Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:28 PM GMT

PDB ID	:	1KHD
Title	:	Crystal Structure Analysis of the anthranilate phosphoribosyltransferase from Erwinia carotovora at 1.9 resolution (current name, Pectobacterium carotovorum)
Authors	:	Kim, C.; Xuong, N.-H.; Edwards, S.; Madhusudan; Yee, M.-C.; Spraggon, G.; Mills, S.E.
Deposited on	:	2001-11-29
Resolution	:	1.86 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 (i)) were used in the production of this report:

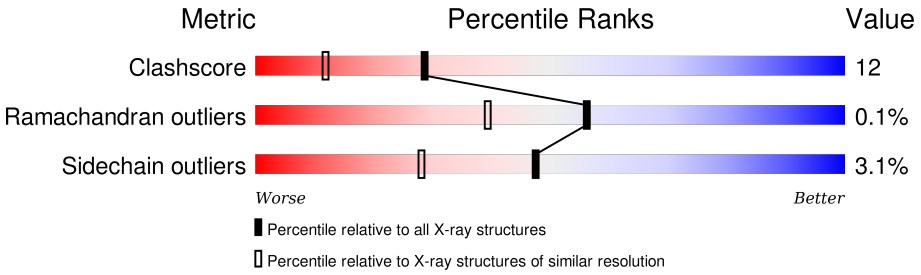
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.86 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))
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)

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	345	78% 15% • 6%
1	B	345	78% 16% • 5%
1	C	345	71% 21% • 7%
1	D	345	74% 19% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10629 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 Anthranilate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2433	1527	435	462	9			
1	B	328	Total	C	N	O	S	0	0	0
			2459	1541	442	467	9			
1	C	320	Total	C	N	O	S	0	0	0
			2391	1504	426	453	8			
1	D	329	Total	C	N	O	S	0	0	0
			2449	1536	439	465	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	251	Total	O	0	0
			251	251		
2	B	224	Total	O	0	0
			224	224		
2	C	222	Total	O	0	0
			222	222		
2	D	200	Total	O	0	0
			200	200		

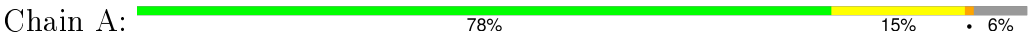
3 Residue-property plots (i)

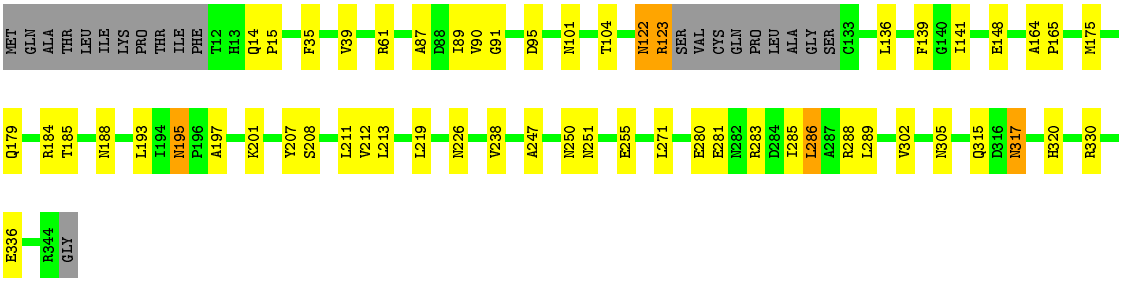
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

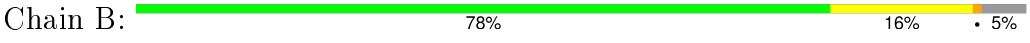
Chain A:

