Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:48 PM GMT

PDB ID	:	1CK4
Title	:	CRYSTAL STRUCTURE OF RAT A1B1 INTEGRIN I-DOMAIN.
Authors	:	Nolte, M.; Pepinsky, R.B.; Venyaminov, S.Y.; Koteliansky, V.; Gotwals, P.J.; Karpusas, M.
Deposited on	:	1999-04-27
Resolution	:	2.20 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:

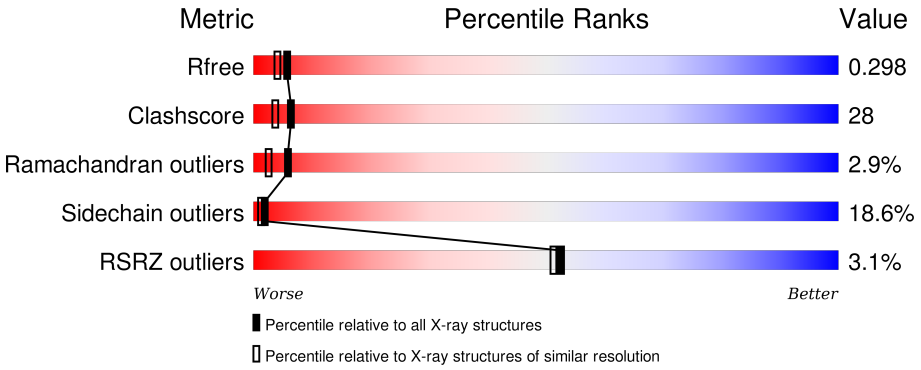
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	198	5% 38% 48% 11%
1	B	198	2% 54% 37% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3968 atoms, of which 710 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 INTEGRIN ALPHA-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	193	Total	C	H	N	O	S	365	0	1
			1869	953	354	264	294	4			
1	B	195	Total	C	H	N	O	S	364	0	1
			1884	962	356	266	296	4			

- Molecule 2 is water.

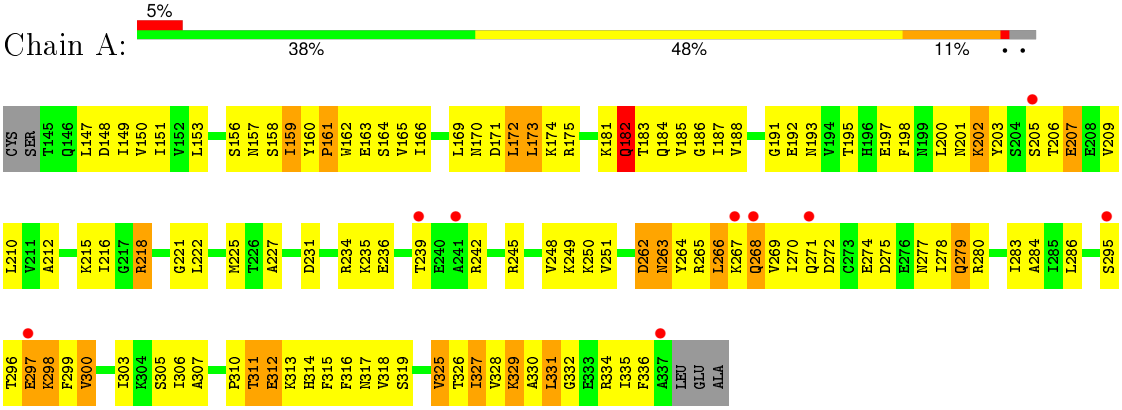
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total	O	0	0
			76	76		
2	B	139	Total	O	0	0
			139	139		

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.

