

Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 03:46 PM EST

PDB ID	:	1J2E
Title	:	Crystal structure of Human Dipeptidyl peptidase IV
Authors	:	Hiramatsu, H.; Kyono, K.; Higashiyama, Y.; Fukushima, C.; Shima, H.;
		Sugiyama, S.; Inaka, K.; Yamamoto, A.; Shimizu, R.
Deposited on	:	2002-12-30
Resolution	:	2.60 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.60 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.



Motric	Whole archive	Similar resolution		
IVIEUIIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455(2.60-2.60)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	А	740	69%	28%			
1	В	740	71%	26%	••		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12355 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	729	Total 5971	C 3831	N 983	0 1131	S 26	0	0	0
1	В	729	Total 5971	C 3831	N 983	0 1131	S 26	0	0	0

• Molecule 1 is a protein called Dipeptidyl peptidase IV.

Chain	Residue	Modelled	Actual	Comment	Reference
А	767	HIS	-	expression tag	UNP P27487
А	768	HIS	-	expression tag	UNP P27487
А	769	HIS	-	expression tag	UNP P27487
А	770	HIS	-	expression tag	UNP P27487
А	771	HIS	-	expression tag	UNP P27487
А	772	HIS	-	expression tag	UNP P27487
В	767	HIS	-	expression tag	UNP P27487
В	768	HIS	-	expression tag	UNP P27487
В	769	HIS	-	expression tag	UNP P27487
В	770	HIS	-	expression tag	UNP P27487
В	771	HIS	-	expression tag	UNP P27487
B	772	HIS	_	expression tag	UNP P27487

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
0	Λ	1	Total	С	Ν	0	0	0	
	A	1	14	8	1	5	0	0	
9	Λ	1	Total	С	Ν	0	0	0	
2	Л	T	14	8	1	5	0	0	
2	Δ	1	Total	С	Ν	0	0	0	
2	Л	T	14	8	1	5	0	0	
9	Λ	1	Total	С	Ν	0	0	0	
	Л	1	14	8	1	5	0	0	
9	Λ	1	Total	С	Ν	0	0	0	
	Л	T	14	8	1	5	0	0	
2	В	1	Total	С	Ν	0	0	Ο	
2	D	L	14	8	1	5	0	0	
2	В	1	Total	С	Ν	0	0	0	
2	D	T	14	8	1	5	0	0	
2	В	1	Total	С	Ν	0	0	0	
2	2 D	I	14	8	1	5	0	0	
2	B	1	Total	С	Ν	0	0	Ο	
	D	1	14	8	1	5	0	U	
2	В	1	Total	С	Ν	0	0	0	
	D		14	8	1	5	0	0	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	136	Total O 136 136	0	0
3	В	137	Total O 137 137	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 geometry. 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. 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: Dipeptidyl peptidase IV

• Molecule 1: Dipeptidyl peptidase IV





Y225 P290 A291 S292 M293 M293 L294 I295 R336 W337 V279 T280 N281 3334 V341 A342 R343 Y24: 1517 1518 1518 1519 N520 E521 L366 S458 V459 S460 F461 K466 Y467 Y468 Q469 L470 L470 **R471** K512 K513 E378 E379 1397 1398 G428 R429 N430 L477 P478 L504 Q505 <mark>N506</mark> V507 Q508 q527 M528 H483 S484 L500 D501 E40 I418 <mark>W563</mark> A564 T565 Y566 N595 R596 R597 R597 R597 R599 R509 F601 F601 F601 F603 R605 D605 K536 K539 R623 1624 <mark>A625</mark> 1626 F730 Q731 A732 M733 W734 W734 H740 G741 I742 E660 Y661 R669 Y670 M671 P766 HIS HIS HIS HIS HIS HIS D725 V726 I 759 K 760 G650 E693



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	118.04Å 125.92Å 136.84Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 2.60	Depositor
% Data completeness	94 4 (10 00-2 60)	Depositor
(in resolution range)	51.1 (10.00 2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.249 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12355	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.35	0/6143	0.62	1/8355~(0.0%)	
1	В	0.35	0/6143	0.62	2/8355~(0.0%)	
All	All	0.35	0/12286	0.62	3/16710~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	458	SER	N-CA-C	-5.16	97.08	111.00
1	В	300	LEU	N-CA-C	-5.14	97.11	111.00
1	А	300	LEU	N-CA-C	-5.13	97.16	111.00