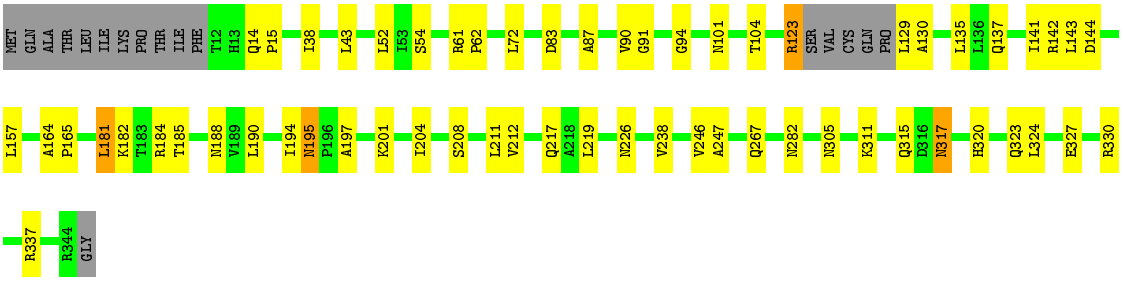




- Molecule 1: Anthranilate phosphoribosyltransferase

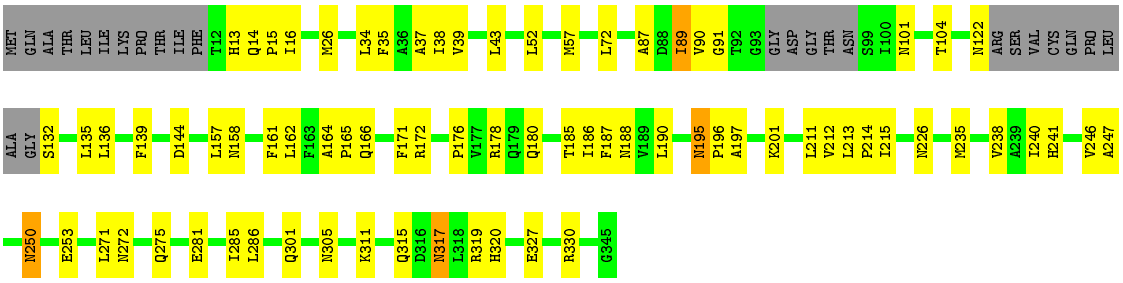
Chain B:





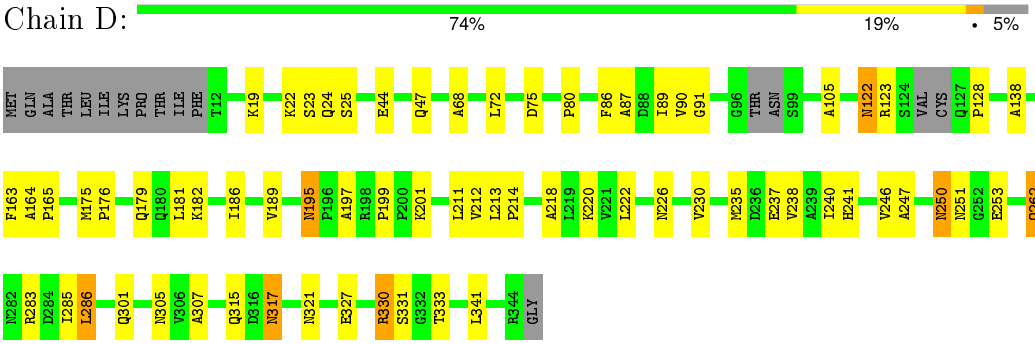
- Molecule 1: Anthranilate phosphoribosyltransferase

Chain C:



• Molecule 1: Anthranilate phosphoribosyltransferase

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.87Å 82.34Å 200.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.86	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-1.86)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10629	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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	0.33	0/2475	0.57	0/3355
1	B	0.32	0/2501	0.57	0/3389
1	C	0.30	0/2432	0.53	0/3296
1	D	0.29	0/2490	0.52	0/3373
All	All	0.31	0/9898	0.55	0/13413

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	2433	0	2411	54	0
1	B	2459	0	2437	48	0
1	C	2391	0	2365	66	0
1	D	2449	0	2415	58	0
2	A	251	0	0	6	0
2	B	224	0	0	6	0
2	C	222	0	0	4	0
2	D	200	0	0	3	0
All	All	10629	0	9628	223	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 12.

