



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 AM GMT

PDB ID : 2FOK
Title : STRUCTURE OF RESTRICTION ENDONUCLEASE FOKI
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Deposited on : 1998-03-30
Resolution : 2.30 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

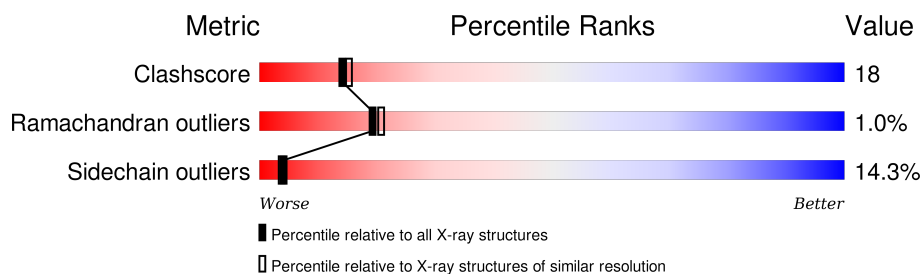
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 $\leq 5\%$. 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	579	
1	B	579	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9427 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 FOKI RESTRICTION ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4458	2859	764	824	11			
1	B	560	Total	C	N	O	S	0	0	0
			4453	2860	759	823	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	LEU	GLY	CONFLICT	UNP P14870
A	381	GLY	VAL	CONFLICT	UNP P14870
A	382	LYS	THR	CONFLICT	UNP P14870
A	383	PRO	LYS	CONFLICT	UNP P14870
A	384	ASP	GLN	CONFLICT	UNP P14870
B	380	LEU	GLY	CONFLICT	UNP P14870
B	381	GLY	VAL	CONFLICT	UNP P14870
B	382	LYS	THR	CONFLICT	UNP P14870
B	383	PRO	LYS	CONFLICT	UNP P14870
B	384	ASP	GLN	CONFLICT	UNP P14870

- Molecule 2 is water.

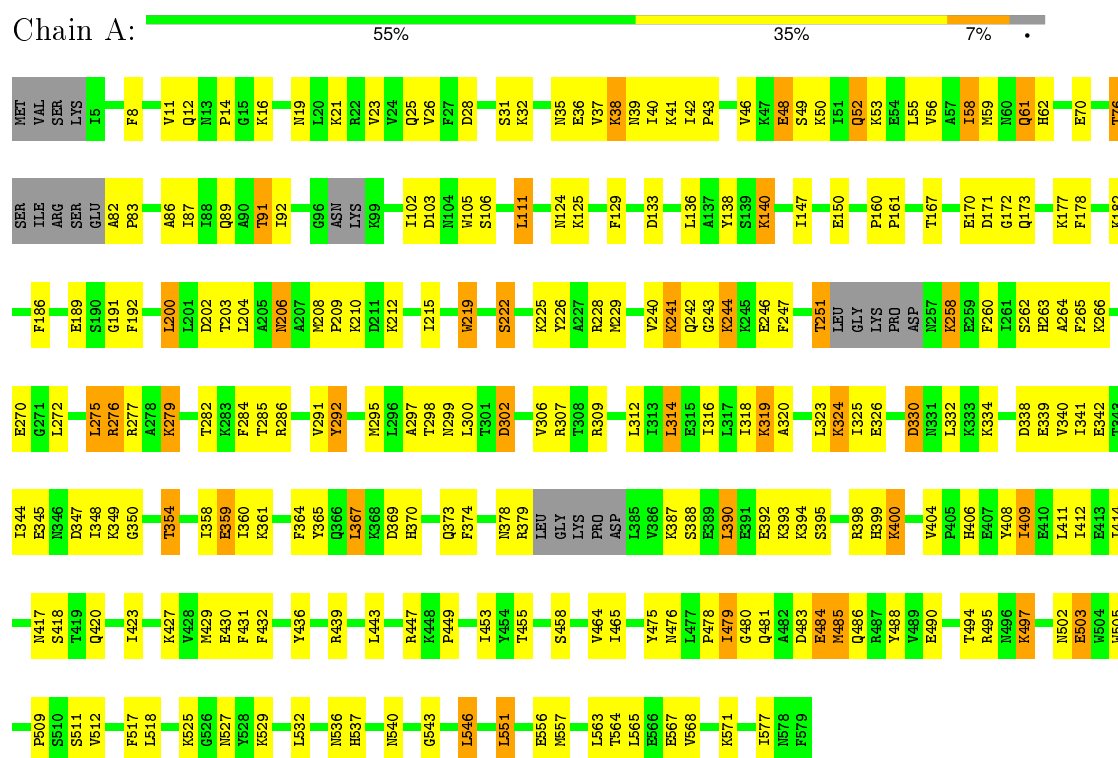
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	282	Total	O	0	0
			282	282		
2	B	234	Total	O	0	0
			234	234		