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	А	5971	0	5684	167	0
1	В	5971	0	5683	164	0
2	А	70	0	65	2	0
2	В	70	0	65	3	0
3	А	136	0	0	0	0
3	В	137	0	0	2	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12355	0	11497	322	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 14.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:219:ASN:H	1:B:308:GLN:HE22	1.07	0.99
1:B:72:GLN:HG3	1:B:73:GLU:H	1.27	0.98
1:A:219:ASN:H	1:A:308:GLN:HE22	1.11	0.93
1:B:429:ARG:HH11	1:B:429:ARG:HG3	1.39	0.87
1:A:428:GLY:O	1:A:429:ARG:HD2	1.78	0.83
1:B:75:ASN:HB3	1:B:92:ASN:N	1.95	0.82
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.62	0.81
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.64	0.80
1:B:91:GLU:O	1:B:94:THR:HG22	1.83	0.79
1:A:316:LEU:HD11	1:A:320:GLN:HA	1.64	0.79
1:B:366:LEU:HD12	1:B:366:LEU:H	1.48	0.78
1:B:75:ASN:HB3	1:B:92:ASN:H	1.50	0.76
1:B:143:ILE:HD12	1:B:178:PRO:HB2	1.67	0.75
1:A:175:LYS:HG2	1:A:182:SER:HB3	1.66	0.75
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.69	0.74
1:B:596:ARG:O	1:B:597:ARG:HD2	1.87	0.73
1:A:501:ASP:O	1:A:505:GLN:HG2	1.88	0.73
1:B:112:GLN:HG2	1:B:138:ASN:HD21	1.55	0.72
1:B:110:ASP:OD1	1:B:112:GLN:HB2	1.90	0.71
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.72	0.70
1:A:75:ASN:HB3	1:A:92:ASN:H	1.55	0.70
1:B:219:ASN:H	1:B:308:GLN:NE2	1.86	0.68
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.23	0.68
1:B:429:ARG:HG3	1:B:429:ARG:NH1	2.06	0.68
1:A:167:VAL:HG21	1:A:198:ILE:HG23	1.76	0.68
1:A:91:GLU:O	1:A:94:THR:HG22	1.95	0.67
1:B:528:MET:CE	1:B:574:ILE:HG21	2.25	0.67
1:A:674:PRO:HG3	1:A:683:TYR:CZ	2.30	0.67
1:B:501:ASP:O	1:B:505:GLN:HG2	1.95	0.66
1:B:107:ILE:HG22	1:B:108:SER:O	1.95	0.66
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.78	0.65
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.27	0.65
1:A:44:THR:O	1:A:47:ASP:HB2	1.96	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:600:THR:O	1:B:604:GLU:HG3	1.95	0.65
1:B:88:VAL:HG11	1:B:91:GLU:OE1	1.97	0.65
1:B:72:GLN:HG3	1:B:73:GLU:N	2.06	0.65
1:B:115:LEU:HD21	1:B:155:VAL:HG11	1.79	0.64
1:B:177:GLU:HB2	1:B:180:LEU:HG	1.79	0.64
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.80	0.63
1:B:135:TYR:HA	1:B:142:LEU:HA	1.81	0.63
1:B:459:VAL:HG22	1:B:460:SER:N	2.14	0.63
1:A:214:LEU:O	1:A:214:LEU:HD12	1.99	0.63
1:A:314:GLN:NE2	1:A:362:PRO:HD3	2.15	0.62
1:A:482:LEU:HD23	1:A:492:ARG:NH1	2.14	0.62
1:B:112:GLN:CG	1:B:138:ASN:HD21	2.12	0.62
1:A:190:LYS:HE2	1:A:193:ILE:HD12	1.82	0.62
1:A:219:ASN:N	1:A:308:GLN:HE22	1.90	0.62
1:A:80:ASN:HB3	1:A:85:ASN:OD1	2.01	0.60
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.35	0.60
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.36	0.60
1:B:281:ASN:ND2	2:B:909:NAG:C7	2.65	0.60
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.84	0.59
1:B:72:GLN:O	1:B:73:GLU:C	2.40	0.59
1:B:94:THR:HG23	1:B:95:PHE:CD1	2.37	0.59
1:A:109:PRO:HG2	1:A:158:SER:O	2.03	0.59
1:A:316:LEU:HD11	1:A:320:GLN:CA	2.32	0.59
1:B:620:ASP:OD1	1:B:623:ARG:HD3	2.03	0.59
1:A:482:LEU:HD23	1:A:492:ARG:HH12	1.68	0.58
1:A:517:ILE:HD12	1:A:517:ILE:O	2.03	0.58
1:A:517:ILE:HD12	1:A:517:ILE:C	2.23	0.58
1:B:512:LYS:HE3	1:B:527:GLN:CD	2.24	0.58
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.85	0.58
1:B:562:ASN:C	1:B:562:ASN:HD22	2.06	0.58
1:B:518:ILE:O	1:B:519:LEU:HD23	2.03	0.58
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.39	0.57
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.87	0.57
1:B:571:GLU:HG3	1:B:760:LYS:HE2	1.85	0.57
1:B:285:ILE:HD12	1:B:285:ILE:N	2.19	0.57
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.24	0.56
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.35	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.87	0.56
1:B:741:GLY:O	1:B:742:ILE:C	2.44	0.56
1:B:341:VAL:O	1:B:343:ARG:N	2.39	0.56
1:B:484:SER:OG	1:B:489:LYS:HG2	2.05	0.56



