	1:D:386:PRO:HA	1.98	0.45
1:B:191:ASP:HA	1:B:192:PRO:HD2	1.82	0.45
1:C:193:LEU:HD21	1:C:199:PHE:CZ	2.51	0.45
1:D:184:ILE:HG13	1:D:389:ALA:HA	1.98	0.45
1:C:172:LEU:O	1:C:175:PHE:HB3	2.17	0.45
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.54	0.45
1:B:305:GLU:HB2	1:C:189:GLN:NE2	2.31	0.44
1:C:202:ILE:HG23	1:C:203:PHE:CD1	2.52	0.44
1:C:133:SER:CB	1:C:140:LEU:HG	2.48	0.44
1:A:343:HIS:NE2	1:A:364:ARG:NH1	2.59	0.44
1:C:173:LEU:C	1:C:175:PHE:N	2.70	0.44
1:D:230:LEU:HA	1:D:260:ILE:HD11	1.99	0.44
1:A:324:ALA:HA	1:A:345:GLY:O	2.17	0.44
2:H:131:ASP:HB3	2:H:134:THR:HG23	1.99	0.44
1:C:224:ALA:HA	1:C:227:GLN:HB2	2.00	0.44
1:A:149:MET:HA	1:A:150:PRO:HD3	1.76	0.44
1:C:177:SER:HB2	1:C:343:HIS:CG	2.53	0.44
1:C:366:SER:HB2	1:C:387:ARG:HE	1.82	0.44
1:B:366:SER:O	1:B:367:TYR:HB3	2.17	0.44
1:C:76:GLN:HE21	1:C:76:GLN:HB3	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:HA	1:D:246:ASN:ND2	2.31	0.44
1:C:132:GLU:O	1:C:137:ASN:ND2	2.52	0.43
1:C:137:ASN:O	1:C:139:LEU:N	2.40	0.43
1:B:123:ASN:O	1:B:124:ASN:CB	2.66	0.43
1:B:199:PHE:O	1:B:200:SER:C	2.56	0.43
1:C:95:VAL:HG21	1:C:144:PRO:HD2	1.99	0.43
1:D:307:ILE:HD13	1:D:346:VAL:HG11	2.00	0.43
1:D:131:LEU:HD12	1:D:132:GLU:H	1.83	0.43
1:C:355:PRO:O	1:C:356:ASN:HB2	2.17	0.43
1:A:218:ASN:OD1	1:A:331:SER:HA	2.18	0.43
1:C:293:GLN:OE1	2:G:129:PHE:CE2	2.72	0.43
1:D:58:LEU:HD22	1:D:142:SER:HB3	2.00	0.43
1:A:88:LEU:CB	1:A:89:PRO:HD2	2.41	0.43
1:A:384:LEU:HD23	1:A:384:LEU:N	2.33	0.43
1:D:297:VAL:O	1:D:298:PRO:C	2.55	0.43
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.80	0.43
1:A:292:TYR:CZ	1:A:294:SER:HB2	2.54	0.43
1:C:229:LEU:CD1	1:C:263:GLU:HG3	2.49	0.43
1:A:186:HIS:CG	1:B:69:ARG:HB2	2.54	0.43
1:B:166:THR:HG22	1:B:169:MET:CE	2.49	0.43
1:A:327:ASN:O	1:A:343:HIS:HB2	2.19	0.43
1:A:42:LYS:HE3	1:A:47:GLU:O	2.19	0.43
1:A:76:GLN:O	1:A:80:THR:HG23	2.17	0.43
1:A:153:GLN:CG	1:A:155:HIS:NE2	2.82	0.43
1:B:161:MET:HG3	1:B:395:LEU:HD13	2.00	0.43
1:A:143:LEU:HA	1:A:144:PRO:HD3	1.85	0.42
1:B:161:MET:N	1:B:161:MET:HE2	2.34	0.42
1:A:278:LEU:C	1:A:280:HIS:H	2.22	0.42
1:B:171:ASN:O	1:B:174:GLY:N	2.52	0.42
1:B:362:THR:O	1:B:390:ALA:HA	2.20	0.42
1:C:81:VAL:HG12	1:C:81:VAL:O	2.18	0.42
1:D:55:PHE:CZ	1:D:129:VAL:HG11	2.54	0.42
1:C:72:ARG:O	1:C:76:GLN:HG3	2.19	0.42
1:D:384:LEU:C	1:D:386:PRO:HD3	2.39	0.42
1:A:377:ILE:HG22	1:A:378:ASP:N	2.34	0.42
1:D:234:LEU:HD23	1:D:252:ILE:HD11	2.02	0.42
1:A:220:VAL:CG2	1:A:270:GLN:HB3	2.49	0.42
1:A:341:THR:CG2	1:A:343:HIS:CE1	3.02	0.42
1:C:173:LEU:C	1:C:175:PHE:H	2.22	0.42
1:D:88:LEU:HA	1:D:88:LEU:HD23	1.82	0.42
1:A:302:LEU:H	1:A:302:LEU:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:OE2	1:B:108:SER:OG	2.32	0.42