3 Residue-property plots

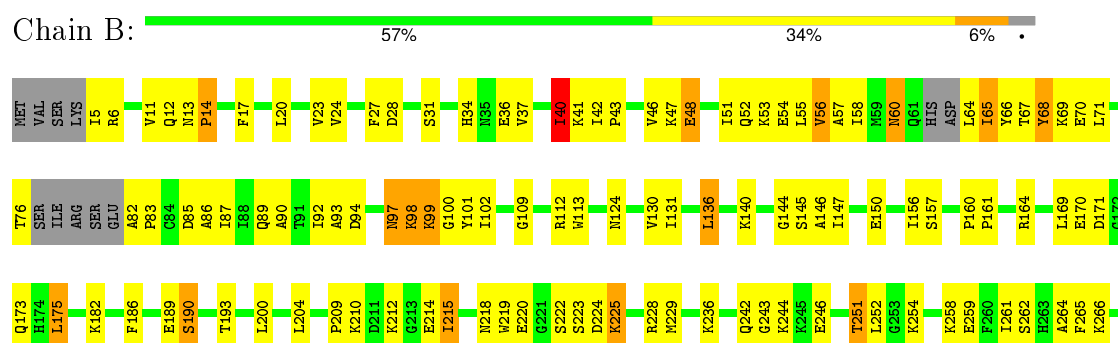
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: FOKI RESTRICTION ENDONUCLEASE



• Molecule 1: FOKI RESTRICTION ENDONUCLEASE



V545	K427	D347	E270
K559	V428	I348	L276
L565	M429	K349	R276
E566	M433	C350	R277
E567	K441	L352	A278
V568		N353	K279
R569		T354	
R570	L453	F357	T282
K571	V454	L358	K283
	T455	E359	F284
I577	S458	L360	T285
N578		K361	R286
F579	Y462	L367	R290
	G463	K368	V291
	V464		T292
		I371	W293
	T468		E294
	K469	V375	M295
		I376	L296
	S472	F377	A297
	G473	N378	T298
	G474	ARG	M299
	Y475	LEU	L300
	N476	GLY	T301
	L477	LYS	K303
		PRO	E304
	Q481	ASP	T305
		LEU	V306
	E484	VAL	R307
		K387	T308
	R487	S388	R309
	Y488	E389	A311
		L390	L312
	K497	E391	L313
	N502	E392	L314
	E503	K393	E315
		K394	I316
	K506	S395	
			K319
	L518	R398	
	F519		S322
	V520	H406	L323
		E407	K324
	H523	Y408	L325
	F524	I409	
	K525		N331
	G526	I412	L332
	N527	E413	K333
	V528	I414	K334
	K529	A415	L335
	A530	R416	
	Q531	N417	V340
	L532	Q420	E342
			T343
	H537	I423	T344

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.01Å 137.17Å 188.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.5 (6.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.211 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9427	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/4543	0.61	0/6118
1	B	0.38	0/4539	0.60	1/6115 (0.0%)
All	All	0.38	0/9082	0.60	1/12233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4458	0	4494	155	0
1	B	4453	0	4486	172	0
2	A	282	0	0	14	0
2	B	234	0	0	8	0
All	All	9427	0	8980	326	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 18.