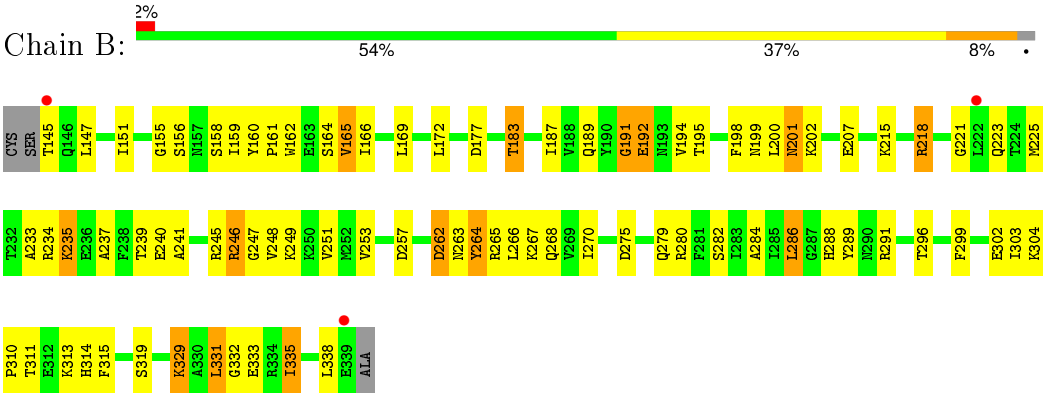
- Molecule 1: INTEGRIN ALPHA-1

Chain A:



- Molecule 1: INTEGRIN ALPHA-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.77Å 85.92Å 132.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20 32.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.3 (100.00-2.20) 90.0 (32.23-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.234 , 0.299 0.230 , 0.298	Depositor DCC
R_{free} test set	1896 reflections (11.12%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 19238 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3968	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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	0.44	0/1536	0.79	2/2073 (0.1%)
1	B	0.48	0/1549	0.74	0/2091
All	All	0.46	0/3085	0.77	2/4164 (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	234	ARG	NE-CZ-NH1	-14.15	113.23	120.30
1	A	234	ARG	NH1-CZ-NH2	7.15	127.27	119.40

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	1515	354	1519	101	0
1	B	1528	356	1535	67	0
2	A	76	0	0	5	0
2	B	139	0	0	6	0
All	All	3258	710	3054	167	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 28.