All (223) 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:122:ASN:HD22	1:A:123:ARG:H	1.13	0.95
1:C:16:ILE:HD11	1:C:26:MET:SD	2.08	0.94
1:C:185:THR:H	1:C:188:ASN:HD22	1.23	0.83
1:D:44:GLU:H	1:D:47:GLN:HE21	1.25	0.83
1:A:122:ASN:ND2	1:A:123:ARG:H	1.77	0.83
1:D:122:ASN:ND2	1:D:123:ARG:H	1.78	0.81
1:A:122:ASN:HD22	1:A:123:ARG:N	1.83	0.76
1:A:148:GLU:HG2	2:A:511:HOH:O	1.84	0.76
1:C:185:THR:H	1:C:188:ASN:ND2	1.84	0.76
1:C:176:PRO:O	1:C:180:GLN:HG3	1.85	0.76
1:D:44:GLU:H	1:D:47:GLN:NE2	1.85	0.75
1:D:87:ALA:HB2	1:D:201:LYS:HB2	1.69	0.75
1:A:208:SER:OG	1:A:211:LEU:HD13	1.87	0.75
1:D:262:GLN:H	1:D:262:GLN:NE2	1.84	0.74
1:C:195:ASN:HD22	1:C:197:ALA:H	1.36	0.73
1:A:195:ASN:HD22	1:A:197:ALA:H	1.35	0.73
1:A:238:VAL:H	1:A:305:ASN:HD21	1.37	0.73
1:B:123:ARG:C	1:B:123:ARG:HE	1.92	0.72
1:B:185:THR:H	1:B:188:ASN:HD22	1.38	0.70
1:D:327:GLU:OE2	1:D:330:ARG:HD2	1.91	0.70
1:C:104:THR:HG1	1:C:132:SER:N	1.88	0.69
1:B:238:VAL:H	1:B:305:ASN:HD21	1.41	0.69
1:C:39:VAL:HG11	1:C:72:LEU:HD22	1.75	0.69
1:A:122:ASN:ND2	1:A:123:ARG:HD2	2.08	0.68
1:A:61:ARG:HH21	1:A:61:ARG:HG3	1.59	0.68
1:A:195:ASN:ND2	1:A:197:ALA:H	1.92	0.68
1:B:195:ASN:HD22	1:B:197:ALA:H	1.42	0.67
1:D:195:ASN:HD22	1:D:197:ALA:H	1.40	0.66
1:D:220:LYS:HB3	1:D:220:LYS:HZ3	1.60	0.66
1:B:208:SER:OG	1:B:211:LEU:HD13	1.95	0.66
1:C:195:ASN:ND2	1:C:197:ALA:H	1.92	0.66
1:B:212:VAL:HG12	1:B:247:ALA:HB2	1.78	0.64
1:A:185:THR:H	1:A:188:ASN:HD22	1.44	0.64
1:D:122:ASN:HD22	1:D:123:ARG:H	1.45	0.64
1:C:172:ARG:HE	1:C:172:ARG:HA	1.61	0.64
1:C:272:ASN:O	1:C:275:GLN:HG2	1.96	0.64
1:D:212:VAL:HG12	1:D:247:ALA:HB2	1.79	0.64
1:A:122:ASN:HD21	1:A:123:ARG:HD2	1.62	0.64
1:C:212:VAL:HG12	1:C:247:ALA:HB2	1.81	0.63
1:C:238:VAL:H	1:C:305:ASN:HD21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD13	2:B:470:HOH:O	1.99	0.62
1:C:13:HIS:O	1:C:16:ILE:HG22	1.99	0.62
1:A:336:GLU:HB3	2:A:381:HOH:O	1.99	0.62
1:D:164:ALA:HB3	1:D:165:PRO:HD3	1.82	0.62
1:A:87:ALA:HB2	1:A:201:LYS:HB2	1.82	0.61
1:D:195:ASN:ND2	1:D:197:ALA:H	1.99	0.61
1:C:317:ASN:ND2	1:C:320:HIS:H	1.99	0.61
1:C:135:LEU:HD13	1:C:286:LEU:HD22	1.82	0.61
1:C:186:ILE:O	1:C:190:LEU:HD13	2.00	0.61
1:C:139:PHE:HE2	1:C:286:LEU:HD23	1.66	0.61
1:D:220:LYS:HB3	1:D:220:LYS:NZ	2.15	0.60
1:D:218:ALA:O	1:D:222:LEU:HD13	2.02	0.60
1:A:317:ASN:C	1:A:317:ASN:HD22	2.06	0.59
1:B:87:ALA:HB2	1:B:201:LYS:HB2	1.84	0.59
1:B:195:ASN:ND2	1:B:197:ALA:H	1.99	0.59
1:D:105:ALA:HB2	1:D:286:LEU:HD11	1.82	0.59
1:D:262:GLN:HE21	1:D:262:GLN:H	1.49	0.59
1:C:172:ARG:NE	1:C:172:ARG:HA	2.17	0.59