1:C:88:LEU:HB3	1:C:89:PRO:HD3	2.02	0.42
1:D:272:ALA:O	1:D:276:GLU:HG2	2.20	0.42
1:B:277:PHE:O	1:B:283:ALA:HB2	2.20	0.41
1:D:68:SER:O	1:D:69:ARG:HB3	2.20	0.41
1:B:166:THR:HG22	1:B:169:MET:HE3	2.02	0.41
1:C:343:HIS:NE2	1:C:364:ARG:HG3	2.36	0.41
1:D:315:ALA:C	1:D:317:ARG:N	2.71	0.41
1:B:300:LEU:O	1:B:304:HIS:HB3	2.21	0.41
1:D:205:ASP:OD1	1:D:293:GLN:HG3	2.21	0.41
1:B:351:PRO:HG3	1:C:188:ALA:HB3	2.02	0.41
1:C:310:ALA:HA	1:C:349:MET:HG2	2.01	0.41
1:C:326:ILE:HG22	1:C:327:ASN:N	2.35	0.41
1:C:323:ASN:N	2:G:128:LYS:O	2.53	0.41
1:A:332:GLN:HA	1:A:337:ASN:O	2.19	0.41
1:D:181:THR:HG22	1:D:391:SER:HB3	2.02	0.41
1:D:343:HIS:NE2	1:D:364:ARG:NH1	2.69	0.41
1:C:324:ALA:HA	1:C:345:GLY:O	2.21	0.41
1:D:216:SER:O	1:D:217:LEU:HD23	2.21	0.41
1:B:81:VAL:O	1:B:81:VAL:HG12	2.21	0.41
1:C:305:GLU:O	1:C:309:LYS:HG3	2.21	0.41
1:A:153:GLN:HG3	1:A:155:HIS:CD2	2.56	0.41
1:B:131:LEU:HD12	1:B:132:GLU:N	2.35	0.41
1:C:277:PHE:HE1	1:C:338:ILE:HD13	1.86	0.41
1:B:64:ASN:HA	1:B:65:PRO:HD3	1.85	0.41
1:D:289:SER:HB3	1:D:380:MET:HE1	2.01	0.41
1:C:277:PHE:O	1:C:283:ALA:HB2	2.21	0.41
1:C:282:GLU:HA	1:C:285:THR:OG1	2.20	0.41
1:C:52:GLU:O	1:C:56:LYS:HB2	2.21	0.41
1:D:59:SER:HB2	1:D:131:LEU:HD21	2.02	0.41
1:A:155:HIS:HE1	1:A:179:LEU:HB3	1.81	0.40
1:D:69:ARG:C	1:D:69:ARG:HD3	2.42	0.40
1:B:143:LEU:HA	1:B:144:PRO:HD3	1.94	0.40
1:B:189:GLN:HE22	1:C:305:GLU:HB3	1.84	0.40
1:B:274:VAL:O	1:B:277:PHE:HB3	2.21	0.40
1:A:310:ALA:O	1:A:314:ASN:HB2	2.21	0.40
1:D:143:LEU:HA	1:D:144:PRO:HD3	1.88	0.40
1:D:112:SER:O	1:D:114:LEU:N	2.54	0.40
1:C:82:LEU:HA	1:C:97:ALA:HB2	2.03	0.40
1:D:202:ILE:HG23	1:D:203:PHE:CD1	2.56	0.40
1:D:202:ILE:CG2	1:D:203:PHE:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:HA	1:D:82:LEU:HD12	1.86	0.40
1:A:155:HIS:ND1	1:A:179:LEU:HB3	2.37	0.40
1:B:161:MET:CB	1:B:395:LEU:HD13	2.49	0.40
1:A:283:ALA:O	1:A:287:ILE:HG13	2.21	0.40
1:C:207:CYS:SG	1:C:231:ARG:HD2	2.62	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	344/357 (96%)	312 (91%)	28 (8%)	4 (1%)	16	44
1	B	353/357 (99%)	314 (89%)	29 (8%)	10 (3%)	6	21
1	C	339/357 (95%)	313 (92%)	21 (6%)	5 (2%)	13	38
1	D	342/357 (96%)	308 (90%)	30 (9%)	4 (1%)	16	44
2	E	12/16 (75%)	11 (92%)	1 (8%)	0	100	100
2	F	10/16 (62%)	10 (100%)	0	0	100	100
2	G	8/16 (50%)	7 (88%)	1 (12%)	0	100	100
2	H	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
All	All	1419/1492 (95%)	1285 (91%)	111 (8%)	23 (2%)	12	36

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	ASN
1	B	377	ILE
1	C	134	ASN
1	D	351	PRO
1	D	377	ILE

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Mol	Chain	Res	Type
1	A	292	TYR
1	C	196	PRO