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:491:LEU:O	1:A:492:ARG:HB3	2.05	0.55
1:B:93:SER:HB2	1:B:96:ASP:OD2	2.06	0.55
1:A:266:VAL:HG22	1:A:267:LYS:N	2.21	0.55
1:A:482:LEU:HG	1:A:491:LEU:HD12	1.88	0.55
1:B:528:MET:HE2	1:B:574:ILE:HG21	1.87	0.55
1:B:517:ILE:HG23	1:B:526:TYR:CE2	2.42	0.55
1:A:246:LEU:HD21	1:A:250:LYS:HG3	1.88	0.55
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.88	0.55
1:B:142:LEU:O	1:B:142:LEU:HD12	2.07	0.55
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.07	0.55
1:A:530:LEU:HD13	1:A:534:PHE:CD2	2.42	0.55
1:B:528:MET:HE3	1:B:574:ILE:HG21	1.88	0.55
1:B:330:TYR:CE2	1:B:332:GLU:HA	2.41	0.54
1:B:513:LYS:O	1:B:527:GLN:HA	2.07	0.54
2:B:910:NAG:O3	2:B:910:NAG:H83	2.07	0.54
1:A:438:ASP:CG	1:A:441:LYS:HD3	2.28	0.54
1:A:626:ILE:O	1:A:650:GLY:HA2	2.08	0.54
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.90	0.54
1:B:517:ILE:HG23	1:B:526:TYR:HE2	1.73	0.54
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.88	0.54
1:A:345:HIS:HE1	1:A:389:ILE:O	1.91	0.53
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.08	0.53
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.08	0.53
1:A:415:LEU:HD23	1:A:415:LEU:C	2.29	0.53
1:A:219:ASN:HB2	2:A:902:NAG:H82	1.91	0.53
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.43	0.53
1:B:285:ILE:HD12	1:B:285:ILE:H	1.71	0.53
1:B:531:PRO:HB3	1:B:568:ALA:O	2.09	0.53
1:A:41:LYS:HE3	1:A:507:VAL:HG22	1.91	0.53
1:A:60:LEU:HD12	1:A:60:LEU:C	2.28	0.53
1:A:72:GLN:HB2	1:A:77:LEU:HD11	1.91	0.53
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.91	0.53
1:B:176:ILE:HG22	1:B:177:GLU:HG2	1.90	0.53
1:B:72:GLN:O	1:B:74:ASN:N	2.41	0.53
1:B:112:GLN:HB3	1:B:113:PHE:CD1	2.45	0.53
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.90	0.52
1:B:539:LYS:HE2	1:B:620:ASP:HA	1.91	0.52
1:A:314:GLN:HE22	1:A:362:PRO:HD3	1.74	0.52
1:A:608:GLU:OE2	1:A:611:ARG:HD2	2.09	0.52
1:B:535:ASP:HB3	1:B:538:LYS:HG2	1.91	0.52
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.40	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:325:MET:HE1	1:A:362:PRO:HB3	1.92	0.52
1:A:516:PHE:CE2	1:A:523:LYS:HD3	2.44	0.52
1:A:119:ASN:HD22	1:A:131:SER:HB2	1.75	0.52
1:A:608:GLU:O	1:A:612:GLN:HG2	2.10	0.52
1:B:197:GLY:C	1:B:213:ALA:HB3	2.31	0.51
1:B:520:ASN:O	1:B:521:GLU:HB3	2.10	0.51
1:A:649:CYS:HB3	1:A:699:GLU:HG3	1.92	0.51
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.91	0.51
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.91	0.51
1:B:281:ASN:OD1	2:B:909:NAG:H82	2.10	0.51
1:A:113:PHE:CE2	1:A:178:PRO:HG3	2.45	0.51
1:A:459:VAL:HG22	1:A:460:SER:N	2.26	0.51
1:A:608:GLU:OE2	1:A:608:GLU:HA	2.11	0.51
1:B:696:LYS:O	1:B:696:LYS:HG3	2.10	0.50
1:A:127:SER:HB3	1:A:211:TYR:CG	2.46	0.50
1:A:718:GLN:HE21	1:B:241:TYR:HB3	1.76	0.50
1:A:487:ASN:HD22	1:A:487:ASN:H	1.59	0.50
1:B:293:MET:CE	1:B:324:VAL:HG12	2.41	0.50