All (167) 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:313:LYS:HB3	1:B:338:LEU:HD11	1.43	0.98
1:A:147:LEU:HD23	1:A:149:ILE:HD11	1.52	0.92
1:A:328:VAL:HG23	1:A:329:LYS:HE2	1.54	0.89
1:B:291:ARG:HD3	2:B:434:HOH:O	1.72	0.87
1:A:318:VAL:HG22	1:A:327:ILE:HD12	1.60	0.83
1:B:199:ASN:H	1:B:202:LYS:HE2	1.44	0.81
1:B:191:GLY:O	1:B:192:GLU:HB2	1.80	0.80
1:B:304:LYS:HD3	2:B:410:HOH:O	1.81	0.80
1:A:182:GLN:O	1:A:182:GLN:HG2	1.85	0.75
1:B:194:VAL:HG23	1:B:228:LEU:HD13	1.68	0.74
1:A:147:LEU:H	1:A:245:ARG:HH22	1.36	0.73
1:A:171:ASP:HB3	1:A:328:VAL:HG11	1.71	0.72
1:A:160:TYR:O	1:A:162:TRP:N	2.23	0.72
1:A:242:ARG:HD2	2:A:353:HOH:O	1.89	0.72
1:B:331:LEU:O	1:B:335:ILE:HG22	1.90	0.71
1:A:191:GLY:O	1:A:192:GLU:HB2	1.90	0.70
1:A:171:ASP:OD2	1:A:328:VAL:HG21	1.92	0.70
1:A:299:PHE:O	1:A:303:ILE:HG12	1.91	0.70
1:A:264:TYR:HB3	1:B:275:ASP:HB3	1.76	0.67
1:B:231:ASP:OD1	1:B:234:ARG:NH1	2.26	0.67
1:A:286:LEU:HD23	1:A:299:PHE:CE2	2.30	0.66
1:A:267:LYS:HE2	2:A:382:HOH:O	1.94	0.66
1:A:160:TYR:HB3	1:A:161:PRO:HD3	1.79	0.65
1:B:245:ARG:HB2	1:B:248:VAL:HG21	1.80	0.64
1:B:239:THR:HG22	1:B:241:ALA:N	2.13	0.64
1:B:218:ARG:HG3	1:B:218:ARG:O	1.97	0.63
1:A:147:LEU:N	1:A:245:ARG:HH22	1.97	0.63
1:A:151:ILE:HD12	1:A:186:GLY:O	1.99	0.62
1:A:206:THR:O	1:A:210:LEU:HG	2.00	0.62
1:A:335:ILE:HG23	1:A:336:PHE:H	1.64	0.62
1:A:184:GLN:HG3	1:A:245:ARG:CZ	2.30	0.62
1:A:172:LEU:HD11	1:A:331:LEU:HD13	1.82	0.62
1:A:169:LEU:O	1:A:173:LEU:HD23	2.00	0.61
1:A:295:SER:HB3	1:A:297:GLU:HG3	1.83	0.61
1:A:151:ILE:HD13	1:A:187:ILE:HG12	1.84	0.60
1:A:153:LEU:HD11	1:A:165:VAL:HG11	1.82	0.60
1:A:303:ILE:HA	1:A:306:ILE:HD12	1.84	0.60
1:B:329:LYS:O	1:B:333:GLU:HG2	2.02	0.59
1:B:145:THR:HA	2:B:430:HOH:O	2.00	0.59
1:A:313:LYS:HE2	1:A:334:ARG:HB3	1.84	0.59
1:B:253:VAL:O	1:B:253:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:O	1:A:215:LYS:HG2	2.02	0.59
1:A:171:ASP:HA	1:A:174:LYS:HE3	1.85	0.58
1:B:160:TYR:HB3	1:B:161:PRO:HD3	1.86	0.58
1:A:251:VAL:HG11	1:A:335:ILE:HD13	1.86	0.58
1:A:329:LYS:NZ	1:A:329:LYS:HA	2.18	0.57
1:A:268:GLN:O	1:A:272:ASP:OD1	2.22	0.57
1:A:265:ARG:O	1:A:269:VAL:HG23	2.04	0.57
1:A:239:THR:OG1	1:A:242:ARG:HG3	2.05	0.56
1:B:302:GLU:O	1:B:306:ILE:HD12	2.05	0.56
1:A:263:ASN:O	1:A:266:LEU:HB2	2.05	0.56
1:B:268:GLN:HA	1:B:268:GLN:NE2	2.20	0.56
1:B:268:GLN:HA	1:B:268:GLN:HE21	1.70	0.56
1:B:239:THR:HG22	1:B:241:ALA:H	1.69	0.56
1:A:231:ASP:OD2	1:A:265:ARG:NH1	2.39	0.55
1:A:157:ASN:ND2	1:A:221:GLY:H	2.05	0.55
1:A:335:ILE:HG23	1:A:336:PHE:N	2.22	0.55
1:B:245:ARG:HB2	1:B:248:VAL:CG2	2.37	0.55
1:B:201:ASN:C	1:B:201:ASN:HD22	2.10	0.54
