Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID	:	1K3Z
Title	:	X-ray crystal structure of the IkBb/NF-kB p65 homodimer complex
Authors	:	Shiva, M.; Huang, D.B.; Chen, Y.; Huxford, T.; Ghosh, S.; Ghosh, G.
Deposited on	:	2001-10-04
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
http://wwpdb.org/validation/2016/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:

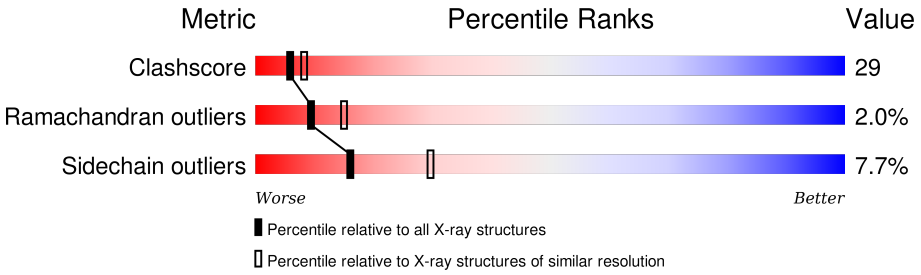
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	136	54% 39%
1	B	136	54% 29% 13%
2	D	282	42% 31% 5% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3769 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 Transcription factor p65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1056	660	191	199	6			
1	B	118	Total	C	N	O	S	0	0	0
			953	590	175	183	5			

- Molecule 2 is a protein called transcription factor inhibitor I-kappa-B-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	221	Total	C	N	O	S	0	0	0
			1661	1041	305	309	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	312	GLU	SER	ENGINEERED	UNP Q60778
D	313	GLU	SER	ENGINEERED	UNP Q60778
D	314	GLU	SER	ENGINEERED	UNP Q60778
D	316	GLU	SER	ENGINEERED	UNP Q60778
D	318	GLU	SER	ENGINEERED	UNP Q60778

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	23	Total	O	0	0
			23	23		
3	D	49	Total	O	0	0
			49	49		

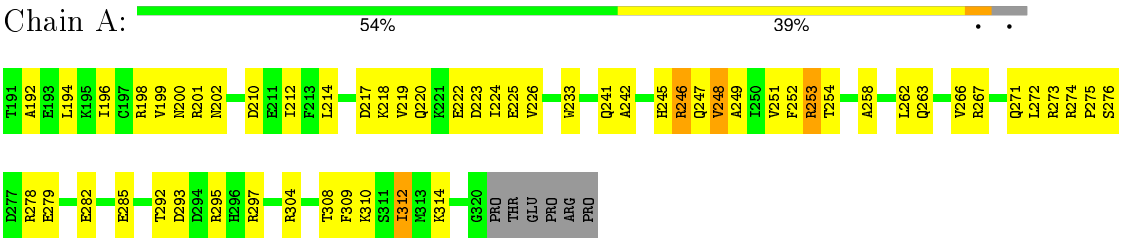
3 Residue-property plots (i)

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.

Note EDS was not executed.

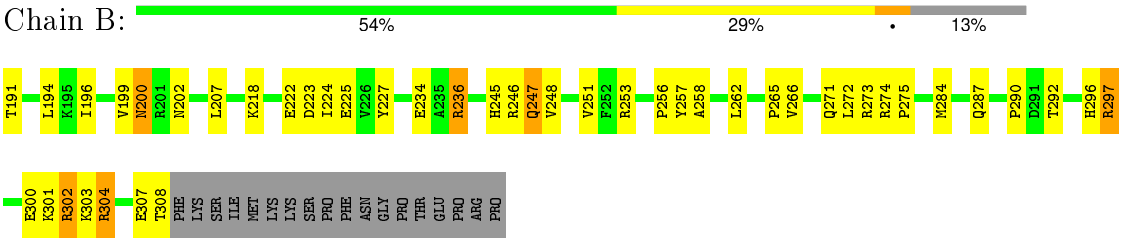
- Molecule 1: Transcription factor p65

Chain A:



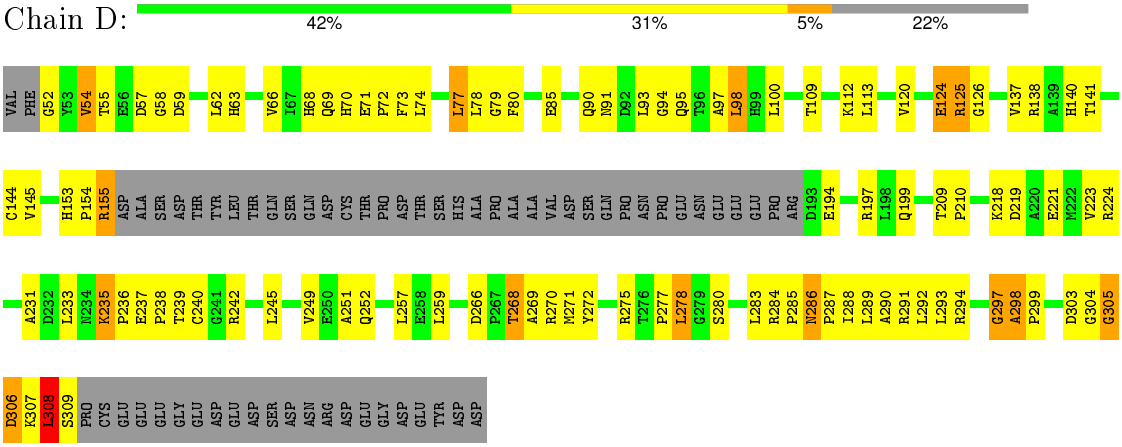
- Molecule 1: Transcription factor p65

Chain B:



- Molecule 2: transcription factor inhibitor I-kappa-B-beta

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	46.40Å 48.92Å 59.47Å 95.17° 91.80° 105.45°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	80.0 (30.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3769	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

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	0.36	0/1079	0.62	0/1453
1	B	0.37	0/972	0.65	0/1312
2	D	0.35	0/1696	0.62	1/2309 (0.0%)
All	All	0.36	0/3747	0.63	1/5074 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	238	PRO	N-CA-C	5.08	125.30	112.10

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	1056	0	1037	82	0
1	B	953	0	927	55	0
2	D	1661	0	1642	98	0
3	A	27	0	0	1	0
3	B	23	0	0	4	0
3	D	49	0	0	3	0
All	All	3769	0	3606	209	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 29.