1:B:129:LEU:N	1:B:129:LEU:HD23	2.18	0.58
1:C:16:ILE:HD13	1:C:34:LEU:HB2	1.84	0.58
1:C:164:ALA:HB3	1:C:165:PRO:HD3	1.86	0.58
1:C:317:ASN:HD22	1:C:317:ASN:C	2.05	0.58
1:A:280:GLU:HG3	1:A:283:ARG:NH2	2.18	0.58
1:B:142:ARG:HG3	1:B:144:ASP:OD2	2.04	0.58
1:A:271:LEU:HD23	1:A:271:LEU:O	2.05	0.57
1:C:101:ASN:ND2	1:C:104:THR:H	2.02	0.57
1:A:195:ASN:HD22	1:A:195:ASN:C	2.08	0.57
1:A:185:THR:H	1:A:188:ASN:ND2	2.02	0.56
1:C:195:ASN:HD22	1:C:195:ASN:C	2.07	0.56
1:C:250:ASN:HD22	1:C:250:ASN:C	2.09	0.56
1:D:186:ILE:O	1:D:189:VAL:HG22	2.06	0.56
1:B:101:ASN:HD21	1:B:104:THR:H	1.53	0.56
1:B:94:GLY:HA2	1:B:184:ARG:HH22	1.69	0.56
1:C:89:ILE:O	1:C:89:ILE:HG23	2.05	0.56
1:D:238:VAL:H	1:D:305:ASN:HD21	1.53	0.55
1:B:323:GLN:HE21	1:B:327:GLU:HG3	1.71	0.55
1:A:285:ILE:HD13	1:A:288:ARG:NH2	2.20	0.55
1:C:213:LEU:HB3	1:C:214:PRO:HD3	1.89	0.55
1:D:211:LEU:HD21	2:D:519:HOH:O	2.06	0.55
1:C:327:GLU:OE1	1:C:330:ARG:HD3	2.07	0.55
1:A:61:ARG:HG3	1:A:61:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LEU:HD12	2:B:456:HOH:O	2.07	0.54
1:A:123:ARG:HG3	1:A:123:ARG:HH21	1.71	0.54
1:C:90:VAL:HG22	1:C:91:GLY:N	2.22	0.54
1:D:281:GLU:O	1:D:285:ILE:HG13	2.08	0.54
1:D:201:LYS:HA	1:D:226:ASN:O	2.08	0.54
1:A:285:ILE:HD13	1:A:288:ARG:HH21	1.72	0.54
1:D:90:VAL:HG22	1:D:91:GLY:N	2.22	0.53
1:B:195:ASN:HD22	1:B:195:ASN:C	2.11	0.53
1:D:250:ASN:HD22	1:D:251:ASN:N	2.06	0.53
1:B:317:ASN:HD22	1:B:317:ASN:C	2.12	0.53
1:D:230:VAL:HG12	1:D:246:VAL:HG22	1.90	0.53
1:D:122:ASN:ND2	1:D:123:ARG:N	2.53	0.53
1:C:144:ASP:HA	1:C:166:GLN:NE2	2.24	0.53
1:D:19:LYS:HE2	1:D:25:SER:O	2.10	0.52
1:D:240:ILE:HG21	1:D:301:GLN:HA	1.92	0.52
1:B:323:GLN:NE2	1:B:327:GLU:HG3	2.24	0.52
1:C:327:GLU:HA	1:C:330:ARG:HG2	1.91	0.52
1:D:240:ILE:CG2	1:D:301:GLN:HA	2.40	0.52
1:A:317:ASN:ND2	1:A:320:HIS:H	2.08	0.51
1:A:175:MET:O	1:A:179:GLN:HG2	2.10	0.51
1:A:271:LEU:HG	2:A:561:HOH:O	2.10	0.51
1:C:201:LYS:HA	1:C:226:ASN:O	2.10	0.51
1:A:212:VAL:HG12	1:A:247:ALA:HB2	1.92	0.51
1:D:212:VAL:HG12	1:D:247:ALA:CB	2.41	0.51
1:C:186:ILE:HG12	1:C:190:LEU:HD13	1.93	0.51
1:C:211:LEU:O	1:C:215:ILE:HG12	2.11	0.51
1:C:162:LEU:HD13	1:C:196:PRO:HG2	1.93	0.50
1:A:89:ILE:O	1:A:89:ILE:HG23	2.11	0.50
1:C:178:ARG:HD2	2:C:559:HOH:O	2.11	0.50
1:D:330:ARG:HD3	1:D:331:SER:N	2.26	0.50
1:C:271:LEU:HD12	1:C:272:ASN:N	2.27	0.50
1:C:89:ILE:HD11	2:C:366:HOH:O	2.12	0.50
1:B:317:ASN:ND2	1:B:320:HIS:H	2.10	0.50
1:D:317:ASN:HD22	1:D:317:ASN:C	2.15	0.50
1:B:185:THR:H	1:B:188:ASN:ND2	2.07	0.49
1:B:14:GLN:HB3	1:B:15:PRO:HD3	1.94	0.49
1:A:101:ASN:HD21	1:A:104:THR:H	1.60	0.49
