Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:58 pm GMT

PDB ID	:	1YF2
Title	:	Three-dimensional structure of DNA sequence specificity (S) subunit of a type I restriction-modification enzyme and its functional implications
Authors	:	Kim, J.S.; Degiovanni, A.; Jancarik, J.; Adams, P.D.; Yokota, H.A.; Kim, R.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2004-12-30
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/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:

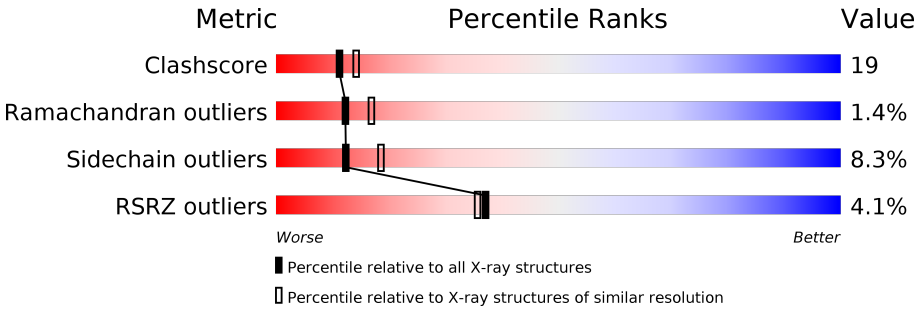
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

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 2.40 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	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	425	7% 60% 36%
1	B	425	2% 61% 33% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7157 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 Type I restriction-modification enzyme, S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3412	2201	558	644	9			
1	B	425	Total	C	N	O	S	0	0	0
			3416	2204	559	644	9			

- Molecule 2 is water.

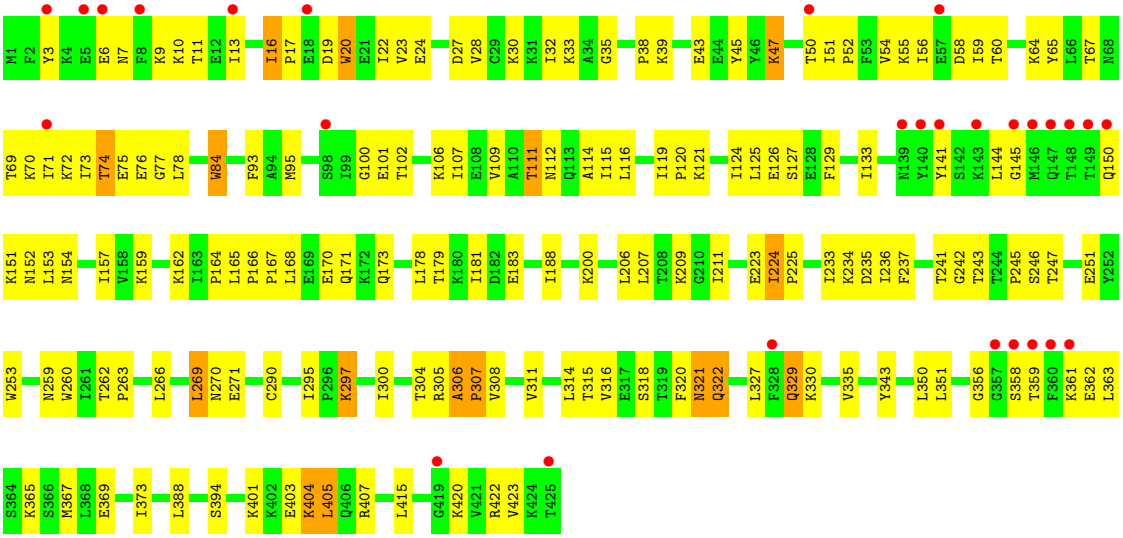
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	179	Total	O	0	0
			179	179		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

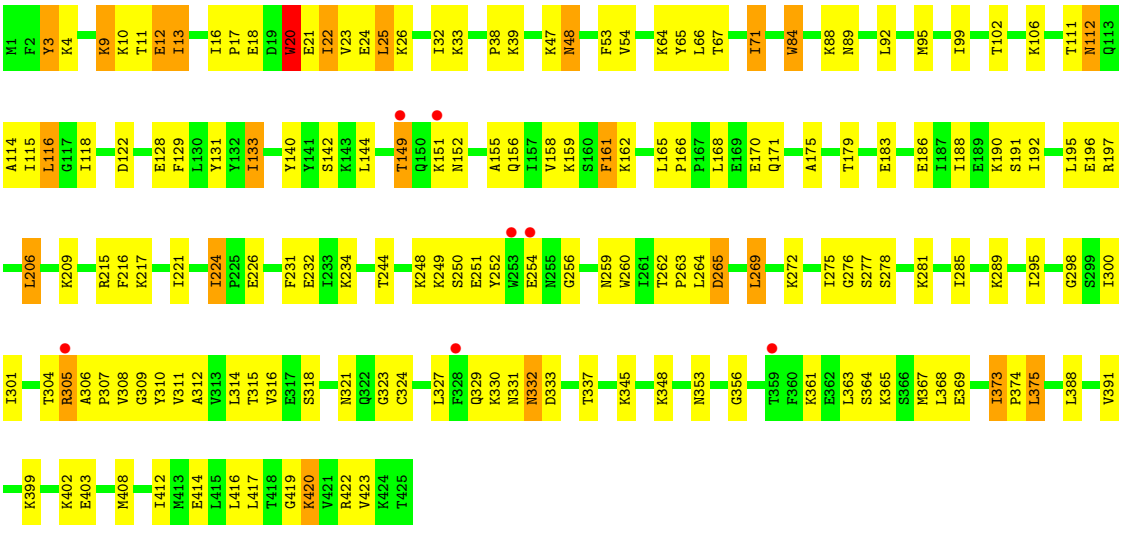
• Molecule 1: Type I restriction-modification enzyme, S subunit

Chain A:



• Molecule 1: Type I restriction-modification enzyme, S subunit

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.97Å 94.22Å 103.52Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	48.52 – 2.40 48.52 – 2.21	Depositor EDS
% Data completeness (in resolution range)	93.7 (48.52-2.40) 81.6 (48.52-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.65 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.279 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.56	0/3469	0.62	0/4661
1	B	0.59	0/3473	0.66	0/4665
All	All	0.58	0/6942	0.64	0/9326

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	3412	0	3574	131	0