1:A:173:LEU:HD11	1:A:185:VAL:HG11	1.89	0.54
1:A:284:ALA:HB2	1:A:303:ILE:HG21	1.88	0.54
1:A:331:LEU:HD22	2:A:392:HOH:O	2.07	0.54
1:A:335:ILE:HB	2:A:392:HOH:O	2.09	0.53
1:B:304:LYS:HE3	1:B:311:THR:OG1	2.08	0.53
1:A:170:ASN:O	1:A:174:LYS:HG2	2.09	0.53
1:B:282:SER:HB2	1:B:303:ILE:HG22	1.91	0.53
1:A:162:TRP:CE3	1:A:218:ARG:HD3	2.43	0.53
1:A:147:LEU:N	1:A:245:ARG:NH2	2.57	0.53
1:B:192:GLU:OE1	1:B:221:GLY:HA2	2.09	0.52
1:A:251:VAL:HG11	1:A:335:ILE:CD1	2.39	0.52
1:B:155:GLY:HA3	1:B:189:GLN:OE1	2.09	0.52
1:B:289:TYR:CD2	1:B:296:THR:HG22	2.45	0.52
1:A:270:ILE:CD1	1:A:306:ILE:HG23	2.40	0.52
1:A:286:LEU:HD23	1:A:299:PHE:HE2	1.73	0.52
1:B:161:PRO:O	1:B:164:SER:HB2	2.10	0.52
1:B:299:PHE:HE1	1:B:303:ILE:HD11	1.75	0.52
1:A:225:MET:CE	1:A:262:ASP:OD1	2.58	0.51
1:A:329:LYS:HZ2	1:A:329:LYS:HA	1.75	0.51
1:B:286:LEU:HD23	1:B:286:LEU:N	2.25	0.51
1:B:160:TYR:O	1:B:162:TRP:N	2.44	0.50
1:A:161:PRO:O	1:A:164:SER:HB2	2.10	0.50
1:B:199:ASN:N	1:B:202:LYS:HE2	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:HE3	1:B:311:THR:CB	2.42	0.50
1:B:299:PHE:CE1	1:B:303:ILE:HD11	2.47	0.50
1:B:314:HIS:CE1	1:B:338:LEU:HD13	2.47	0.50
1:A:231:ASP:O	1:A:235:LYS:HB2	2.11	0.50
1:B:194:VAL:CG2	1:B:228:LEU:HD13	2.40	0.49
1:B:251:VAL:HG11	1:B:335:ILE:HD13	1.93	0.49
1:A:318:VAL:CG2	1:A:327:ILE:HD12	2.38	0.49
1:A:331:LEU:O	1:A:335:ILE:HG22	2.13	0.49
1:A:202:LYS:HG2	1:A:203:TYR:CE2	2.47	0.49
1:A:286:LEU:HD22	1:A:296:THR:CG2	2.43	0.48
1:B:241:ALA:HB2	2:B:422:HOH:O	2.14	0.48
1:A:227:ALA:HB3	1:A:262:ASP:HB3	1.94	0.48
1:A:330:ALA:O	1:A:334:ARG:HG3	2.13	0.48
1:A:286:LEU:HD22	1:A:296:THR:HG21	1.95	0.48
1:A:327:ILE:O	1:A:327:ILE:HG23	2.12	0.48
1:B:304:LYS:HE3	1:B:311:THR:HB	1.95	0.48
1:B:233:ALA:O	1:B:237:ALA:HB3	2.14	0.48
1:B:264:TYR:CE1	1:B:265:ARG:HG2	2.49	0.48
1:A:225:MET:HE3	1:A:262:ASP:OD1	2.14	0.47
1:B:267:LYS:HE3	2:B:350:HOH:O	2.13	0.47
1:B:284:ALA:HB2	1:B:303:ILE:HG13	1.95	0.47
1:B:199:ASN:H	1:B:202:LYS:CE	2.23	0.47
1:A:171:ASP:OD2	1:A:328:VAL:HG11	2.15	0.47
1:A:158:SER:O	1:A:160:TYR:N	2.47	0.47
1:A:236:GLU:O	1:A:239:THR:HG23	2.15	0.47
1:A:278:ILE:O	1:A:280:ARG:HG3	2.15	0.47
1:A:245:ARG:HB2	1:A:248:VAL:HG21	1.97	0.46
1:A:300:VAL:HG22	1:A:315:PHE:CZ	2.51	0.46
1:A:318:VAL:HG22	1:A:327:ILE:CD1	2.41	0.45
1:B:304:LYS:HD2	1:B:315:PHE:CD2	2.51	0.45
1:B:231:ASP:O	1:B:235:LYS:HB2	2.16	0.45
1:A:203:TYR:HB2	1:A:209:VAL:HG23	1.97	0.45
1:B:267:LYS:HG3	2:B:409:HOH:O	2.16	0.45
1:A:271:GLN:OE1	1:A:274:GLU:OE1	2.33	0.45
1:A:150:VAL:CG2	1:A:200:LEU:HD11	2.47	0.45
1:A:307:ALA:HB1	1:A:314:HIS:HB2	1.97	0.45
1:B:151:ILE:HD13	1:B:169:LEU:HD22	1.98	0.45
1:B:177:ASP:O	1:B:183:THR:HG23	2.16	0.45