All (326) 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:497:LYS:HD2	1:A:497:LYS:H	1.35	0.91
1:B:417:ASN:HB2	1:B:420:GLN:HG2	1.54	0.89
1:B:390:LEU:HD21	1:B:413:GLU:HG2	1.53	0.88
1:B:37:VAL:HA	1:B:41:LYS:HB2	1.55	0.88
1:B:131:ILE:HD13	1:B:136:LEU:HD13	1.53	0.88
1:B:209:PRO:HA	1:B:212:LYS:HG3	1.58	0.86
1:A:325:ILE:HG23	1:A:341:ILE:HD12	1.55	0.86
1:A:340:VAL:HG11	1:A:399:HIS:HB2	1.57	0.86
1:A:350:GLY:O	1:A:354:THR:HG22	1.79	0.83
1:A:325:ILE:HG12	1:A:341:ILE:HG23	1.63	0.78
1:B:42:ILE:HB	1:B:43:PRO:HD3	1.65	0.78
1:B:36:GLU:O	1:B:40:ILE:HG23	1.85	0.76
1:B:41:LYS:HD2	1:B:90:ALA:O	1.86	0.76
1:A:87:ILE:O	1:A:91:THR:HG23	1.86	0.75
1:B:334:LYS:HD2	1:B:335:LEU:HD23	1.70	0.74
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.53	0.73
1:A:35:ASN:O	1:A:39:ASN:HB2	1.88	0.73
1:A:417:ASN:HB3	1:A:420:GLN:HG3	1.69	0.73
1:A:302:ASP:O	1:A:306:VAL:HG23	1.88	0.73
1:A:349:LYS:HE3	2:A:1023:HOH:O	1.89	0.72
1:A:443:LEU:HB2	1:A:449:PRO:O	1.89	0.72
1:B:277:ARG:HA	1:B:282:THR:CG2	2.20	0.72
1:B:414:ILE:HG23	1:B:420:GLN:HB3	1.71	0.71
1:A:358:ILE:HG12	1:A:367:LEU:HD12	1.73	0.70
1:B:277:ARG:HA	1:B:282:THR:HG21	1.74	0.69
1:B:204:LEU:HA	1:B:215:ILE:HD11	1.73	0.69
1:A:172:GLY:O	1:A:266:LYS:HE3	1.92	0.69
1:B:85:ASP:HA	2:B:1336:HOH:O	1.90	0.69
1:A:14:PRO:HA	1:A:229:MET:HE1	1.74	0.69
1:B:225:LYS:HG3	1:B:228:ARG:HH21	1.58	0.69
1:A:564:THR:OG1	1:A:567:GLU:HG3	1.93	0.69
1:B:453:ILE:HG13	1:B:464:VAL:HB	1.74	0.68
1:A:58:ILE:O	1:A:61:GLN:HG3	1.94	0.68
1:B:76:THR:CB	1:B:82:ALA:HB2	2.23	0.68
1:A:475:TYR:CZ	1:A:478:PRO:HD2	2.29	0.68
1:B:160:PRO:HB2	1:B:161:PRO:HD3	1.76	0.68
1:A:359:GLU:HG3	1:A:361:LYS:NZ	2.09	0.68
1:A:228:ARG:NH1	1:A:229:MET:SD	2.68	0.67
1:A:465:ILE:HG22	1:A:485:MET:HE1	1.77	0.66
1:B:147:ILE:H	1:B:147:ILE:HD12	1.60	0.66
1:A:485:MET:HA	1:A:485:MET:HE3	1.76	0.66
1:B:476:ASN:HA	1:B:525:LYS:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:CD2	1:B:236:LYS:HD2	2.31	0.66
1:A:136:LEU:O	1:A:140:LYS:HG2	1.96	0.66
1:B:186:PHE:O	1:B:189:GLU:HG2	1.96	0.66
1:B:343:THR:HG21	1:B:395:SER:OG	1.97	0.65
1:B:474:GLY:HA3	1:B:525:LYS:HG2	1.80	0.64
1:B:5:ILE:HD13	1:B:304:GLU:HG3	1.80	0.64
1:B:527:ASN:HD21	1:B:530:ALA:HB3	1.62	0.64
1:A:58:ILE:O	1:A:61:GLN:NE2	2.31	0.64
1:B:297:ALA:HB3	1:B:307:ARG:HG3	1.80	0.63
1:B:11:VAL:HG11	1:B:14:PRO:HB3	1.81	0.63
1:A:200:LEU:HD11	1:A:219:TRP:HB3	1.81	0.63
1:A:76:THR:OG1	1:A:82:ALA:HB2	1.99	0.62
1:B:414:ILE:HG23	1:B:420:GLN:CB	2.30	0.62
1:B:343:THR:HG22	1:B:398:ARG:HH11	1.65	0.62
1:B:315:GLU:O	1:B:319:LYS:HD2	1.99	0.62
1:A:518:LEU:HD11	1:A:546:LEU:HB2	1.82	0.61
1:B:566:GLU:OE2	1:B:569:ARG:NH1	2.31	0.61
1:B:13:ASN:HD22	1:B:229:MET:HE3	1.65	0.61
1:B:293:TRP:CE3	1:B:377:PRO:HG2	2.35	0.61
1:B:406:HIS:HA	1:B:409:ILE:HD12	1.82	0.61
1:B:394:LYS:HE2	1:B:413:GLU:HG3	1.82	0.60
1:A:299:ASN:HB3	2:A:1216:HOH:O	2.01	0.60
1:A:320:ALA:HB2	2:A:1197:HOH:O	2.01	0.60
1:A:243:GLY:O	1:A:264:ALA:HB3	2.01	0.60
1:A:186:PHE:O	1:A:189:GLU:HG2	2.02	0.60
1:B:348:ILE:O	1:B:352:ILE:HD12	2.03	0.59
1:B:97:ASN:ND2	1:B:100:GLY:HA2	2.18	0.58
1:B:305:TYR:CE2	1:B:387:LYS:HB3	2.38	0.58
1:A:430:GLU:HG3	2:A:1142:HOH:O	2.03	0.58
1:A:398:ARG:HG2	1:A:406:HIS:CG	2.38	0.58
1:A:206:ASN:ND2	1:A:206:ASN:C	2.56	0.58
1:A:476:ASN:HA	1:A:525:LYS:O	2.02	0.58
1:A:43:PRO:HA	1:A:52:GLN:OE1	2.03	0.58
1:A:495:ARG:O	1:A:497:LYS:HE2	2.03	0.58
1:B:559:LYS:CE	1:B:559:LYS:HA	2.34	0.58
1:B:371:ILE:O	1:B:371:ILE:HG13	2.04	0.58
1:A:393:LYS:HD2	1:A:412:ILE:HD13	1.86	0.57
1:A:453:ILE:HG12	1:A:464:VAL:HB	1.86	0.57
1:B:53:LYS:O	1:B:56:VAL:HG12	2.05	0.57
1:A:70:GLU:O	1:A:86:ALA:HB1	2.05	0.57
1:B:527:ASN:ND2	1:B:530:ALA:HB3	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HG23	1:B:92:ILE:HD11	1.86	0.56