1	B	3416	0	3585	137	0
2	A	150	0	0	3	0
2	B	179	0	0	2	0
All	All	7157	0	7159	267	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 19.

All (267) 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:269:LEU:HD21	1:B:275:ILE:HG22	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:N	1:A:329:GLN:OE1	1.99	0.95
1:A:70:LYS:HG3	1:A:71:ILE:HG13	1.53	0.90
1:B:275:ILE:HD11	1:B:314:LEU:HD12	1.56	0.88
1:B:215:ARG:HD2	2:B:574:HOH:O	1.76	0.85
1:B:234:LYS:HB3	1:B:369:GLU:HB2	1.59	0.84
1:A:145:GLY:HA2	1:A:150:GLN:HA	1.60	0.83
1:B:12:GLU:HG2	1:B:22:ILE:HG21	1.61	0.82
1:B:269:LEU:HB2	1:B:272:LYS:HB2	1.61	0.82
1:A:329:GLN:CD	1:A:329:GLN:H	1.83	0.81
1:A:16:ILE:HD11	1:A:164:PRO:HB3	1.63	0.80
1:A:306:ALA:HB1	1:A:307:PRO:CD	2.10	0.80
1:B:259:ASN:HB2	1:B:318:SER:CB	2.13	0.77
1:B:259:ASN:HB2	1:B:318:SER:HB2	1.64	0.77
1:A:154:ASN:H	1:A:157:ILE:HD12	1.51	0.76
1:A:129:PHE:O	1:A:133:ILE:HD13	1.87	0.75
1:B:10:LYS:HE2	1:B:18:GLU:HA	1.67	0.75
1:B:263:PRO:HG2	1:B:264:LEU:HD22	1.69	0.74
1:A:306:ALA:HB1	1:A:307:PRO:HD3	1.69	0.74
1:B:263:PRO:HG3	1:B:305:ARG:HD2	1.69	0.74
1:B:306:ALA:HB3	1:B:307:PRO:HD3	1.69	0.74
1:B:26:LYS:HB3	1:B:159:LYS:HB3	1.68	0.74
1:A:188:ILE:HD11	1:A:401:LYS:HE3	1.69	0.73
1:A:179:THR:O	1:A:183:GLU:HG3	1.89	0.72
1:A:30:LYS:HE2	1:A:119:ILE:HG21	1.70	0.72
1:B:112:ASN:C	1:B:112:ASN:HD22	1.93	0.72
1:A:9:LYS:HB2	1:A:16:ILE:O	1.90	0.71
1:B:365:LYS:O	1:B:369:GLU:HG2	1.91	0.71
1:A:55:LYS:HA	1:A:112:ASN:HD21	1.56	0.71
1:B:263:PRO:HG3	1:B:305:ARG:HH11	1.57	0.69
1:A:55:LYS:HA	1:A:112:ASN:ND2	2.08	0.69
1:B:304:THR:HG22	1:B:363:LEU:HB3	1.76	0.67
1:B:12:GLU:OE1	1:B:13:ILE:HG23	1.95	0.66
1:B:269:LEU:CD2	1:B:275:ILE:HG22	2.23	0.66
1:A:173:GLN:HB3	1:A:423:VAL:HG21	1.76	0.66
1:B:234:LYS:O	1:B:330:LYS:HE3	1.97	0.64
1:A:266:LEU:O	1:A:269:LEU:HB2	1.97	0.64
1:A:22:ILE:HD12	1:A:22:ILE:H	1.63	0.64
1:A:121:LYS:HB2	1:A:124:ILE:HB	1.78	0.64
1:A:32:ILE:HD12	1:A:159:LYS:HG2	1.79	0.63
1:A:306:ALA:CB	1:A:307:PRO:CD	2.76	0.63
1:A:403:GLU:HB3	1:A:407:ARG:HH12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HG2	1:B:171:GLN:HG3	1.81	0.63