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.46	0.50
1:B:710:ASN:C	1:B:710:ASN:HD22	2.14	0.50
1:A:138:ASN:C	1:A:140:ARG:H	2.15	0.50
1:B:469:GLN:HE21	1:B:494:LEU:HD12	1.77	0.50
1:B:562:ASN:HD22	1:B:565:THR:H	1.60	0.50
1:B:60:LEU:C	1:B:60:LEU:HD12	2.32	0.50
1:A:58:TYR:CZ	1:A:494:LEU:HD22	2.47	0.49
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.94	0.49
1:A:542:LEU:HD23	1:A:542:LEU:C	2.33	0.49
1:A:554:LYS:HB3	1:A:577:SER:HB3	1.94	0.49
1:A:418:ILE:HA	1:A:430:ASN:O	2.12	0.49
1:A:467:TYR:CD2	1:A:491:LEU:HD11	2.47	0.49
1:A:95:PHE:CE2	1:A:116:LEU:HD11	2.48	0.49
1:B:109:PRO:HD2	1:B:161:GLY:O	2.12	0.49
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.47	0.49
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.93	0.49
1:A:703:ILE:HA	1:A:733:MET:O	2.12	0.48
1:A:291:ALA:O	1:A:295:ILE:HG23	2.14	0.48
1:B:703:ILE:HA	1:B:733:MET:O	2.13	0.48
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.95	0.48
1:B:630:SER:OG	1:B:740:HIS:NE2	2.39	0.48
1:A:244:GLU:HG2	1:B:658:ARG:NH1	2.28	0.48
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.48	0.48
1:A:658:ARG:HD3	1:A:661:TYR:CE1	2.49	0.48
1:A:530:LEU:HD23	1:A:574:ILE:HG23	1.96	0.48
1:B:334:SER:OG	1:B:336:ARG:HG3	2.14	0.48
1:B:598:LEU:HB2	1:B:671:MET:SD	2.53	0.47
1:B:459:VAL:HG22	1:B:460:SER:H	1.79	0.47
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.96	0.47
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.14	0.47
1:B:624:ILE:HD12	3:B:1029:HOH:O	2.12	0.47
1:A:41:LYS:HE3	1:A:53:TYR:OH	2.14	0.47
1:A:266:VAL:CG2	1:A:267:LYS:N	2.77	0.47
1:A:531:PRO:HB3	1:A:568:ALA:O	2.15	0.47
1:A:598:LEU:HG	1:A:631:TYR:OH	2.14	0.47
1:B:602:GLU:HG2	1:B:603:VAL:N	2.28	0.47
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.45	0.47
1:A:710:ASN:HD22	1:A:710:ASN:C	2.16	0.47
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.14	0.47
1:B:82:GLU:HB2	1:B:467:TYR:OH	2.15	0.47
1:B:259:ALA:HB3	1:B:660:GLU:HA	1.97	0.47
1:A:370:SER:HB2	1:A:387:PHE:O	2.15	0.47
1:B:127:SER:O	1:B:128:TYR:HB3	2.14	0.47
1:A:544:LEU:HG	1:A:546:VAL:CG2	2.45	0.47
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.45	0.47
1:B:418:ILE:HA	1:B:430:ASN:O	2.14	0.47
1:A:701:LEU:HD12	1:A:702:LEU:N	2.29	0.46
1:A:72:GLN:HB2	1:A:77:LEU:CD1	2.45	0.46
1:B:361:GLU:O	1:B:361:GLU:HG2	2.14	0.46
1:B:95:PHE:CE2	1:B:116:LEU:HD11	2.49	0.46
1:B:693:GLU:HG3	1:B:726:VAL:HG11	1.98	0.46
1:B:428:GLY:O	1:B:429:ARG:HG3	2.16	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.53	0.46
1:B:562:ASN:ND2	1:B:565:THR:H	2.13	0.46
1:A:660:GLU:OE2	1:A:684:ARG:NE	2.44	0.46
1:B:176:ILE:HD13	1:B:183:TYR:CE1	2.51	0.46
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.81	0.46
1:B:600:THR:OG1	1:B:601:PHE:N	2.47	0.46
1:A:263:ASN:HD21	1:A:664:SER:CB	2.29	0.46
1:A:562:ASN:C	1:A:562:ASN:HD22	2.19	0.46
1:B:293:MET:HE2	1:B:324:VAL:HG12	1.97	0.46
1:A:237:GLU:OE1	1:A:253:ARG:HD3	2.16	0.46