1:A:178:PHE:CZ	1:A:200:LEU:HD22	2.39	0.56
1:A:8:PHE:HB3	2:A:1009:HOH:O	2.05	0.56
1:A:103:ASP:OD2	1:A:105:TRP:HB2	2.05	0.56
1:A:251:THR:HG22	2:A:1449:HOH:O	2.05	0.56
1:A:160:PRO:HB2	1:A:161:PRO:HD3	1.88	0.56
1:A:209:PRO:HA	1:A:212:LYS:HG3	1.88	0.56
1:B:270:GLU:HG3	2:B:1050:HOH:O	2.04	0.56
1:B:37:VAL:O	1:B:42:ILE:HG13	2.06	0.56
1:B:58:ILE:HD11	1:B:87:ILE:HD11	1.88	0.56
1:A:497:LYS:CD	1:A:497:LYS:H	2.15	0.56
1:A:42:ILE:O	1:A:46:VAL:HB	2.06	0.55
1:A:291:VAL:O	1:A:374:PHE:HB3	2.07	0.55
1:B:340:VAL:CG2	1:B:343:THR:HG23	2.37	0.55
1:B:527:ASN:HD21	1:B:530:ALA:CB	2.19	0.55
1:A:270:GLU:HG2	2:A:1313:HOH:O	2.06	0.55
1:A:398:ARG:HG2	1:A:406:HIS:CD2	2.41	0.55
1:A:89:GLN:HG2	1:A:102:ILE:O	2.06	0.55
1:A:242:GLN:HG3	1:A:265:PHE:CE2	2.41	0.55
1:B:305:TYR:OH	1:B:387:LYS:HD2	2.07	0.55
1:A:497:LYS:N	1:A:497:LYS:HD2	2.15	0.54
1:B:93:ALA:HB1	1:B:97:ASN:ND2	2.22	0.54
1:A:340:VAL:HG11	1:A:399:HIS:CB	2.36	0.54
1:A:36:GLU:OE2	1:A:41:LYS:NZ	2.40	0.54
1:B:322:SER:O	1:B:323:LEU:HD23	2.08	0.54
1:B:305:TYR:CZ	1:B:387:LYS:HD2	2.42	0.54
1:B:57:ALA:O	1:B:60:ASN:HB2	2.07	0.54
1:A:298:THR:OG1	1:A:299:ASN:N	2.41	0.54
1:B:277:ARG:HG3	1:B:282:THR:HG21	1.90	0.54
1:B:13:ASN:HD22	1:B:229:MET:CE	2.20	0.54
1:A:556:GLU:O	1:A:556:GLU:HG3	2.06	0.54
1:B:86:ALA:HB3	1:B:89:GLN:HG3	1.89	0.53
1:A:432:PHE:O	1:A:436:TYR:HB2	2.08	0.53
1:A:373:GLN:HB2	2:A:1332:HOH:O	2.08	0.53
1:A:12:GLN:HG3	1:A:226:TYR:CE1	2.43	0.53
1:A:319:LYS:HE2	2:A:1347:HOH:O	2.07	0.53
1:A:309:ARG:HD2	1:A:347:ASP:OD2	2.09	0.53
1:A:359:GLU:HG3	1:A:361:LYS:HZ3	1.73	0.53
1:A:431:PHE:CD2	1:A:551:LEU:HD22	2.44	0.53
1:A:49:SER:O	1:A:53:LYS:HG3	2.08	0.53
1:B:190:SER:HB3	1:B:299:ASN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HG3	1:A:138:TYR:CZ	2.43	0.53
1:A:177:LYS:HE2	1:A:263:HIS:ND1	2.23	0.53
1:B:204:LEU:HD22	1:B:259:GLU:OE1	2.08	0.53
1:B:28:ASP:HB3	1:B:31:SER:HB2	1.90	0.53
1:A:297:ALA:HB3	1:A:307:ARG:HG3	1.92	0.52
1:A:276:ARG:HG3	1:A:276:ARG:NH1	2.21	0.52
1:B:215:ILE:HA	1:B:219:TRP:CD1	2.44	0.52
1:A:286:ARG:NH1	1:A:369:ASP:HA	2.24	0.52
1:A:388:SER:O	1:A:392:GLU:HG3	2.09	0.52
1:B:17:PHE:HD2	1:B:236:LYS:HD2	1.74	0.52
1:B:17:PHE:CE2	1:B:236:LYS:HD2	2.43	0.52
1:A:373:GLN:HG3	1:A:373:GLN:O	2.08	0.52
1:B:112:ARG:NH1	2:B:1509:HOH:O	2.41	0.52
1:B:66:TYR:HB2	1:B:71:LEU:HD21	1.91	0.52
1:B:258:LYS:HB3	2:B:1145:HOH:O	2.10	0.52
1:A:206:ASN:HD22	1:A:206:ASN:C	2.11	0.52
1:A:37:VAL:HG21	1:A:91:THR:HB	1.91	0.52
1:A:359:GLU:HG3	1:A:361:LYS:HZ2	1.75	0.52
1:A:455:THR:HG22	1:A:565:LEU:HD13	1.92	0.52
1:B:506:LYS:CB	1:B:506:LYS:HZ3	2.23	0.52
1:B:214:GLU:O	1:B:218:ASN:HB2	2.09	0.51
1:B:565:LEU:HA	1:B:568:VAL:HG13	1.91	0.51
1:B:571:LYS:HB3	1:B:577:ILE:HG12	1.92	0.51
1:B:58:ILE:CD1	1:B:87:ILE:HD11	2.40	0.51
1:A:228:ARG:NH1	2:A:1078:HOH:O	2.43	0.51
1:A:325:ILE:CG2	1:A:341:ILE:HD12	2.36	0.51
1:B:308:THR:O	1:B:312:LEU:HG	2.10	0.51
1:A:275:LEU:HD22	1:A:279:LYS:HD2	1.93	0.51
1:B:40:ILE:HG12	1:B:41:LYS:N	2.25	0.51
1:A:39:ASN:O	1:A:40:ILE:HG13	2.10	0.51
1:A:341:ILE:O	1:A:345:GLU:HG3	2.11	0.51
1:B:277:ARG:CG	1:B:282:THR:HG21	2.40	0.51
1:A:52:GLN:O	1:A:56:VAL:HG13	2.11	0.51
1:B:334:LYS:HD2	1:B:335:LEU:CD2	2.39	0.50
1:B:506:LYS:HB2	1:B:506:LYS:HZ3	1.76	0.50
1:B:164:ARG:HG2	1:B:353:ASN:O	2.11	0.50
1:B:357:PHE:O	1:B:367:LEU:HD12	2.11	0.50
1:B:242:GLN:HG3	1:B:265:PHE:CE1	2.46	0.50
1:A:571:LYS:HB3	1:A:577:ILE:HG12	1.93	0.50
1:A:83:PRO:HD2	2:A:1164:HOH:O	2.10	0.50
1:B:12:GLN:O	1:B:229:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HA	1:B:215:ILE:CD1	2.41	0.50
1:B:66:TYR:CB	1:B:71:LEU:HD21	2.42	0.50
1:B:55:LEU:O	1:B:58:ILE:HG13	2.12	0.50