1:A:111:THR:HB	1:A:115:ILE:HB	1.81	0.63
1:B:231:PHE:CE1	1:B:375:LEU:HD12	2.34	0.63
1:A:13:ILE:HG21	1:A:162:LYS:HB3	1.81	0.63
1:A:59:ILE:HG22	1:A:101:GLU:HG3	1.81	0.63
1:B:16:ILE:HG23	1:B:20:TRP:HB2	1.80	0.62
1:A:236:ILE:CG2	1:A:335:VAL:HG21	2.29	0.62
1:B:259:ASN:ND2	1:B:277:SER:HA	2.14	0.62
1:B:221:ILE:HG13	1:B:224:ILE:HD13	1.82	0.62
1:B:231:PHE:HE1	1:B:375:LEU:HD12	1.65	0.61
1:A:404:LYS:HD2	1:A:405:LEU:N	2.16	0.61
1:A:236:ILE:HG21	1:A:335:VAL:HG21	1.83	0.61
1:B:306:ALA:HB3	1:B:307:PRO:CD	2.31	0.61
1:A:52:PRO:HG2	1:A:109:VAL:HG12	1.82	0.60
1:B:329:GLN:CD	1:B:329:GLN:H	2.04	0.60
1:B:22:ILE:HD11	1:B:162:LYS:HD2	1.82	0.60
1:A:211:ILE:HD11	1:B:206:LEU:HD13	1.82	0.60
1:B:192:ILE:HD13	1:B:399:LYS:HG2	1.84	0.60
1:B:12:GLU:O	1:B:13:ILE:HG13	2.02	0.60
1:A:23:VAL:HG21	1:A:28:VAL:HG13	1.85	0.59
1:A:243:THR:HA	1:A:322:GLN:HG3	1.84	0.59
1:B:259:ASN:HB2	1:B:318:SER:HB3	1.84	0.59
1:B:20:TRP:CE2	1:B:166:PRO:HB3	2.37	0.59
1:B:20:TRP:CZ2	1:B:166:PRO:HB3	2.38	0.58
1:B:24:GLU:OE1	1:B:26:LYS:HE3	2.03	0.58
1:A:154:ASN:HB3	1:A:157:ILE:HG13	1.86	0.58
1:B:262:THR:HB	1:B:263:PRO:HD2	1.83	0.58
1:A:223:GLU:O	1:A:224:ILE:HD12	2.03	0.58
1:A:305:ARG:HG2	1:A:362:GLU:HG3	1.85	0.58
1:B:329:GLN:NE2	1:B:332:ASN:HD22	2.02	0.58
1:B:275:ILE:HD11	1:B:314:LEU:CD1	2.29	0.58
1:A:74:THR:HG22	1:A:75:GLU:H	1.69	0.58
1:A:359:THR:HG23	2:A:514:HOH:O	2.05	0.57
1:B:275:ILE:O	1:B:275:ILE:HG13	2.03	0.57
1:A:188:ILE:HD13	1:A:401:LYS:HG2	1.86	0.57
1:B:20:TRP:HH2	1:B:170:GLU:OE1	1.88	0.57
1:A:67:THR:HG22	1:A:106:LYS:HB2	1.87	0.56
1:A:356:GLY:HA2	1:A:361:LYS:HG2	1.85	0.56
1:A:150:GLN:O	1:A:151:LYS:HD2	2.05	0.56
1:B:158:VAL:HG13	1:B:161:PHE:CZ	2.40	0.56
1:A:23:VAL:HG11	1:A:28:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:TYR:HB3	1:B:423:VAL:HA	1.88	0.56
1:A:112:ASN:OD1	1:A:114:ALA:HB3	2.05	0.56
1:B:140:TYR:CE2	1:B:144:LEU:HD11	2.40	0.56
1:B:311:VAL:O	1:B:345:LYS:HE3	2.06	0.56
1:A:209:LYS:NZ	1:A:223:GLU:HB3	2.20	0.56
1:A:64:LYS:HE2	1:A:65:TYR:CZ	2.41	0.56