1	D	113	GLU
1	A	313	TYR
1	A	377	ILE
1	B	144	PRO
1	B	309	LYS
1	C	333	SER
1	D	316	GLU
1	B	73	GLN
1	B	160	GLU
1	B	292	TYR
1	B	318	SER
1	A	196	PRO
1	B	196	PRO
1	B	351	PRO
1	C	138	ARG
1	C	377	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	310/317 (98%)	291 (94%)	19 (6%)	23 52
1	B	315/317 (99%)	300 (95%)	15 (5%)	31 65
1	C	305/317 (96%)	289 (95%)	16 (5%)	29 60
1	D	308/317 (97%)	299 (97%)	9 (3%)	50 81
2	E	13/15 (87%)	13 (100%)	0	100 100
2	F	11/15 (73%)	11 (100%)	0	100 100
2	G	10/15 (67%)	9 (90%)	1 (10%)	9 26
2	H	12/15 (80%)	10 (83%)	2 (17%)	3 6
All	All	1284/1328 (97%)	1222 (95%)	62 (5%)	31 65

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	82	LEU
1	A	104	SER
1	A	112	SER
1	A	118	GLU
1	A	123	ASN
1	A	130	LEU
1	A	135	GLU
1	A	158	LEU
1	A	168	SER
1	A	187	ASN
1	A	193	LEU
1	A	201	SER
1	A	216	SER
1	A	302	LEU
1	A	311	SER
1	A	338	ILE
1	A	353	ASP
1	A	366	SER
1	B	92	LEU
1	B	134	ASN
1	B	161	MET
1	B	164	THR
1	B	168	SER
1	B	194	SER
1	B	201	SER
1	B	202	ILE
1	B	207	CYS
1	B	245	ARG
1	B	265	SER
1	B	325	CYS
1	B	341	THR
1	B	371	GLN
1	B	395	LEU
1	C	49	SER
1	C	92	LEU
1	C	96	SER
1	C	108	SER
1	C	142	SER
1	C	143	LEU
1	C	153	GLN
1	C	163	LEU
1	C	168	SER

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Mol	Chain	Res	Type
1	C	265	SER
1	C	285	THR
1	C	304	HIS
1	C	331	SER
1	C	341	THR
1	C	378	ASP
1	C	382	SER
1	D	96	SER
1	D	128	THR
1	D	163	LEU
1	D	204	MET
1	D	245	ARG
1	D	265	SER
1	D	311	SER
1	D	329	SER
1	D	366	SER
2	G	132	SER
2	H	133	ASN
2	H	134	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	B	141	GLN
1	B	189	GLN
1	B	293	GLN
1	B	327	ASN
1	B	337	ASN
1	C	76	GLN
1	C	141	GLN
1	C	153	GLN
1	C	189	GLN
1	D	76	GLN
1	D	141	GLN
1	D	171	ASN
1	D	246	ASN
1	D	255	HIS
1	D	280	HIS
1	D	332	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	350/357 (98%)	-0.45	2 (0%) 90 89	26, 60, 104, 159	0
1	B	355/357 (99%)	-0.41	3 (0%) 87 86	39, 68, 129, 180	0
1	C	345/357 (96%)	-0.25	3 (0%) 85 84	41, 77, 126, 149	0
1	D	348/357 (97%)	-0.21	8 (2%) 64 59	44, 73, 142, 183	0
2	E	14/16 (87%)	-0.04	0 100 100	61, 84, 99, 102	0
2	F	12/16 (75%)	-0.12	0 100 100	64, 86, 111, 130	0
2	G	10/16 (62%)	1.01	0 100 100	95, 124, 142, 143	0
2	H	13/16 (81%)	-0.60	0 100 100	74, 92, 105, 130	0
All	All	1447/1492 (96%)	-0.32	16 (1%) 82 80	26, 70, 129, 183	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	316	GLU	6.3
1	D	240	HIS	4.1
1	D	151	TYR	3.6
1	B	397	ASN	3.3
1	C	164	THR	3.2
1	A	317	ARG	2.6
1	C	136	GLN	2.6
1	C	166	THR	2.4
1	D	239	THR	2.4
1	B	318	SER	2.4
1	D	315	ALA	2.3
1	A	315	ALA	2.3
1	D	114	LEU	2.2
1	D	317	ARG	2.2
1	D	356	ASN	2.1
1	B	317	ARG	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.