All (209) 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:246:ARG:HG3	1:B:248:VAL:HG21	1.34	1.07
2:D:55:THR:HG22	2:D:59:ASP:H	1.18	1.02
1:A:218:LYS:NZ	1:B:246:ARG:HE	1.63	0.95
1:A:278:ARG:HB3	1:A:278:ARG:HH11	1.30	0.94
2:D:55:THR:HG23	2:D:57:ASP:H	1.35	0.92
2:D:308:LEU:HD22	2:D:308:LEU:H	1.33	0.92
2:D:294:ARG:HA	2:D:298:ALA:HB2	1.52	0.88
1:A:267:ARG:HH22	1:A:285:GLU:HG3	1.39	0.85
1:A:246:ARG:HG3	1:B:248:VAL:CG2	2.08	0.84
1:A:218:LYS:HZ2	1:B:246:ARG:HE	1.22	0.84
2:D:55:THR:HG22	2:D:59:ASP:N	1.92	0.83
2:D:297:GLY:C	2:D:299:PRO:HD3	1.98	0.83
1:A:248:VAL:HG21	1:B:246:ARG:HG2	1.63	0.80
1:A:219:VAL:O	1:A:247:GLN:HB2	1.83	0.79
2:D:257:LEU:HD22	2:D:289:LEU:HD23	1.64	0.79
1:A:278:ARG:HB3	1:A:278:ARG:NH1	1.98	0.78
2:D:70:HIS:HD2	2:D:73:PHE:H	1.31	0.78
1:A:218:LYS:HD2	1:A:218:LYS:H	1.51	0.74
1:B:199:VAL:HG11	1:B:284:MET:HE3	1.70	0.74
1:B:297:ARG:HD2	1:B:297:ARG:N	2.03	0.73
2:D:294:ARG:CA	2:D:298:ALA:HB2	2.19	0.73
1:B:297:ARG:HD2	1:B:297:ARG:H	1.52	0.73
2:D:266:ASP:OD2	2:D:268:THR:HB	1.88	0.73
1:B:265:PRO:HB3	1:B:287:GLN:NE2	2.02	0.73
1:B:191:THR:HA	3:B:601:HOH:O	1.88	0.73
1:A:199:VAL:HG12	1:A:201:ARG:H	1.52	0.72
2:D:194:GLU:HA	2:D:197:ARG:HD2	1.72	0.72
2:D:219:ASP:O	2:D:223:VAL:HG23	1.89	0.72
2:D:288:ILE:O	2:D:292:LEU:HD13	1.89	0.72
2:D:74:LEU:HD23	2:D:78:LEU:HD13	1.72	0.71
1:B:304:ARG:HH11	1:B:304:ARG:HG3	1.55	0.71
1:A:218:LYS:HZ2	1:B:246:ARG:NE	1.89	0.70
2:D:55:THR:CG2	2:D:59:ASP:H	2.00	0.70
2:D:278:LEU:HD21	2:D:294:ARG:NH1	2.07	0.70
1:A:267:ARG:HH22	1:A:285:GLU:CG	2.06	0.69
2:D:257:LEU:HD22	2:D:289:LEU:CD2	2.24	0.68
1:B:304:ARG:NH1	1:B:304:ARG:HG3	2.10	0.67
2:D:55:THR:HG23	2:D:57:ASP:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:294:ARG:HA	2:D:298:ALA:CB	2.25	0.67
1:A:251:VAL:HG12	1:A:253:ARG:NH2	2.11	0.66
1:A:222:GLU:HA	1:A:241:GLN:HE21	1.59	0.66
2:D:120:VAL:HG21	2:D:199:GLN:OE1	1.96	0.66
1:A:267:ARG:HH12	1:A:285:GLU:HB2	1.60	0.66
1:B:199:VAL:CG1	1:B:284:MET:HE3	2.24	0.66
1:A:293:ASP:O	1:A:297:ARG:HB2	1.96	0.65
1:A:309:PHE:HA	1:A:312:ILE:HD11	1.77	0.65
1:A:297:ARG:HD3	3:A:633:HOH:O	1.97	0.64
1:A:218:LYS:NZ	1:B:246:ARG:NE	2.41	0.63
2:D:288:ILE:HD13	2:D:291:ARG:NH1	2.13	0.63
1:A:192:ALA:HB3	1:A:274:ARG:HH12	1.62	0.63
2:D:140:HIS:HE1	2:D:219:ASP:OD2	1.80	0.63
2:D:306:ASP:OD1	2:D:308:LEU:HD13	1.98	0.62
2:D:63:HIS:O	2:D:66:VAL:HG22	1.99	0.62
2:D:91:ASN:HD21	2:D:95:GLN:HE21	1.45	0.62
1:B:265:PRO:HB3	1:B:287:GLN:HE21	1.65	0.62
2:D:221:GLU:HB2	3:D:630:HOH:O	1.99	0.61
2:D:54:VAL:HG12	2:D:58:GLY:HA2	1.83	0.61
2:D:71:GLU:HB3	2:D:72:PRO:HD3	1.82	0.60
2:D:141:THR:O	2:D:145:VAL:HG23	2.00	0.60