1:B:506:LYS:NZ	1:B:506:LYS:CB	2.73	0.50
1:B:244:LYS:HA	1:B:261:ILE:O	2.11	0.50
1:A:191:GLY:O	1:A:222:SER:HB2	2.12	0.49
1:B:462:TYR:CE1	1:B:569:ARG:HB2	2.46	0.49
1:A:167:THR:O	1:A:170:GLU:HG2	2.12	0.49
1:A:568:VAL:O	1:A:571:LYS:HB2	2.12	0.49
1:B:34:HIS:CE1	1:B:64:LEU:HD11	2.46	0.49
1:B:359:GLU:OE2	1:B:361:LYS:HG3	2.12	0.49
1:A:484:GLU:HG3	1:A:488:TYR:CE2	2.47	0.49
1:B:220:GLU:HB2	1:B:224:ASP:HB2	1.94	0.49
1:A:171:ASP:HB2	1:A:173:GLN:NE2	2.27	0.49
1:B:566:GLU:CD	1:B:569:ARG:HH12	2.16	0.49
1:B:423:ILE:O	1:B:427:LYS:HB2	2.12	0.49
1:B:6:ARG:HD2	1:B:68:TYR:CE2	2.48	0.49
1:B:169:LEU:HD23	1:B:175:LEU:HD22	1.95	0.49
1:B:477:LEU:HD23	1:B:528:TYR:O	2.13	0.49
1:A:292:TYR:O	1:A:295:MET:HG2	2.14	0.48
1:A:406:HIS:O	1:A:409:ILE:HG23	2.13	0.48
1:B:455:THR:HG22	1:B:565:LEU:HD13	1.96	0.48
1:B:47:LYS:O	1:B:48:GLU:HB2	2.12	0.48
1:A:87:ILE:O	1:A:91:THR:CG2	2.60	0.48
1:B:566:GLU:CD	1:B:569:ARG:NH1	2.66	0.48
1:B:24:VAL:O	1:B:27:PHE:HB2	2.13	0.48
1:A:282:THR:HG23	1:A:284:PHE:O	2.14	0.48
1:A:509:PRO:HD2	1:A:512:VAL:HG21	1.95	0.48
1:A:247:PHE:O	1:A:258:LYS:HD3	2.13	0.48
1:A:359:GLU:HG2	1:A:360:ILE:N	2.27	0.48
1:B:204:LEU:HG	1:B:215:ILE:HD11	1.94	0.47
1:A:344:ILE:O	1:A:348:ILE:HG13	2.13	0.47
1:B:43:PRO:HA	1:B:52:GLN:CD	2.35	0.47
1:B:46:VAL:HG13	2:B:1336:HOH:O	2.14	0.47
1:A:453:ILE:CG1	1:A:464:VAL:HB	2.44	0.47
1:B:506:LYS:NZ	2:B:1388:HOH:O	2.47	0.47
1:B:484:GLU:HG3	1:B:487:ARG:NH2	2.29	0.47
1:B:98:LYS:HD2	1:B:99:LYS:HD2	1.96	0.47
1:B:412:ILE:O	1:B:416:ARG:HD2	2.14	0.47
1:A:390:LEU:HD21	1:A:412:ILE:HG22	1.96	0.47
1:B:502:ASN:C	1:B:502:ASN:OD1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HE3	1:B:54:GLU:OE2	2.15	0.47
1:A:475:TYR:CE1	1:A:478:PRO:HD2	2.50	0.47
1:A:171:ASP:HB2	1:A:173:GLN:CD	2.35	0.47
1:A:447:ARG:HD2	1:A:447:ARG:HA	1.70	0.47
1:A:388:SER:O	1:A:392:GLU:CG	2.63	0.47
1:A:62:HIS:HB3	2:A:1353:HOH:O	2.15	0.46
1:B:275:LEU:HD21	1:B:279:LYS:HZ2	1.80	0.46
1:B:83:PRO:HA	1:B:101:TYR:OH	2.15	0.46
1:A:272:LEU:O	1:A:276:ARG:HB2	2.15	0.46
1:A:244:LYS:NZ	1:A:246:GLU:OE2	2.49	0.46
1:A:423:ILE:O	1:A:427:LYS:HB2	2.16	0.46
1:B:502:ASN:O	1:B:503:GLU:C	2.52	0.46
1:B:170:GLU:OE1	1:B:279:LYS:NZ	2.46	0.46
1:A:486:GLN:O	1:A:490:GLU:HG3	2.15	0.46
1:B:97:ASN:HD21	1:B:100:GLY:HA2	1.79	0.46
1:B:367:LEU:HD12	1:B:368:LYS:N	2.31	0.46
1:B:23:VAL:CG2	1:B:92:ILE:HD11	2.45	0.46
1:B:5:ILE:CD1	1:B:304:GLU:HG3	2.46	0.45
1:B:67:THR:OG1	1:B:70:GLU:HG3	2.16	0.45
1:B:244:LYS:CB	1:B:262:SER:HA	2.47	0.45
1:B:171:ASP:HB2	1:B:173:GLN:CD	2.37	0.45
1:A:393:LYS:HD2	1:A:412:ILE:HG21	1.97	0.45
1:A:369:ASP:OD1	1:A:370:HIS:N	2.42	0.45
1:B:94:ASP:OD2	1:B:98:LYS:HG3	2.15	0.45
1:B:20:LEU:HD22	1:B:113:TRP:CE2	2.51	0.45
1:A:340:VAL:CG1	1:A:342:GLU:OE2	2.65	0.45
1:B:186:PHE:CD1	1:B:350:GLY:HA3	2.52	0.45
1:A:203:THR:HG22	1:A:215:ILE:HD13	1.99	0.45
1:A:394:LYS:HA	1:A:409:ILE:HD13	1.98	0.45
1:B:92:ILE:HB	1:B:102:ILE:HD11	1.99	0.45
1:B:334:LYS:HB3	1:B:334:LYS:HE2	1.64	0.45
1:A:314:LEU:O	1:A:318:ILE:HG13	2.17	0.45
1:B:529:LYS:O	1:B:532:LEU:N	2.49	0.45
1:B:37:VAL:CA	1:B:41:LYS:HB2	2.37	0.44
1:A:38:LYS:HB3	1:A:59:MET:HE2	1.98	0.44
1:B:290:ARG:HD3	2:B:1429:HOH:O	2.16	0.44
1:B:354:THR:HG22	1:B:354:THR:O	2.17	0.44
1:A:536:ASN:O	1:A:540:ASN:HA	2.18	0.44
1:A:215:ILE:O	1:A:219:TRP:HB2	2.17	0.44
1:A:490:GLU:O	1:A:494:THR:HG23	2.18	0.44
1:A:404:VAL:HG23	1:A:556:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HG23	1:B:331:ASN:HD22	1.82	0.44
1:A:360:ILE:HG12	1:A:365:TYR:CD2	2.53	0.44
1:B:93:ALA:HB1	1:B:97:ASN:HD22	1.82	0.44
1:B:193:THR:O	1:B:223:SER:HB2	2.17	0.44
1:A:28:ASP:OD1	1:A:28:ASP:C	2.55	0.44
1:B:309:ARG:HD2	1:B:347:ASP:OD2	2.17	0.44