1:B:305:ARG:O	1:B:308:VAL:HG23	2.06	0.56
1:A:35:GLY:HA3	1:A:111:THR:O	2.06	0.55
1:B:133:ILE:HD12	1:B:417:LEU:HD22	1.88	0.55
1:B:54:VAL:HB	1:B:111:THR:HG22	1.87	0.55
1:B:95:MET:O	1:B:99:ILE:HG12	2.06	0.55
1:A:16:ILE:HG23	1:A:20:TRP:HB2	1.87	0.55
1:A:93:PHE:HE2	1:A:153:LEU:HD13	1.72	0.55
1:A:260:TRP:CZ2	1:A:321:ASN:HB3	2.42	0.55
1:B:17:PRO:HD3	1:B:419:GLY:CA	2.36	0.54
1:A:107:ILE:O	1:A:109:VAL:HG13	2.07	0.54
1:B:95:MET:SD	1:B:116:LEU:HD22	2.47	0.54
1:A:95:MET:SD	1:A:116:LEU:HD13	2.48	0.54
1:A:52:PRO:CG	1:A:109:VAL:HG12	2.38	0.54
1:A:23:VAL:HG22	1:A:24:GLU:N	2.23	0.54
1:A:20:TRP:CE2	1:A:166:PRO:HB3	2.43	0.53
1:B:129:PHE:CG	1:B:171:GLN:HG2	2.44	0.53
1:A:115:ILE:N	1:A:115:ILE:HD12	2.24	0.53
1:B:22:ILE:HD13	1:B:22:ILE:C	2.28	0.53
1:B:217:LYS:HD3	1:B:226:GLU:HA	1.90	0.53
1:B:48:ASN:ND2	1:B:48:ASN:H	2.06	0.52
1:A:234:LYS:HG3	1:A:235:ASP:N	2.24	0.52
1:B:311:VAL:HB	1:B:345:LYS:HG3	1.91	0.52
1:B:112:ASN:C	1:B:112:ASN:ND2	2.63	0.51
1:B:262:THR:H	1:B:265:ASP:HB2	1.75	0.51
1:B:329:GLN:CD	1:B:329:GLN:N	2.60	0.51
1:B:414:GLU:OE2	1:B:420:LYS:HE2	2.11	0.51
1:A:93:PHE:CD1	1:A:102:THR:HG22	2.45	0.51
1:A:43:GLU:HG2	1:A:47:LYS:HB2	1.92	0.51
1:A:38:PRO:HG3	1:A:73:ILE:HD12	1.92	0.51
1:B:88:LYS:O	1:B:89:ASN:HB2	2.11	0.51
1:A:120:PRO:HB2	1:A:125:LEU:O	2.09	0.51
1:A:245:PRO:HG2	1:A:253:TRP:CZ2	2.46	0.50
1:B:232:GLU:OE1	1:B:234:LYS:HE2	2.11	0.50
1:A:126:GLU:H	1:A:171:GLN:NE2	2.09	0.50
1:A:32:ILE:HB	1:A:159:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HG22	1:A:363:LEU:HB3	1.93	0.50
1:A:224:ILE:HD11	2:A:435:HOH:O	2.12	0.50
1:A:270:ASN:O	1:A:271:GLU:HB2	2.12	0.50
1:B:264:LEU:HD22	1:B:264:LEU:H	1.76	0.50
1:B:305:ARG:HB2	1:B:323:GLY:HA3	1.93	0.50
1:B:151:LYS:O	1:B:152:ASN:HB2	2.12	0.50
1:A:363:LEU:HD23	1:A:367:MET:HB2	1.93	0.50
1:A:28:VAL:HG11	1:A:165:LEU:HD22	1.94	0.50
1:A:304:THR:O	1:A:362:GLU:HA	2.12	0.50
1:B:92:LEU:O	1:B:102:THR:HA	2.12	0.50
1:B:329:GLN:OE1	1:B:329:GLN:N	2.33	0.50
1:A:20:TRP:HE3	1:A:20:TRP:N	2.09	0.49
1:A:93:PHE:HD1	1:A:102:THR:HG22	1.76	0.49
1:B:298:GLY:O	1:B:337:THR:HG21	2.13	0.49