1:B:262:LEU:HD11	1:B:266:VAL:CG2	2.32	0.60
1:B:246:ARG:C	1:B:247:GLN:HG3	2.22	0.60
2:D:286:ASN:HD21	2:D:288:ILE:HG12	1.65	0.60
1:A:253:ARG:HD2	1:A:253:ARG:N	2.17	0.60
2:D:308:LEU:H	2:D:308:LEU:CD2	2.11	0.59
1:B:224:ILE:HD12	1:B:273:ARG:O	2.01	0.59
2:D:68:HIS:O	2:D:69:GLN:HB2	2.02	0.59
2:D:55:THR:HG21	3:D:646:HOH:O	2.02	0.59
1:A:225:GLU:HG2	1:A:273:ARG:O	2.02	0.59
1:B:301:LYS:C	1:B:303:LYS:H	2.05	0.59
1:B:223:ASP:OD2	1:B:275:PRO:HD2	2.02	0.59
1:B:246:ARG:O	1:B:247:GLN:HG3	2.02	0.59
1:B:262:LEU:HD11	1:B:266:VAL:HG21	1.83	0.58
1:B:297:ARG:H	1:B:297:ARG:CD	2.16	0.58
1:A:310:LYS:O	1:A:314:LYS:HB2	2.03	0.58
1:A:218:LYS:HZ2	1:B:246:ARG:HH21	1.50	0.57
2:D:62:LEU:HD22	2:D:97:ALA:CB	2.33	0.57
1:B:304:ARG:NH2	2:D:58:GLY:CA	2.68	0.57
1:A:248:VAL:HG13	1:A:248:VAL:O	2.04	0.57
2:D:294:ARG:O	2:D:298:ALA:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:CYS:HB3	3:D:635:HOH:O	2.04	0.57
1:A:212:ILE:CD1	1:A:254:THR:HG23	2.35	0.57
2:D:70:HIS:CD2	2:D:73:PHE:HB2	2.39	0.56
1:A:267:ARG:NH2	1:A:285:GLU:HG3	2.17	0.56
1:B:196:ILE:HD11	1:B:271:GLN:HA	1.88	0.55
2:D:286:ASN:HB3	2:D:289:LEU:HD12	1.89	0.55
2:D:70:HIS:CD2	2:D:73:PHE:H	2.19	0.55
1:B:202:ASN:HD21	2:D:239:THR:HA	1.72	0.55
2:D:280:SER:O	2:D:284:ARG:HG2	2.07	0.55
1:A:218:LYS:HZ1	1:B:246:ARG:HE	1.52	0.54
1:A:194:LEU:HD23	1:A:279:GLU:CG	2.37	0.54
2:D:240:CYS:O	2:D:271:MET:HB2	2.08	0.54
2:D:74:LEU:O	2:D:74:LEU:HD23	2.08	0.53
1:B:218:LYS:HA	1:B:247:GLN:O	2.09	0.53
1:A:218:LYS:HZ2	1:B:246:ARG:NH2	2.07	0.53
1:A:267:ARG:HB3	1:A:267:ARG:HH11	1.73	0.53
1:B:297:ARG:N	1:B:297:ARG:CD	2.71	0.53
2:D:231:ALA:O	2:D:233:LEU:HD13	2.07	0.53
1:A:245:HIS:NE2	1:B:248:VAL:HG22	2.24	0.53
2:D:109:THR:HA	2:D:112:LYS:HD2	1.91	0.52
2:D:290:ALA:O	2:D:294:ARG:HG2	2.09	0.52
2:D:70:HIS:HD2	2:D:73:PHE:N	2.04	0.52
1:A:223:ASP:OD1	1:A:276:SER:HB2	2.08	0.52
1:A:308:THR:O	1:A:312:ILE:HG12	2.09	0.52
1:A:226:VAL:HG21	1:A:252:PHE:CD2	2.45	0.52
1:A:297:ARG:HD2	2:D:93:LEU:HD11	1.90	0.52
2:D:252:GLN:HA	2:D:289:LEU:HD11	1.92	0.51
2:D:278:LEU:HA	2:D:293:LEU:HD13	1.91	0.51
2:D:98:LEU:HA	2:D:113:LEU:HD13	1.93	0.51
1:B:300:GLU:HG2	1:B:304:ARG:NH1	2.26	0.51
2:D:298:ALA:N	2:D:299:PRO:HD3	2.25	0.50
1:B:227:TYR:OH	1:B:234:GLU:HG2	2.11	0.50
1:B:200:ASN:HD22	1:B:200:ASN:N	2.08	0.50
1:B:304:ARG:HH21	2:D:58:GLY:CA	2.25	0.50
2:D:245:LEU:O	2:D:249:VAL:HG23	2.11	0.50
1:B:308:THR:HG21	2:D:52:GLY:HA2	1.93	0.49
1:B:236:ARG:HB2	3:B:609:HOH:O	2.10	0.49
1:B:297:ARG:O	1:B:301:LYS:N	2.41	0.49
1:A:267:ARG:NH1	1:A:267:ARG:HB3	2.27	0.49
1:A:267:ARG:NH1	1:A:285:GLU:HB2	2.27	0.49
1:A:295:ARG:HH21	2:D:137:VAL:CG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ALA:O	2:D:277:PRO:HD3	2.13	0.49