1:B:312:LEU:O	1:B:316:ILE:HD12	2.17	0.44
1:B:146:ALA:O	1:B:150:GLU:HG3	2.18	0.44
1:A:37:VAL:CG2	1:A:91:THR:HB	2.47	0.43
1:B:94:ASP:N	1:B:94:ASP:OD1	2.52	0.43
1:B:215:ILE:HA	1:B:219:TRP:CG	2.53	0.43
1:B:243:GLY:O	1:B:264:ALA:HB3	2.17	0.43
1:B:331:ASN:HA	1:B:334:LYS:HE2	2.00	0.43
1:A:409:ILE:HD12	1:A:409:ILE:O	2.19	0.43
1:B:359:GLU:CD	1:B:361:LYS:HG3	2.39	0.43
1:B:109:GLY:O	1:B:113:TRP:HB2	2.19	0.43
1:A:240:VAL:HG13	1:A:241:LYS:N	2.33	0.43
1:A:186:PHE:CD1	1:A:350:GLY:HA3	2.54	0.43
1:A:502:ASN:O	1:A:503:GLU:C	2.56	0.43
1:B:474:GLY:CA	1:B:525:LYS:HG2	2.47	0.43
1:B:341:ILE:HA	1:B:344:ILE:HD12	2.00	0.43
1:B:566:GLU:OE1	1:B:569:ARG:NH1	2.52	0.43
1:A:244:LYS:HE2	1:A:260:PHE:CD2	2.54	0.43
1:B:283:LYS:HA	1:B:283:LYS:HD3	1.69	0.43
1:B:251:THR:CG2	1:B:252:LEU:N	2.82	0.43
1:A:25:GLN:O	1:A:31:SER:OG	2.32	0.43
1:B:387:LYS:HB2	1:B:391:GLU:HB2	2.01	0.43
1:B:200:LEU:O	1:B:200:LEU:HD13	2.19	0.43
1:A:61:GLN:HG3	1:A:61:GLN:H	1.51	0.42
1:A:503:GLU:HA	1:A:505:TRP:CH2	2.54	0.42
1:A:192:PHE:CZ	1:A:298:THR:HG23	2.55	0.42
1:B:244:LYS:HB3	1:B:262:SER:HA	2.00	0.42
1:A:91:THR:O	1:A:92:ILE:HD13	2.19	0.42
1:B:98:LYS:HD2	1:B:99:LYS:CD	2.49	0.42
1:B:42:ILE:HG23	1:B:46:VAL:HG21	2.01	0.42
1:B:302:ASP:HB2	2:B:1001:HOH:O	2.19	0.42
1:A:517:PHE:CE1	1:A:543:GLY:HA3	2.54	0.42
1:A:204:LEU:O	1:A:212:LYS:HE3	2.19	0.42
1:A:111:LEU:HD21	1:A:129:PHE:CZ	2.55	0.42
1:A:46:VAL:HG12	1:A:52:GLN:HB2	2.02	0.42
1:B:48:GLU:HG2	1:B:51:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HG	2:A:1074:HOH:O	2.20	0.42
1:B:97:ASN:HD22	1:B:97:ASN:HA	1.69	0.42
1:A:537:HIS:O	1:A:537:HIS:HD2	2.03	0.42
1:B:484:GLU:HG2	1:B:488:TYR:CE2	2.55	0.41
1:B:497:LYS:O	1:B:497:LYS:HG3	2.19	0.41
1:B:474:GLY:HA3	1:B:525:LYS:HD3	2.02	0.41
1:B:468:THR:HG22	1:B:520:VAL:HB	2.02	0.41
1:A:326:GLU:O	1:A:330:ASP:HB2	2.20	0.41
1:B:36:GLU:HG2	1:B:36:GLU:O	2.19	0.41
1:B:340:VAL:HG22	1:B:343:THR:HG23	2.02	0.41
1:A:124:ASN:O	1:A:125:LYS:CB	2.68	0.41
1:A:58:ILE:O	1:A:61:GLN:CG	2.65	0.41
1:B:469:LYS:HA	1:B:469:LYS:HE2	2.03	0.41
1:A:408:TYR:O	1:A:411:LEU:HG	2.21	0.41
1:B:42:ILE:HG22	1:B:52:GLN:CG	2.51	0.41
1:A:200:LEU:CD1	1:A:219:TRP:HB3	2.50	0.41
1:A:529:LYS:HB2	2:A:1127:HOH:O	2.19	0.41
1:B:277:ARG:O	1:B:286:ARG:HG2	2.21	0.41
1:B:474:GLY:HA3	1:B:525:LYS:CG	2.48	0.41
1:A:431:PHE:HD2	1:A:551:LEU:HD22	1.85	0.41
1:B:65:ILE:HG13	1:B:66:TYR:N	2.36	0.41
1:A:324:LYS:HG3	1:A:364:PHE:CE1	2.56	0.41
1:A:55:LEU:HD22	1:A:87:ILE:HG13	2.03	0.41
1:B:42:ILE:HG22	1:B:52:GLN:HG2	2.02	0.41
1:B:290:ARG:NH1	1:B:290:ARG:HG2	2.36	0.41
1:B:200:LEU:C	1:B:200:LEU:HD13	2.41	0.41
1:A:557:MET:HB3	1:A:563:LEU:CB	2.50	0.41
1:A:480:GLY:O	1:A:483:ASP:HB2	2.21	0.41
1:A:312:LEU:O	1:A:316:ILE:HG13	2.20	0.41
1:B:136:LEU:O	1:B:140:LYS:HG3	2.20	0.40
1:A:453:ILE:O	1:A:464:VAL:N	2.51	0.40
1:B:325:ILE:HD11	1:B:344:ILE:CG2	2.51	0.40
1:A:479:ILE:O	1:A:479:ILE:HG13	2.20	0.40
1:A:19:ASN:O	1:A:23:VAL:HG23	2.21	0.40
1:B:277:ARG:CA	1:B:282:THR:HG21	2.47	0.40
1:B:367:LEU:HD12	1:B:368:LYS:H	1.85	0.40
1:B:306:VAL:O	1:B:310:ARG:HG3	2.21	0.40
1:B:420:GLN:O	1:B:423:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	548/579 (95%)	514 (94%)	31 (6%)	3 (0%)	34	41
1	B	552/579 (95%)	512 (93%)	32 (6%)	8 (1%)	14	13
All	All	1100/1158 (95%)	1026 (93%)	63 (6%)	11 (1%)	19	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	GLU
1	A	400	LYS
1	A	48	GLU
1	B	503	GLU
1	B	14	PRO
1	B	145	SER
1	A	503	GLU
1	B	124	ASN
1	B	144	GLY
1	B	377	PRO
1	B	40	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	478/503 (95%)	406 (85%)	72 (15%)	3	3
1	B	475/503 (94%)	411 (86%)	64 (14%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	953/1006 (95%)	817 (86%)	136 (14%)	4 4