1:B:177:GLU:HB2	1:B:180:LEU:CG	2.44	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:218:PRO:HB2	1:B:308:GLN:OE1	2.16	0.46
1:A:200:ASP:OD1	1:A:203:TYR:HB2	2.15	0.46
1:A:361:GLU:CD	1:A:361:GLU:H	2.14	0.46
1:B:71:LYS:HG2	1:B:105:TYR:OH	2.16	0.45
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.51	0.45
1:B:115:LEU:HD21	1:B:155:VAL:CG1	2.45	0.45
1:A:107:ILE:N	1:A:107:ILE:HD12	2.32	0.45
1:B:109:PRO:HG2	1:B:158:SER:O	2.15	0.45
1:A:422:TYR:CZ	1:A:423:LYS:HE3	2.51	0.45
1:A:348:MET:CE	2:A:905:NAG:H83	2.46	0.45
1:B:143:ILE:HD13	1:B:179:ASN:HB3	1.98	0.45
1:B:378:GLU:HG3	1:B:379:GLU:H	1.82	0.45
1:B:512:LYS:HE3	1:B:527:GLN:NE2	2.30	0.45
1:A:545:ASP:HB3	1:A:577:SER:OG	2.16	0.45
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.51	0.45
1:B:341:VAL:C	1:B:343:ARG:H	2.19	0.45
1:B:341:VAL:C	1:B:343:ARG:N	2.70	0.45
1:B:459:VAL:CG2	1:B:460:SER:N	2.80	0.45
1:A:467:TYR:HD2	1:A:491:LEU:HD11	1.80	0.45
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.17	0.45
1:A:276:LEU:HD23	1:A:282:ALA:HB2	1.99	0.45
1:B:176:ILE:HD12	1:B:176:ILE:N	2.32	0.44
1:A:138:ASN:O	1:A:140:ARG:HG3	2.18	0.44
1:A:91:GLU:O	1:A:93:SER:N	2.50	0.44
1:A:279:VAL:CG1	1:A:280:THR:N	2.81	0.44
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.52	0.44
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.52	0.44
1:A:91:GLU:C	1:A:93:SER:H	2.21	0.44
1:A:751:ILE:HG23	1:A:752:TYR:N	2.32	0.44
1:A:113:PHE:CZ	1:A:178:PRO:HG3	2.53	0.44
1:A:606:GLN:O	1:A:609:ALA:HB3	2.18	0.44
1:A:627:TRP:HB2	1:A:651:ILE:HB	2.00	0.44
1:B:734:TRP:CD1	1:B:734:TRP:C	2.91	0.44
1:A:596:ARG:HA	1:A:670:TYR:O	2.17	0.44
1:A:56:LYS:O	1:A:57:LEU:HD23	2.17	0.44
1:B:63:ILE:CG2	1:B:69:LEU:HG	2.48	0.44
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.53	0.43
1:B:97:GLU:N	1:B:97:GLU:OE2	2.51	0.43
1:B:378:GLU:HG3	1:B:379:GLU:N	2.33	0.43
1:B:535:ASP:HB3	1:B:538:LYS:CG	2.47	0.43
1:A:94:THR:HG23	1:A:95:PHE:CD1	2.54	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:258:LYS:HD2	1:B:248:TYR:CE1	2.53	0.43
1:A:542:LEU:HD23	1:A:543:LEU:N	2.32	0.43
1:A:718:GLN:NE2	1:B:241:TYR:HB3	2.33	0.43
1:B:214:LEU:HD23	1:B:225:TYR:CB	2.48	0.43
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.47	0.43
1:A:454:CYS:HB3	1:A:457:TYR:CZ	2.53	0.43
1:B:63:ILE:HG21	1:B:69:LEU:HG	2.00	0.43
1:B:143:ILE:CD1	1:B:178:PRO:HB2	2.41	0.43
1:B:507:VAL:HG12	1:B:508:GLN:N	2.33	0.43
1:A:138:ASN:C	1:A:140:ARG:N	2.72	0.43
1:A:438:ASP:OD1	1:A:441:LYS:HD3	2.19	0.43
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.18	0.43
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.53	0.43
1:B:107:ILE:HD12	1:B:107:ILE:N	2.34	0.43
1:B:222:PHE:HB2	1:B:305:TRP:CH2	2.53	0.43
1:B:291:ALA:O	1:B:295:ILE:HG23	2.19	0.43
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.00	0.43
1:A:272:ASN:OD1	1:A:274:ASP:HB2	2.19	0.43
1:A:750:HIS:CD2	1:B:724:VAL:HG22	2.54	0.43