1:A:246:ARG:O	1:A:247:GLN:HG2	2.12	0.48
1:A:212:ILE:HD13	1:A:254:THR:HG23	1.94	0.48
2:D:304:GLY:O	2:D:306:ASP:N	2.47	0.48
1:A:293:ASP:OD1	1:A:295:ARG:N	2.47	0.48
1:A:278:ARG:HH11	1:A:278:ARG:CB	2.15	0.48
2:D:62:LEU:HD22	2:D:97:ALA:HB2	1.95	0.48
1:A:218:LYS:CD	1:A:218:LYS:H	2.23	0.47
1:A:242:ALA:HB2	2:D:283:LEU:HD12	1.96	0.47
1:A:218:LYS:HD2	1:A:218:LYS:N	2.24	0.47
1:A:309:PHE:HA	1:A:312:ILE:CD1	2.44	0.47
2:D:74:LEU:O	2:D:78:LEU:HD13	2.14	0.47
1:B:300:GLU:HG2	1:B:304:ARG:HH11	1.80	0.47
1:A:226:VAL:HG11	1:A:252:PHE:CZ	2.50	0.47
1:A:218:LYS:HA	1:A:247:GLN:O	2.15	0.47
1:B:303:LYS:O	1:B:307:GLU:HB2	2.15	0.47
2:D:194:GLU:O	2:D:197:ARG:HB2	2.15	0.46
1:A:218:LYS:HZ2	1:B:246:ARG:CZ	2.28	0.46
1:A:246:ARG:HB3	2:D:309:SER:HB2	1.98	0.46
2:D:287:PRO:O	2:D:291:ARG:HG3	2.15	0.46
1:B:304:ARG:NH2	2:D:58:GLY:HA2	2.30	0.46
1:B:194:LEU:HD11	1:B:274:ARG:HG3	1.96	0.46
1:A:273:ARG:HH21	1:A:278:ARG:NH2	2.13	0.46
1:A:248:VAL:CG1	1:A:248:VAL:O	2.64	0.46
2:D:137:VAL:O	2:D:137:VAL:HG12	2.16	0.46
1:A:233:TRP:CD1	1:A:258:ALA:HB2	2.51	0.46
1:A:309:PHE:HA	1:A:312:ILE:CG1	2.46	0.45
1:A:224:ILE:HG13	1:A:225:GLU:N	2.31	0.45
1:A:222:GLU:HB3	1:A:241:GLN:NE2	2.31	0.45
1:B:200:ASN:H	1:B:200:ASN:HD22	1.62	0.45
2:D:124:GLU:OE1	2:D:126:GLY:N	2.48	0.45
1:A:198:ARG:HD3	1:B:251:VAL:HG21	1.97	0.45
1:A:273:ARG:O	1:A:275:PRO:HD3	2.17	0.45
1:A:242:ALA:HB2	2:D:283:LEU:CD1	2.48	0.44
1:A:217:ASP:O	1:A:219:VAL:HG13	2.18	0.44
2:D:237:GLU:HG3	2:D:242:ARG:O	2.17	0.44
1:A:274:ARG:HG2	1:A:276:SER:HB3	2.00	0.44
2:D:74:LEU:C	2:D:74:LEU:HD23	2.38	0.44
1:A:194:LEU:HD23	1:A:279:GLU:HG2	2.00	0.44
1:A:297:ARG:HD2	2:D:93:LEU:CD1	2.48	0.43
2:D:304:GLY:O	2:D:305:GLY:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HH22	1:A:285:GLU:CB	2.31	0.43
1:A:222:GLU:CB	1:A:241:GLN:NE2	2.82	0.43
2:D:270:ARG:HA	2:D:275:ARG:O	2.18	0.43
2:D:288:ILE:HD13	2:D:291:ARG:HH12	1.80	0.43
2:D:240:CYS:HA	2:D:272:TYR:CD1	2.53	0.43
1:B:194:LEU:HD21	1:B:274:ARG:HG3	2.01	0.43
1:A:214:LEU:O	1:A:249:ALA:HA	2.19	0.43
1:A:200:ASN:HB2	3:B:625:HOH:O	2.18	0.43
2:D:294:ARG:HH11	2:D:294:ARG:HG2	1.84	0.43
1:A:267:ARG:HH12	1:A:285:GLU:CB	2.29	0.43
2:D:218:LYS:HE2	2:D:251:ALA:O	2.19	0.43
1:A:297:ARG:HH11	1:A:297:ARG:HG2	1.85	0.42
1:B:262:LEU:O	1:B:290:PRO:HB3	2.19	0.42
1:A:212:ILE:N	1:A:212:ILE:HD12	2.34	0.42
2:D:137:VAL:O	2:D:138:ARG:HB2	2.20	0.42
1:A:192:ALA:HB3	1:A:274:ARG:NH1	2.31	0.42
2:D:124:GLU:CD	2:D:126:GLY:H	2.22	0.42
2:D:94:GLY:O	2:D:124:GLU:HA	2.19	0.42
2:D:57:ASP:O	2:D:91:ASN:HB2	2.20	0.42
1:B:302:ARG:HA	1:B:302:ARG:NE	2.31	0.42