1:A:14:GLN:HB3	1:A:15:PRO:HD3	1.94	0.49
1:A:122:ASN:ND2	1:A:123:ARG:N	2.51	0.49
1:B:238:VAL:H	1:B:305:ASN:ND2	2.10	0.49
1:B:94:GLY:CA	1:B:184:ARG:HH12	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:N	1:A:255:GLU:OE2	2.46	0.49
1:D:86:PHE:CE1	1:D:199:PRO:HB3	2.48	0.49
1:B:123:ARG:NE	1:B:123:ARG:C	2.65	0.49
1:C:14:GLN:N	1:C:15:PRO:CD	2.76	0.49
1:D:138:ALA:HB1	1:D:283:ARG:HD2	1.95	0.49
1:C:186:ILE:HG12	1:C:190:LEU:CD1	2.44	0.48
1:B:164:ALA:HB3	1:B:165:PRO:HD3	1.95	0.48
1:D:213:LEU:N	1:D:214:PRO:HD2	2.28	0.48
1:D:195:ASN:C	1:D:195:ASN:HD22	2.17	0.48
1:D:307:ALA:HA	1:D:321:ASN:HB3	1.95	0.48
1:C:271:LEU:HD12	1:C:271:LEU:C	2.34	0.48
1:A:90:VAL:HG22	1:A:91:GLY:N	2.28	0.48
1:C:101:ASN:ND2	1:C:104:THR:OG1	2.47	0.47
1:C:87:ALA:HB2	1:C:201:LYS:HB2	1.97	0.47
1:D:283:ARG:HH11	1:D:283:ARG:HG2	1.78	0.47
1:B:184:ARG:HG2	2:B:414:HOH:O	2.14	0.47
1:C:89:ILE:C	1:C:89:ILE:HD13	2.35	0.47
1:C:144:ASP:HA	1:C:166:GLN:HE22	1.80	0.47
1:A:238:VAL:H	1:A:305:ASN:ND2	2.06	0.47
1:B:101:ASN:ND2	1:B:104:THR:H	2.13	0.47
1:B:94:GLY:C	1:B:184:ARG:HH12	2.17	0.47
1:B:61:ARG:CZ	2:B:525:HOH:O	2.63	0.46
1:D:19:LYS:HG3	1:D:24:GLN:NE2	2.30	0.46
1:A:315:GLN:HG3	2:A:513:HOH:O	2.15	0.46
1:B:330:ARG:HG2	2:B:394:HOH:O	2.15	0.46
1:A:184:ARG:HD3	1:A:207:TYR:CE1	2.50	0.46
1:D:331:SER:OG	1:D:333:THR:HG22	2.16	0.46
1:C:178:ARG:HD3	1:C:187:PHE:CB	2.45	0.46
1:D:330:ARG:C	1:D:330:ARG:HD3	2.36	0.46
1:D:237:GLU:HB2	1:D:305:ASN:HD21	1.79	0.46
1:B:72:LEU:HD13	1:B:194:ILE:HD13	1.98	0.46
1:C:39:VAL:CG1	1:C:72:LEU:HD22	2.43	0.46
1:C:311:LYS:HA	1:C:315:GLN:O	2.16	0.45
1:D:68:ALA:O	1:D:72:LEU:HD23	2.16	0.45
1:C:212:VAL:HG12	1:C:247:ALA:CB	2.46	0.45
1:A:289:LEU:HD21	1:A:302:VAL:HG21	1.98	0.45
1:A:193:LEU:HD22	1:A:219:LEU:HD21	1.99	0.45
1:C:241:HIS:HD2	2:C:372:HOH:O	2.00	0.45
1:A:201:LYS:HA	1:A:226:ASN:O	2.17	0.45
1:B:14:GLN:N	1:B:15:PRO:CD	2.80	0.45
1:C:13:HIS:HE1	1:C:37:ALA:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ALA:CB	1:B:282:ASN:HD22	2.30	0.45
1:B:201:LYS:HA	1:B:226:ASN:O	2.16	0.44
1:D:89:ILE:O	1:D:89:ILE:HG23	2.17	0.44
1:A:271:LEU:HD23	1:A:271:LEU:C	2.37	0.44
1:D:19:LYS:HG3	1:D:24:GLN:HE21	1.82	0.44
1:A:101:ASN:ND2	1:A:104:THR:H	2.15	0.44
1:D:327:GLU:O	1:D:330:ARG:HG3	2.17	0.44
1:B:246:VAL:HG12	1:B:247:ALA:N	2.32	0.44
1:A:250:ASN:HD22	1:A:251:ASN:N	2.16	0.44
1:D:220:LYS:HE3	2:D:511:HOH:O	2.18	0.43
1:A:213:LEU:HD23	2:A:553:HOH:O	2.17	0.43
1:C:101:ASN:HD21	1:C:104:THR:H	1.63	0.43
1:A:14:GLN:OE1	1:D:182:LYS:HE3	2.19	0.43
1:D:315:GLN:HB3	1:D:321:ASN:HD21	1.83	0.43
1:D:241:HIS:CD2	1:D:271:LEU:HB2	2.53	0.43