1:B:54:ARG:NH1	1:B:54:ARG:HG2	2.34	0.43
1:A:251:THR:HG21	1:A:253:ARG:NH1	2.34	0.43
1:A:78:VAL:O	1:A:86:SER:HB2	2.18	0.43
1:A:123:GLN:HG2	1:A:124:TRP:CD2	2.54	0.43
1:A:219:ASN:H	1:A:308:GLN:NE2	1.94	0.42
1:B:546:VAL:HG22	1:B:606:GLN:OE1	2.19	0.42
1:A:75:ASN:CB	1:A:91:GLU:HA	2.49	0.42
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.19	0.42
1:A:75:ASN:HB3	1:A:91:GLU:HA	2.00	0.42
1:A:661:TYR:OH	1:A:718:GLN:HG3	2.19	0.42
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.01	0.42
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.55	0.42
1:B:521:GLU:O	1:B:521:GLU:HG2	2.18	0.42
1:A:249:PRO:HD3	1:B:714:GLN:NE2	2.34	0.42
1:A:148:ILE:HD11	1:A:164:LEU:HD13	2.02	0.42
1:A:674:PRO:O	1:A:680:LEU:HD13	2.20	0.42
1:A:71:LYS:HE3	1:A:105:TYR:HE2	1.85	0.42
1:A:487:ASN:H	1:A:487:ASN:ND2	2.18	0.42
1:A:487:ASN:ND2	1:A:487:ASN:N	2.68	0.42
1:A:735:TYR:OH	1:A:751:ILE:HA	2.20	0.42
1:A:41:LYS:CE	1:A:53:TYR:OH	2.67	0.42
1:A:550:PRO:HG3	1:A:594:ILE:HD12	2.02	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:54:ARG:HG2	1:B:54:ARG:HH11	1.84	0.42
1:B:548:ALA:HA	3:B:933:HOH:O	2.20	0.42
1:A:330:TYR:CE1	1:A:335:GLY:HA2	2.55	0.41
1:B:730:PHE:HE1	1:B:732:ALA:HB2	1.85	0.41
1:A:344:GLN:O	1:A:392:LYS:HE2	2.20	0.41
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.55	0.41
1:B:598:LEU:HD22	1:B:671:MET:HG2	2.01	0.41
1:B:169:ASN:N	1:B:169:ASN:HD22	2.18	0.41
1:B:542:LEU:C	1:B:542:LEU:HD23	2.41	0.41
1:A:41:LYS:NZ	1:A:53:TYR:OH	2.52	0.41
1:B:571:GLU:OE2	1:B:760:LYS:NZ	2.53	0.41
1:B:631:TYR:O	1:B:634:TYR:HB3	2.20	0.41
1:B:658:ARG:HD3	1:B:661:TYR:CZ	2.55	0.41
1:A:658:ARG:HD3	1:A:661:TYR:CZ	2.55	0.41
1:A:696:LYS:HG2	1:A:728:VAL:HG22	2.02	0.41
1:B:107:ILE:CG2	1:B:111:GLY:HA2	2.51	0.41
1:B:198:ILE:HA	1:B:211:TYR:O	2.20	0.41
1:A:127:SER:N	1:A:204:GLU:OE1	2.52	0.41
1:B:119:ASN:HD22	1:B:131:SER:CB	2.34	0.41
1:A:73:GLU:HA	1:A:73:GLU:OE2	2.20	0.41
1:A:253:ARG:NH1	1:B:253:ARG:HH12	2.18	0.41
1:A:480:TYR:HD2	1:A:495:GLU:HB3	1.86	0.41
1:A:658:ARG:NH2	1:A:684:ARG:NE	2.69	0.41
1:A:750:HIS:CD2	1:B:724:VAL:HA	2.56	0.41
1:A:253:ARG:HH12	1:B:253:ARG:NH1	2.18	0.41
1:A:674:PRO:HG3	1:A:683:TYR:CE1	2.56	0.41
1:A:739:ASP:C	1:A:739:ASP:OD2	2.59	0.41
1:B:429:ARG:NH1	1:B:429:ARG:CG	2.78	0.41
1:B:466:LYS:HG2	1:B:467:TYR:CE1	2.56	0.41
1:A:276:LEU:HD23	1:A:282:ALA:CB	2.52	0.40
1:A:424:GLY:O	1:A:426:PRO:HD3	2.20	0.40
1:A:635:VAL:O	1:A:639:VAL:HG23	2.21	0.40
1:B:290:PRO:HD3	1:B:315:TRP:CD1	2.56	0.40
1:A:219:ASN:OD1	1:A:219:ASN:C	2.60	0.40
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.56	0.40
1:B:477:LEU:HA	1:B:478:PRO:HD3	1.97	0.40
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.20	0.40
1:B:102:ILE:O	1:B:102:ILE:HG13	2.21	0.40
1:B:118:TYR:CE2	1:B:119:ASN:ND2	2.90	0.40
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.37	0.40
1:B:519:LEU:HD21	1:B:612:GLN:HE22	1.86	0.40



Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:CG2	1:A:69:LEU:HG	2.51	0.40
1:B:594:ILE:C	1:B:594:ILE:HD12	2.42	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	Perce	entiles
1	А	727/740~(98%)	671 (92%)	52 (7%)	4 (1%)	25	47
1	В	727/740~(98%)	678 (93%)	41 (6%)	8 (1%)	14	30
All	All	1454/1480 (98%)	1349 (93%)	93 (6%)	12 (1%)	19	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	92	ASN
1	А	320	GLN
1	В	73	GLU
1	В	279	VAL
1	В	342	ALA
1	А	389	ILE
1	А	664	SER
1	В	74	ASN
1	В	124	TRP
1	В	320	GLN
1	В	218	PRO
1	В	742	ILE



5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	654/663~(99%)	642 (98%)	12 (2%)	59 80		
1	В	654/663~(99%)	638~(98%)	16 (2%)	49 74		
All	All	1308/1326~(99%)	1280~(98%)	28 (2%)	53 77		

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	96	ASP
1	А	230	ASP
1	А	385	CYS
1	А	388	GLN
1	А	487	ASN
1	А	504	LEU
1	А	506	ASN
1	А	562	ASN
1	А	566	TYR
1	А	627	TRP
1	А	699	GLU
1	А	710	ASN
1	В	41	LYS
1	В	71	LYS
1	В	74	ASN
1	В	112	GLN
1	В	133	ASP
1	В	244	GLU
1	В	326	ASP
1	В	472	CYS
1	В	504	LEU
1	В	562	ASN
1	В	566	TYR
1	В	597	ARG
1	В	696	LYS
1	В	710	ASN
1	В	759	ILE