2:D:209:THR:O	2:D:210:PRO:C	2.58	0.42
2:D:90:GLN:HA	2:D:95:GLN:O	2.19	0.42
2:D:252:GLN:HE22	2:D:284:ARG:CB	2.33	0.42
1:B:304:ARG:HH21	2:D:58:GLY:C	2.22	0.42
2:D:77:LEU:C	2:D:79:GLY:H	2.23	0.42
1:A:196:ILE:HD11	1:A:271:GLN:HA	2.02	0.42
2:D:286:ASN:HD22	2:D:286:ASN:C	2.23	0.41
1:A:220:GLN:HB2	1:A:223:ASP:HB3	2.02	0.41
1:A:292:THR:HG22	1:A:292:THR:O	2.19	0.41
2:D:153:HIS:O	2:D:155:ARG:N	2.42	0.41
1:A:212:ILE:HD11	1:A:254:THR:HG23	2.03	0.41
2:D:71:GLU:N	2:D:72:PRO:CD	2.84	0.41
1:A:267:ARG:HH22	1:A:285:GLU:HB2	1.85	0.41
1:B:207:LEU:O	1:B:256:PRO:HB3	2.21	0.41
1:A:199:VAL:HG13	1:A:212:ILE:HG23	2.01	0.41
2:D:66:VAL:HG21	2:D:100:LEU:HB2	2.03	0.41
1:A:248:VAL:HG13	1:B:245:HIS:CD2	2.56	0.41
2:D:197:ARG:HG2	2:D:197:ARG:NH1	2.36	0.41
1:A:210:ASP:O	1:A:253:ARG:HA	2.21	0.41
2:D:224:ARG:NH1	2:D:259:LEU:HD21	2.36	0.41
1:B:257:TYR:CG	1:B:258:ALA:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:GLU:CD	2:D:85:GLU:H	2.23	0.41
1:A:262:LEU:HD11	1:A:266:VAL:CG2	2.51	0.40
2:D:235:LYS:HA	2:D:236:PRO:HD3	1.85	0.40
1:B:225:GLU:HB2	3:B:609:HOH:O	2.20	0.40
2:D:285:PRO:O	2:D:287:PRO:HD3	2.21	0.40
2:D:93:LEU:HB3	2:D:125:ARG:NH1	2.35	0.40
2:D:305:GLY:O	2:D:307:LYS:N	2.54	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	128/136 (94%)	117 (91%)	10 (8%)	1 (1%)	24 41
1	B	116/136 (85%)	101 (87%)	14 (12%)	1 (1%)	21 37
2	D	217/282 (77%)	195 (90%)	15 (7%)	7 (3%)	5 6
All	All	461/554 (83%)	413 (90%)	39 (8%)	9 (2%)	9 15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	303	ASP
2	D	305	GLY
2	D	308	LEU
1	B	292	THR
2	D	306	ASP
1	A	304	ARG
2	D	298	ALA
2	D	154	PRO
2	D	297	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	117/123 (95%)	109 (93%)	8 (7%)	20	36
1	B	105/123 (85%)	95 (90%)	10 (10%)	11	20
2	D	168/225 (75%)	156 (93%)	12 (7%)	18	34
All	All	390/471 (83%)	360 (92%)	30 (8%)	16	30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	246	ARG
1	A	248	VAL
1	A	253	ARG
1	A	263	GLN
1	A	272	LEU
1	A	282	GLU
1	A	312	ILE
1	B	200	ASN
1	B	222	GLU
1	B	236	ARG
1	B	247	GLN
1	B	253	ARG
1	B	272	LEU
1	B	296	HIS
1	B	297	ARG
1	B	302	ARG
1	B	304	ARG
2	D	54	VAL
2	D	77	LEU
2	D	80	PHE
2	D	98	LEU
2	D	124	GLU
2	D	125	ARG
2	D	155	ARG
2	D	235	LYS

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Mol	Chain	Res	Type
2	D	268	THR
2	D	278	LEU
2	D	286	ASN
2	D	308	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	241	GLN
1	A	247	GLN
1	A	296	HIS
1	B	200	ASN
1	B	202	ASN
1	B	220	GLN
1	B	287	GLN
2	D	69	GLN
2	D	70	HIS
2	D	95	GLN
2	D	140	HIS
2	D	286	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 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.