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	16	LYS
1	A	26	VAL
1	A	32	LYS
1	A	38	LYS
1	A	48	GLU
1	A	52	GLN
1	A	58	ILE
1	A	61	GLN
1	A	76	THR
1	A	91	THR
1	A	106	SER
1	A	111	LEU
1	A	133	ASP
1	A	140	LYS
1	A	147	ILE
1	A	150	GLU
1	A	182	LYS
1	A	200	LEU
1	A	202	ASP
1	A	206	ASN
1	A	208	MET
1	A	210	LYS
1	A	219	TRP
1	A	222	SER
1	A	225	LYS
1	A	241	LYS
1	A	244	LYS
1	A	251	THR
1	A	258	LYS
1	A	262	SER
1	A	275	LEU
1	A	276	ARG
1	A	277	ARG
1	A	279	LYS
1	A	285	THR
1	A	292	TYR

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Mol	Chain	Res	Type
1	A	302	ASP
1	A	314	LEU
1	A	319	LYS
1	A	323	LEU
1	A	324	LYS
1	A	330	ASP
1	A	332	LEU
1	A	334	LYS
1	A	338	ASP
1	A	339	GLU
1	A	354	THR
1	A	359	GLU
1	A	367	LEU
1	A	378	ASN
1	A	379	ARG
1	A	387	LYS
1	A	390	LEU
1	A	395	SER
1	A	400	LYS
1	A	409	ILE
1	A	414	ILE
1	A	418	SER
1	A	429	MET
1	A	439	ARG
1	A	458	SER
1	A	479	ILE
1	A	481	GLN
1	A	484	GLU
1	A	485	MET
1	A	497	LYS
1	A	511	SER
1	A	527	ASN
1	A	532	LEU
1	A	546	LEU
1	A	551	LEU
1	B	40	ILE
1	B	56	VAL
1	B	60	ASN
1	B	65	ILE
1	B	68	TYR
1	B	69	LYS
1	B	97	ASN