1:B:310:PRO:HG2	1:B:313:LYS:HB2	1.98	0.44
1:B:160:TYR:CD1	1:B:160:TYR:C	2.90	0.44
1:B:225:MET:HB3	1:B:262:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HD11	1:A:306:ILE:HG23	1.99	0.44
1:A:187:ILE:HG13	1:A:198:PHE:CZ	2.52	0.44
1:A:197:GLU:O	1:A:198:PHE:HB3	2.18	0.44
1:B:332:GLY:O	1:B:335:ILE:HG23	2.17	0.44
1:B:187:ILE:HD12	1:B:198:PHE:CE2	2.52	0.44
1:B:201:ASN:C	1:B:201:ASN:ND2	2.71	0.44
1:B:165:VAL:HG12	1:B:166:ILE:HD13	1.99	0.44
1:B:279:GLN:OE1	1:B:314:HIS:HE1	2.01	0.44
1:A:316:PHE:HB3	1:A:327:ILE:HD13	2.00	0.44
1:A:249:LYS:HE3	1:A:277:ASN:O	2.18	0.44
1:A:297:GLU:CD	1:A:298:LYS:H	2.20	0.44
1:A:203:TYR:HB2	1:A:209:VAL:CG2	2.48	0.44
1:A:160:TYR:C	1:A:160:TYR:CD1	2.90	0.43
1:B:158:SER:HB2	1:B:288:HIS:CG	2.54	0.43
1:A:186:GLY:HA3	1:A:200:LEU:HD12	2.00	0.43
1:A:311:THR:HG23	1:A:312:GLU:OE1	2.18	0.43
1:A:159:ILE:O	1:A:218:ARG:CZ	2.67	0.43
1:B:246:ARG:HD2	1:B:247:GLY:N	2.33	0.43
1:B:201:ASN:HD22	1:B:202:LYS:N	2.17	0.43
1:A:310:PRO:O	1:A:314:HIS:HD2	2.02	0.42
1:B:151:ILE:HD12	1:B:187:ILE:HG12	2.01	0.42
1:B:246:ARG:HH11	1:B:246:ARG:HG2	1.84	0.42
1:A:249:LYS:NZ	1:A:279:GLN:HG3	2.35	0.42
1:A:162:TRP:CE3	1:A:218:ARG:CD	3.02	0.42
1:A:148:ASP:OD1	1:A:184:GLN:HB2	2.19	0.42
1:A:147:LEU:HD23	1:A:149:ILE:CD1	2.38	0.42
1:B:331:LEU:HD22	1:B:331:LEU:O	2.19	0.42
1:A:286:LEU:CD2	1:A:299:PHE:CE2	3.01	0.42
1:A:207:GLU:O	1:A:210:LEU:HB2	2.20	0.41
1:B:158:SER:O	1:B:160:TYR:N	2.53	0.41
1:B:332:GLY:O	1:B:335:ILE:CG2	2.68	0.41
1:A:197:GLU:HA	1:A:197:GLU:OE1	2.19	0.41
1:A:173:LEU:CD2	1:A:173:LEU:N	2.84	0.41
1:A:317:ASN:C	1:A:317:ASN:OD1	2.58	0.41
1:B:266:LEU:HA	1:B:266:LEU:HD23	1.92	0.41
1:A:166:ILE:HD11	1:A:216:ILE:O	2.21	0.41
1:A:251:VAL:HG22	1:A:279:GLN:HB2	2.03	0.41
1:A:212:ALA:HA	1:A:215:LYS:HD3	2.03	0.41
1:A:236:GLU:HG2	2:A:353:HOH:O	2.20	0.40
1:A:227:ALA:HB1	1:A:265:ARG:HG3	2.04	0.40
1:B:191:GLY:O	1:B:192:GLU:CB	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HG23	1:A:316:PHE:HB2	2.03	0.40
1:A:332:GLY:C	1:A:335:ILE:HG22	2.42	0.40
1:A:310:PRO:HG2	1:A:313:LYS:HB2	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	191/198 (96%)	170 (89%)	15 (8%)	6 (3%)	5	2
1	B	193/198 (98%)	182 (94%)	6 (3%)	5 (3%)	7	3
All	All	384/396 (97%)	352 (92%)	21 (6%)	11 (3%)	6	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	THR
1	B	263	ASN
1	A	263	ASN
1	B	192	GLU
1	A	182	GLN
1	B	156	SER
1	B	191	GLY
1	A	161	PRO
1	A	325	VAL
1	B	264	TYR
1	A	159	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	166/170 (98%)	132 (80%)	34 (20%)	1	1
1	B	167/170 (98%)	139 (83%)	28 (17%)	2	2
All	All	333/340 (98%)	271 (81%)	62 (19%)	2	1