1:A:415:LEU:HA	1:A:420:LYS:HG3	1.94	0.49
1:A:55:LYS:HG2	1:A:112:ASN:HD22	1.76	0.49
1:B:155:ALA:O	1:B:159:LYS:HG3	2.13	0.49
1:A:259:ASN:HB2	1:A:318:SER:HB2	1.94	0.49
1:A:351:LEU:HD22	1:A:363:LEU:HD11	1.95	0.49
1:B:263:PRO:CG	1:B:305:ARG:HD2	2.41	0.49
1:A:6:GLU:OE2	1:A:420:LYS:HA	2.12	0.48
1:A:356:GLY:C	1:A:358:SER:H	2.16	0.48
1:A:297:LYS:NZ	1:A:297:LYS:HB2	2.29	0.48
1:A:52:PRO:HB3	1:A:69:THR:HG21	1.95	0.48
1:A:73:ILE:HD11	1:A:77:GLY:C	2.34	0.48
1:B:197:ARG:HG3	2:B:572:HOH:O	2.13	0.48
1:B:221:ILE:HD12	1:B:374:PRO:HG3	1.94	0.48
1:B:48:ASN:HD22	1:B:48:ASN:H	1.62	0.48
1:A:56:ILE:N	1:A:115:ILE:HD11	2.29	0.47
1:A:356:GLY:HA3	1:A:361:LYS:HE2	1.95	0.47
1:B:149:THR:HB	1:B:151:LYS:HG3	1.96	0.47
1:B:186:GLU:HG3	1:B:190:LYS:NZ	2.29	0.47
1:A:45:TYR:CE1	1:A:76:GLU:HG2	2.49	0.47
1:B:256:GLY:HA3	1:B:281:LYS:HB2	1.95	0.47
1:B:300:ILE:HB	1:B:327:LEU:HB2	1.97	0.47
1:A:401:LYS:O	1:A:404:LYS:HG3	2.14	0.47
1:B:301:ILE:HD11	1:B:324:CYS:HB3	1.95	0.47
1:A:24:GLU:HB2	1:A:27:ASP:OD2	2.15	0.47
1:B:158:VAL:HA	1:B:161:PHE:CE2	2.50	0.47
1:B:17:PRO:HD3	1:B:419:GLY:HA2	1.95	0.47
1:A:126:GLU:H	1:A:171:GLN:HE22	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PRO:HG3	1:B:305:ARG:NH1	2.28	0.46
1:A:60:THR:HA	1:A:101:GLU:OE1	2.15	0.46
1:B:23:VAL:O	1:B:162:LYS:HA	2.14	0.46
1:B:25:LEU:HD22	1:B:161:PHE:CE1	2.50	0.46
1:B:275:ILE:HG23	1:B:312:ALA:HB1	1.97	0.46
1:B:20:TRP:CH2	1:B:170:GLU:OE1	2.67	0.46
1:B:64:LYS:HD3	1:B:65:TYR:CE1	2.51	0.46
1:A:245:PRO:HB3	1:A:290:CYS:SG	2.56	0.46
1:B:129:PHE:CZ	1:B:133:ILE:HD13	2.50	0.46
1:B:331:ASN:HD21	1:B:333:ASP:HB2	1.80	0.46
1:B:64:LYS:HG3	1:B:131:TYR:CZ	2.51	0.46
1:A:262:THR:HB	1:A:263:PRO:HD2	1.98	0.46
1:B:3:TYR:CB	1:B:422:ARG:O	2.64	0.46
1:A:58:ASP:OD2	1:A:69:THR:HA	2.16	0.46
1:B:158:VAL:HG13	1:B:161:PHE:HZ	1.79	0.46
1:B:264:LEU:HD22	1:B:264:LEU:N	2.30	0.46
1:B:252:TYR:OH	1:B:289:LYS:HD3	2.16	0.46
1:B:276:GLY:O	1:B:316:VAL:HG12	2.16	0.46
1:B:179:THR:O	1:B:183:GLU:HG3	2.16	0.45
1:B:112:ASN:ND2	1:B:114:ALA:H	2.14	0.45
1:B:251:GLU:O	1:B:285:ILE:HD12	2.16	0.45