1:C:272:ASN:HA	1:C:275:GLN:HG2	2.01	0.43
1:A:250:ASN:ND2	1:A:251:ASN:N	2.66	0.43
1:B:267:GLN:HG3	2:B:436:HOH:O	2.18	0.43
1:B:182:LYS:HE3	1:C:14:GLN:OE1	2.19	0.43
1:B:204:ILE:HD12	1:B:219:LEU:HD11	2.00	0.43
1:C:136:LEU:HD11	1:C:161:PHE:CD2	2.54	0.42
1:B:62:PRO:HG2	1:B:217:GLN:NE2	2.33	0.42
1:D:235:MET:HE1	1:D:271:LEU:HD21	2.01	0.42
1:C:157:LEU:O	1:C:158:ASN:HB2	2.19	0.42
1:D:80:PRO:HG2	1:D:151:ARG:HB2	2.01	0.42
1:A:164:ALA:HB3	1:A:165:PRO:HD3	2.00	0.42
1:B:141:ILE:N	1:B:141:ILE:HD12	2.35	0.42
1:B:90:VAL:HG22	1:B:91:GLY:N	2.34	0.42
1:C:281:GLU:O	1:C:285:ILE:HG13	2.20	0.42
1:A:139:PHE:HE2	1:A:286:LEU:HD13	1.84	0.42
1:D:90:VAL:HG22	1:D:91:GLY:H	1.84	0.42
1:B:38:ILE:HG12	1:B:43:LEU:HD22	2.01	0.42
1:C:38:ILE:HG12	1:C:43:LEU:HD22	2.02	0.42
1:B:137:GLN:HG3	1:B:143:LEU:HD11	2.00	0.42
1:C:101:ASN:HD22	1:C:104:THR:HB	1.85	0.41
1:A:123:ARG:NH2	1:A:123:ARG:HG3	2.35	0.41
1:D:175:MET:HB3	1:D:176:PRO:HD3	2.01	0.41
1:C:250:ASN:ND2	1:C:250:ASN:C	2.72	0.41
1:B:54:SER:HA	1:C:57:MET:SD	2.60	0.41
1:A:250:ASN:HD22	1:A:251:ASN:H	1.67	0.41
1:C:240:ILE:CG2	1:C:301:GLN:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASN:ND2	1:C:104:THR:CB	2.83	0.41
1:C:35:PHE:O	1:C:39:VAL:HG22	2.21	0.41
1:D:253:GLU:HG3	2:D:398:HOH:O	2.19	0.41
1:B:181:LEU:HA	1:B:181:LEU:HD12	1.93	0.41
1:D:163:PHE:CG	1:D:165:PRO:HD2	2.56	0.41
1:A:281:GLU:O	1:A:285:ILE:HG12	2.21	0.41
1:A:184:ARG:HD3	1:A:207:TYR:CZ	2.55	0.41
1:A:136:LEU:HD22	1:A:141:ILE:HD13	2.02	0.41
1:D:179:GLN:O	1:D:182:LYS:HG3	2.21	0.41
1:D:22:LYS:O	1:D:23:SER:HB2	2.21	0.41
1:B:311:LYS:HA	1:B:315:GLN:O	2.21	0.41
1:A:330:ARG:HD2	2:A:517:HOH:O	2.21	0.41
1:C:246:VAL:HG12	1:C:247:ALA:N	2.36	0.40
1:D:141:ILE:HD13	1:D:341:LEU:HD23	2.03	0.40
1:C:319:ARG:HB2	2:C:488:HOH:O	2.20	0.40
1:B:62:PRO:HG2	1:B:217:GLN:HE21	1.87	0.40
1:B:157:LEU:HB3	1:B:337:ARG:HD2	2.04	0.40
1:A:35:PHE:O	1:A:39:VAL:HG22	2.21	0.40
1:C:90:VAL:HG22	1:C:91:GLY:H	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	320/345 (93%)	311 (97%)	9 (3%)	0	100	100
1	B	324/345 (94%)	318 (98%)	6 (2%)	0	100	100
1	C	314/345 (91%)	309 (98%)	5 (2%)	0	100	100
1	D	323/345 (94%)	312 (97%)	10 (3%)	1 (0%)	46	29
All	All	1281/1380 (93%)	1250 (98%)	30 (2%)	1 (0%)	56	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	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	249/271 (92%)	243 (98%)	6 (2%)	57	39
1	B	251/271 (93%)	244 (97%)	7 (3%)	51	33
1	C	243/271 (90%)	234 (96%)	9 (4%)	41	20
1	D	248/271 (92%)	239 (96%)	9 (4%)	42	21
All	All	991/1084 (91%)	960 (97%)	31 (3%)	47	28