Continued from previous page...

Mol	Chain	Res	Type
1	В	760	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	112	GLN
1	А	119	ASN
1	А	141	GLN
1	А	263	ASN
1	А	286	GLN
1	А	308	GLN
1	А	314	GLN
1	А	345	HIS
1	А	388	GLN
1	А	487	ASN
1	А	506	ASN
1	А	562	ASN
1	А	572	ASN
1	А	679	ASN
1	А	694	ASN
1	А	697	GLN
1	А	710	ASN
1	В	119	ASN
1	В	138	ASN
1	В	169	ASN
1	В	263	ASN
1	В	286	GLN
1	В	308	GLN
1	В	469	GLN
1	В	487	ASN
1	В	506	ASN
1	В	562	ASN
1	В	612	GLN
1	В	679	ASN
1	В	694	ASN
1	В	710	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	ths	B	ond ang	les
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	901	1	$14,\!14,\!15$	0.51	0	17,19,21	0.69	0
2	NAG	В	910	1	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
2	NAG	А	905	1	14,14,15	0.59	0	17,19,21	1.33	2 (11%)
2	NAG	В	909	1	14,14,15	0.54	0	17,19,21	0.56	0
2	NAG	А	902	1	$14,\!14,\!15$	0.49	0	17,19,21	0.71	0
2	NAG	А	904	1	14,14,15	0.53	0	17,19,21	0.90	1 (5%)
2	NAG	В	908	1	14,14,15	0.48	0	17,19,21	0.72	1 (5%)
2	NAG	A	903	1	$14,\!14,\!15$	0.44	0	17,19,21	0.72	0
2	NAG	В	906	1	14,14,15	0.47	0	17,19,21	0.67	0
2	NAG	В	907	1	14,14,15	0.49	0	17,19,21	0.94	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	А	901	1	-	3/6/23/26	0/1/1/1
2	NAG	В	910	1	-	2/6/23/26	0/1/1/1
2	NAG	А	905	1	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	909	1	-	4/6/23/26	0/1/1/1
2	NAG	А	902	1	-	2/6/23/26	0/1/1/1
2	NAG	А	904	1	-	0/6/23/26	0/1/1/1
2	NAG	В	908	1	-	2/6/23/26	0/1/1/1
2	NAG	А	903	1	-	3/6/23/26	0/1/1/1
2	NAG	В	906	1	-	3/6/23/26	0/1/1/1
2	NAG	В	907	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	А	905	NAG	C4-C3-C2	-3.59	105.75	111.02
2	В	907	NAG	C2-N2-C7	-2.65	119.13	122.90
2	А	905	NAG	C2-N2-C7	-2.61	119.19	122.90
2	В	910	NAG	C2-N2-C7	-2.34	119.58	122.90
2	В	908	NAG	C2-N2-C7	-2.15	119.84	122.90
2	А	904	NAG	C2-N2-C7	-2.09	119.93	122.90

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	901	NAG	C8-C7-N2-C2
2	А	901	NAG	O7-C7-N2-C2
2	А	902	NAG	C8-C7-N2-C2
2	А	902	NAG	O7-C7-N2-C2
2	А	903	NAG	C8-C7-N2-C2
2	А	903	NAG	O7-C7-N2-C2
2	В	908	NAG	C8-C7-N2-C2
2	В	908	NAG	O7-C7-N2-C2
2	В	909	NAG	C8-C7-N2-C2
2	В	909	NAG	O7-C7-N2-C2
2	В	910	NAG	C8-C7-N2-C2
2	В	910	NAG	O7-C7-N2-C2
2	А	905	NAG	C8-C7-N2-C2
2	А	905	NAG	O7-C7-N2-C2
2	В	907	NAG	C8-C7-N2-C2
2	В	909	NAG	C1-C2-N2-C7
2	В	906	NAG	C8-C7-N2-C2

All (24) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	В	907	NAG	O7-C7-N2-C2
2	В	906	NAG	O7-C7-N2-C2
2	А	901	NAG	O5-C5-C6-O6
2	А	903	NAG	O5-C5-C6-O6
2	В	909	NAG	O5-C5-C6-O6
2	В	907	NAG	C4-C5-C6-O6
2	В	906	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	910	NAG	1	0
2	А	905	NAG	1	0
2	В	909	NAG	2	0
2	А	902	NAG	1	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