1:A:365:LYS:HE2	1:A:369:GLU:OE2	2.16	0.45
1:A:38:PRO:HG3	1:A:73:ILE:CD1	2.46	0.45
1:A:51:ILE:HD13	1:A:78:LEU:HD22	1.98	0.45
1:B:305:ARG:HB2	1:B:323:GLY:CA	2.47	0.45
1:A:24:GLU:O	1:A:28:VAL:HG22	2.17	0.45
1:A:306:ALA:O	1:A:308:VAL:N	2.50	0.45
1:B:9:LYS:HA	1:B:17:PRO:HA	1.98	0.45
1:A:17:PRO:HG2	1:A:20:TRP:CD2	2.51	0.45
1:A:125:LEU:HA	1:A:171:GLN:HE22	1.81	0.45
1:A:71:ILE:HG22	1:A:72:LYS:N	2.32	0.45
1:B:54:VAL:HG12	1:B:115:ILE:HD13	1.99	0.45
1:A:33:LYS:O	1:A:84:TRP:CH2	2.70	0.44
1:B:412:ILE:HG23	1:B:416:LEU:CD2	2.47	0.44
1:A:300:ILE:HB	1:A:327:LEU:HB2	1.99	0.44
1:B:129:PHE:CD2	1:B:171:GLN:HG2	2.53	0.44
1:B:248:LYS:O	1:B:250:SER:N	2.49	0.44
1:B:188:ILE:HG21	1:B:402:LYS:HB2	1.99	0.44
1:A:295:ILE:HG13	1:A:314:LEU:CD2	2.48	0.44
1:A:52:PRO:CB	1:A:69:THR:HG21	2.47	0.44
1:B:151:LYS:O	1:B:152:ASN:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LYS:O	1:B:403:GLU:HG3	2.17	0.44
1:B:305:ARG:CG	1:B:306:ALA:H	2.31	0.44
1:A:403:GLU:HB3	1:A:407:ARG:NH1	2.30	0.44
1:A:242:GLY:O	1:A:243:THR:HG23	2.18	0.43
1:A:75:GLU:O	1:A:78:LEU:HB3	2.18	0.43
1:B:140:TYR:O	1:B:144:LEU:HG	2.18	0.43
1:A:166:PRO:HG2	1:A:171:GLN:CG	2.48	0.43
1:B:38:PRO:O	1:B:39:LYS:C	2.57	0.43
1:A:6:GLU:HB3	1:A:9:LYS:NZ	2.33	0.43
1:A:167:PRO:HD2	1:A:170:GLU:OE1	2.19	0.42
1:B:209:LYS:HG3	1:B:216:PHE:CE2	2.54	0.42
1:A:233:ILE:HD13	1:A:373:ILE:HD13	2.00	0.42
1:B:95:MET:CE	1:B:116:LEU:HD13	2.49	0.42
1:B:188:ILE:O	1:B:191:SER:HB3	2.19	0.42
1:B:295:ILE:HG13	1:B:314:LEU:HD22	2.00	0.42
1:B:373:ILE:HA	1:B:374:PRO:HD3	1.84	0.42
1:B:353:ASN:O	1:B:356:GLY:N	2.51	0.42
1:B:53:PHE:HB3	1:B:71:ILE:HG22	2.01	0.42
1:A:166:PRO:HG2	1:A:171:GLN:HG3	2.02	0.42
1:B:128:GLU:HB3	1:B:175:ALA:HB1	2.00	0.42
1:B:22:ILE:HD11	1:B:162:LYS:HB3	2.01	0.42
1:B:364:SER:H	1:B:367:MET:HE3	1.85	0.42
1:B:309:GLY:HA3	1:B:348:LYS:HG3	2.01	0.42
1:B:329:GLN:HE21	1:B:332:ASN:HD22	1.66	0.42
1:B:106:LYS:HB3	1:B:106:LYS:HE3	1.84	0.42
1:B:32:ILE:O	1:B:32:ILE:HG22	2.19	0.42
1:A:207:LEU:HD13	1:A:343:TYR:HA	2.02	0.41
1:B:361:LYS:HD2	1:B:361:LYS:N	2.35	0.41