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Mol	Chain	Res	Type
1	B	98	LYS
1	B	99	LYS
1	B	130	VAL
1	B	136	LEU
1	B	156	ILE
1	B	157	SER
1	B	175	LEU
1	B	182	LYS
1	B	190	SER
1	B	210	LYS
1	B	215	ILE
1	B	222	SER
1	B	225	LYS
1	B	246	GLU
1	B	251	THR
1	B	254	LYS
1	B	266	LYS
1	B	276	ARG
1	B	285	THR
1	B	292	TYR
1	B	295	MET
1	B	301	THR
1	B	303	LYS
1	B	310	ARG
1	B	314	LEU
1	B	319	LYS
1	B	322	SER
1	B	332	LEU
1	B	334	LYS
1	B	359	GLU
1	B	368	LYS
1	B	371	ILE
1	B	375	VAL
1	B	387	LYS
1	B	389	GLU
1	B	393	LYS
1	B	407	GLU
1	B	412	ILE
1	B	413	GLU
1	B	416	ARG
1	B	429	MET
1	B	433	MET

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Mol	Chain	Res	Type
1	B	441	LYS
1	B	458	SER
1	B	469	LYS
1	B	472	SER
1	B	481	GLN
1	B	497	LYS
1	B	503	GLU
1	B	506	LYS
1	B	518	LEU
1	B	523	HIS
1	B	525	LYS
1	B	532	LEU
1	B	537	HIS
1	B	545	VAL
1	B	559	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	19	ASN
1	A	34	HIS
1	A	206	ASN
1	A	331	ASN
1	A	366	GLN
1	A	406	HIS
1	A	527	ASN
1	A	578	ASN
1	B	13	ASN
1	B	39	ASN
1	B	60	ASN
1	B	97	ASN
1	B	331	ASN
1	B	373	GLN
1	B	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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