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	122	ASN
1	A	123	ARG
1	A	195	ASN
1	A	286	LEU
1	A	317	ASN
1	B	52	LEU
1	B	83	ASP
1	B	123	ARG
1	B	181	LEU
1	B	190	LEU
1	B	195	ASN
1	B	317	ASN
1	C	52	LEU
1	C	89	ILE
1	C	122	ASN
1	C	171	PHE
1	C	195	ASN
1	C	235	MET

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Mol	Chain	Res	Type
1	C	250	ASN
1	C	253	GLU
1	C	317	ASN
1	D	75	ASP
1	D	122	ASN
1	D	181	LEU
1	D	195	ASN
1	D	250	ASN
1	D	262	GLN
1	D	286	LEU
1	D	317	ASN
1	D	330	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	GLN
1	A	101	ASN
1	A	120	HIS
1	A	122	ASN
1	A	168	HIS
1	A	180	GLN
1	A	188	ASN
1	A	195	ASN
1	A	217	GLN
1	A	226	ASN
1	A	250	ASN
1	A	251	ASN
1	A	267	GLN
1	A	305	ASN
1	A	317	ASN
1	A	323	GLN
1	B	28	GLN
1	B	33	GLN
1	B	101	ASN
1	B	120	HIS
1	B	137	GLN
1	B	168	HIS
1	B	180	GLN
1	B	188	ASN
1	B	195	ASN

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Mol	Chain	Res	Type
1	B	217	GLN
1	B	250	ASN
1	B	251	ASN
1	B	272	ASN
1	B	305	ASN
1	B	315	GLN
1	B	317	ASN
1	B	323	GLN
1	C	13	HIS
1	C	24	GLN
1	C	28	GLN
1	C	101	ASN
1	C	120	HIS
1	C	122	ASN
1	C	166	GLN
1	C	168	HIS
1	C	188	ASN
1	C	195	ASN
1	C	217	GLN
1	C	241	HIS
1	C	250	ASN
1	C	251	ASN
1	C	267	GLN
1	C	305	ASN
1	C	317	ASN
1	D	24	GLN
1	D	28	GLN
1	D	47	GLN
1	D	122	ASN
1	D	168	HIS
1	D	179	GLN
1	D	180	GLN
1	D	195	ASN
1	D	250	ASN
1	D	251	ASN
1	D	258	GLN
1	D	262	GLN
1	D	291	GLN
1	D	305	ASN
1	D	317	ASN
1	D	321	ASN
1	D	323	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

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.