1:B:33:LYS:HB3	1:B:84:TRP:CZ3	2.54	0.41
1:A:242:GLY:HA3	1:A:320:PHE:O	2.20	0.41
1:B:259:ASN:HD22	1:B:278:SER:H	1.68	0.41
1:B:32:ILE:HG12	1:B:118:ILE:HG23	2.02	0.41
1:A:45:TYR:HE1	1:A:76:GLU:HG2	1.85	0.41
1:A:50:THR:HG23	1:A:51:ILE:HG13	2.01	0.41
1:B:250:SER:C	1:B:252:TYR:H	2.23	0.41
1:B:251:GLU:HA	1:B:254:GLU:CG	2.51	0.41
1:B:304:THR:CG2	1:B:363:LEU:HB3	2.47	0.41
1:B:21:GLU:O	1:B:165:LEU:HB3	2.20	0.41
1:A:95:MET:HB3	1:A:153:LEU:O	2.20	0.41
1:A:30:LYS:HE2	1:A:119:ILE:CG2	2.45	0.41
1:A:350:LEU:HD23	1:A:350:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:THR:HG23	1:B:260:TRP:CZ2	2.55	0.41
1:A:178:LEU:HD23	1:A:181:ILE:HD12	2.03	0.41
1:B:16:ILE:HG23	1:B:20:TRP:CB	2.48	0.41
1:A:100:GLY:O	1:A:102:THR:HG23	2.21	0.41
1:A:111:THR:CB	1:A:115:ILE:HB	2.48	0.41
1:A:141:TYR:O	1:A:144:LEU:HG	2.21	0.41
1:B:275:ILE:HD13	1:B:301:ILE:HG21	2.03	0.41
1:A:51:ILE:HB	1:A:73:ILE:HG23	2.03	0.41
1:A:224:ILE:HG23	1:A:225:PRO:N	2.35	0.41
1:A:51:ILE:O	1:A:73:ILE:HG22	2.21	0.41
1:B:66:LEU:HD13	1:B:66:LEU:C	2.41	0.41
1:A:173:GLN:NE2	1:A:423:VAL:HG11	2.37	0.40
1:A:3:TYR:CB	1:A:422:ARG:HB2	2.51	0.40
1:A:54:VAL:HG21	1:A:109:VAL:HG21	2.03	0.40
1:A:290:CYS:SG	2:A:432:HOH:O	2.63	0.40
1:B:275:ILE:O	1:B:315:THR:HB	2.20	0.40
1:A:13:ILE:HG23	1:A:22:ILE:HG21	2.04	0.40
1:A:245:PRO:O	1:A:246:SER:C	2.60	0.40
1:A:237:PHE:CE2	1:A:329:GLN:HG3	2.56	0.40
1:B:307:PRO:HB2	1:B:310:TYR:HE1	1.87	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	423/425 (100%)	378 (89%)	38 (9%)	7 (2%)	10	13
1	B	423/425 (100%)	379 (90%)	39 (9%)	5 (1%)	14	20
All	All	846/850 (100%)	757 (90%)	77 (9%)	12 (1%)	12	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	B	47	LYS
1	B	420	LYS
1	A	11	THR
1	A	39	LYS
1	A	306	ALA
1	B	12	GLU
1	B	249	LYS
1	A	10	LYS
1	B	20	TRP
1	A	47	LYS
1	A	307	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	385/387 (100%)	357 (93%)	28 (7%)	15 24
1	B	386/387 (100%)	350 (91%)	36 (9%)	10 14
All	All	771/774 (100%)	707 (92%)	64 (8%)	12 18

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	16	ILE
1	A	19	ASP
1	A	20	TRP