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

Mol	Chain	Res	Type
1	A	156	SER
1	A	163	GLU
1	A	172	LEU
1	A	173	LEU
1	A	175	ARG
1	A	181	LYS
1	A	182	GLN
1	A	188	VAL
1	A	193	ASN
1	A	195	THR
1	A	201	ASN
1	A	202	LYS
1	A	205	SER
1	A	207	GLU
1	A	218	ARG
1	A	222	LEU
1	A	250	LYS
1	A	262	ASP
1	A	266	LEU
1	A	268	GLN
1	A	275	ASP
1	A	279	GLN
1	A	297	GLU
1	A	298	LYS
1	A	300	VAL
1	A	305	SER
1	A	311	THR

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	319	SER
1	A	325	VAL
1	A	326	THR
1	A	327	ILE
1	A	329	LYS
1	A	331	LEU
1	B	147	LEU
1	B	159	ILE
1	B	165	VAL
1	B	172	LEU
1	B	183	THR
1	B	195	THR
1	B	200	LEU
1	B	201	ASN
1	B	207	GLU
1	B	215	LYS
1	B	218	ARG
1	B	223	GLN
1	B	228	LEU
1	B	235	LYS
1	B	240	GLU
1	B	246	ARG
1	B	249	LYS
1	B	257	ASP
1	B	262	ASP
1	B	270	ILE
1	B	280	ARG
1	B	286	LEU
1	B	305	SER
1	B	309	GLU
1	B	319	SER
1	B	329	LYS
1	B	331	LEU
1	B	335	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	182	GLN
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	268	GLN
1	A	271	GLN
1	A	314	HIS
1	B	157	ASN
1	B	182	GLN
1	B	201	ASN
1	B	268	GLN
1	B	279	GLN
1	B	314	HIS

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	193/198 (97%)	0.53	9 (4%) 35 34	15, 34, 49, 55	5 (2%)
1	B	195/198 (98%)	0.07	3 (1%) 76 75	12, 21, 33, 48	3 (1%)
All	All	388/396 (97%)	0.30	12 (3%) 52 51	12, 27, 46, 55	8 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	GLU	3.5
1	A	205	SER	3.4
1	A	268	GLN	3.3
1	B	339	GLU	3.0
1	A	295	SER	2.4
1	A	239	THR	2.4
1	B	145	THR	2.2
1	A	337	ALA	2.2
1	A	267	LYS	2.1
1	A	271	GLN	2.1
1	A	241	ALA	2.1
1	B	222	LEU	2.0

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.