1	A	74	THR
1	A	84	TRP
1	A	111	THR
1	A	127	SER
1	A	168	LEU
1	A	200	LYS
1	A	206	LEU
1	A	224	ILE

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Mol	Chain	Res	Type
1	A	241	THR
1	A	247	THR
1	A	251	GLU
1	A	269	LEU
1	A	297	LYS
1	A	311	VAL
1	A	315	THR
1	A	316	VAL
1	A	321	ASN
1	A	322	GLN
1	A	329	GLN
1	A	330	LYS
1	A	388	LEU
1	A	394	SER
1	A	404	LYS
1	A	405	LEU
1	B	3	TYR
1	B	4	LYS
1	B	9	LYS
1	B	11	THR
1	B	13	ILE
1	B	20	TRP
1	B	22	ILE
1	B	25	LEU
1	B	48	ASN
1	B	67	THR
1	B	71	ILE
1	B	84	TRP
1	B	112	ASN
1	B	116	LEU
1	B	122	ASP
1	B	133	ILE
1	B	142	SER
1	B	149	THR
1	B	156	GLN
1	B	161	PHE
1	B	168	LEU
1	B	195	LEU
1	B	196	GLU
1	B	206	LEU
1	B	224	ILE
1	B	265	ASP

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	305	ARG
1	B	321	ASN
1	B	332	ASN
1	B	368	LEU
1	B	373	ILE
1	B	375	LEU
1	B	388	LEU
1	B	391	VAL
1	B	408	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	89	ASN
1	A	139	ASN
1	A	171	GLN
1	A	255	ASN
1	A	270	ASN
1	A	321	ASN
1	A	400	GLN
1	A	406	GLN
1	B	48	ASN
1	B	68	ASN
1	B	112	ASN
1	B	147	GLN
1	B	255	ASN
1	B	259	ASN
1	B	293	ASN
1	B	331	ASN
1	B	332	ASN
1	B	353	ASN
1	B	370	ASN
1	B	400	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	425/425 (100%)	0.15	28 (6%) 18 16	37, 73, 144, 187	0
1	B	425/425 (100%)	-0.16	7 (1%) 72 69	38, 62, 114, 154	0
All	All	850/850 (100%)	-0.00	35 (4%) 37 36	37, 66, 128, 187	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	TYR	6.2
1	A	8	PHE	5.8
1	A	419	GLY	5.8
1	A	149	THR	5.7
1	A	148	THR	5.4
1	A	98	SER	5.1
1	A	143	LYS	5.0
1	A	140	TYR	4.9
1	A	150	GLN	4.7
1	A	359	THR	4.6
1	A	139	ASN	4.1
1	A	360	PHE	3.8
1	A	13	ILE	3.7
1	A	3	TYR	3.6
1	B	149	THR	3.4
1	A	18	GLU	3.4
1	B	328	PHE	3.3
1	B	253	TRP	3.2
1	A	361	LYS	3.0
1	A	147	GLN	2.9
1	A	328	PHE	2.9
1	B	359	THR	2.9
1	A	5	GLU	2.8
1	A	145	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	ILE	2.6
1	A	425	THR	2.4
1	A	357	GLY	2.3
1	B	151	LYS	2.3
1	B	254	GLU	2.3
1	B	305	ARG	2.3
1	A	146	MET	2.3
1	A	50	THR	2.3
1	A	358	SER	2.2
1	A	6	GLU	2.1
1	A	57	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.