

# Full wwPDB X-ray Structure Validation Report (i)

### Sep 22, 2020 – 06:09 PM BST

PDB ID	:	6QZV
$\operatorname{Title}$	:	DPP9 bound to a dipeptide (MP) from the N-terminus of BRCA2
Authors	:	Ross, B.; Geiss-Friedlander, R.; Huber, R.
Deposited on	:	2019-03-12
Resolution	:	3.00  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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

# 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 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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% 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	А	898	% • 71%	18%	• 10%	
1	В	898	% 69%	20%	• 10%	
1	С	898	% 69%	20%	• 10%	
1	D	898	% 69%	20%	• 10%	
2	Е	2	50%	50%		
2	F	2	50%	50%		



Mol	Chain	Length	Quality of chain		
2	G	2	50%	50%	
2	Н	2	50%	50%	



#### $6 \mathrm{QZV}$

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26316 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	Λ	808	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	л	000	6563	4226	1123	1186	28	0	0	0
1	В	805	Total	С	Ν	Ο	S	0	0	0
1	D	805	6540	4213	1115	1184	28	0	0	U
1	C	808	Total	С	Ν	Ο	S	0	0	0
		000	6560	4222	1118	1192	28	0	U	U
1	р	Q10	Total	С	Ν	Ο	S	0	0	0
	812	6585	4236	1122	1199	28		U		

• Molecule 1 is a protein called Dipeptidyl peptidase 9.

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	864	HIS	-	expression tag	UNP Q86TI2
A	865	HIS	-	expression tag	UNP Q86TI2
A	866	HIS	-	expression tag	UNP Q86TI2
А	867	HIS	-	expression tag	UNP Q86TI2
A	868	HIS	-	expression tag	UNP Q86TI2
A	869	HIS	-	expression tag	UNP Q86TI2
В	864	HIS	-	expression tag	UNP Q86TI2
В	865	HIS	-	expression tag	UNP Q86TI2
В	866	HIS	-	expression tag	UNP Q86TI2
В	867	HIS	-	expression tag	UNP Q86TI2
В	868	HIS	-	expression tag	UNP Q86TI2
В	869	HIS	-	expression tag	UNP Q86TI2
С	864	HIS	-	expression tag	UNP Q86TI2
С	865	HIS	-	expression tag	UNP Q86TI2
С	866	HIS	-	expression tag	UNP Q86TI2
С	867	HIS	-	expression tag	UNP Q86TI2
С	868	HIS	-	expression tag	UNP Q86TI2
С	869	HIS	-	expression tag	UNP Q86TI2
D	864	HIS	-	expression tag	UNP Q86TI2
D	865	HIS	-	expression tag	UNP Q86TI2
D	866	HIS	-	expression tag	UNP Q86TI2



00100100								
Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference			
D	867	HIS	-	expression tag	UNP Q86TI2			
D	868	HIS	-	expression tag	UNP Q86TI2			
D	869	HIS	-	expression tag	UNP Q86TI2			

• Molecule 2 is a protein called MET-PRO.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0	F	0	Total	С	Ν	Ο	S	0	0	0
		2	16	10	2	3	1	0	0	0
9	F	9	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	T,	2	16	10	2	3	1	0	0	0
9	С	9	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	G	2	16	10	2	3	1	0	0	U
9	Ц	9	Total	С	Ν	Ο	S	0	0	0
	11	Δ	16	10	2	3	1	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	2	Total O 2 2	0	0
3	D	2	Total O 2 2	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 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.



• Molecule 1: Dipeptidyl peptidase 9







• Molecule 1: Dipeptidyl peptidase 9



%				
Chain D:	69%		20% •	10%
MET ARG VAL VAL VAL VAL VAL VAL VAL VAS VAS VAS VAS VAS VAS VAS	GLY SER SER SER SER SER SER SER SER SER SER	ALLA THR THR GLT FR CHT FR FR FR ALLA ALLA ALLA ALLA ALLA ALLA	ALA ALA ALA ASP ASP P20 D27 D27	K28 K43 TYR SER GIN LEU ILEU
VAL ASM ASM LYS A52 A55 F56 G55 F58 F58 F58 F58 F58 F63 F61 F61 F63	SER 666 666 666 773 777 777 777 877 817 82 83 83 882 83 883 83 83 83 83 83 83 83 83 83 83 83	ARG ARG GLU GLU GLU GLU GLU LIU ILU EL2 EL25 EL25 EL25 EL25 AL31	R133 F151 A155 A155 N157 N157 S158 S158	L159 F160 H161 G165 M168 M168 F170
E179 E179 C184 N188 M188 F200 F200 F200	1200 1200 12112 12119 1223 1223 1223 1223 1223 12	V233 1233 1233 1233 1233 1233 1233 1233	C259 C259 C266 C266 C266 C100 C100 C100 C100 C100 C100 C100 C1	GLY 1270 V280 S283 R307 T308
6309 3310 1313 1324 1319 1324 0334 7334 8339 8343	2344 1.345 1.345 1.345 1.3555 1.3555 1.3555 1.3555 1.35555 1.35555 1.35555555555	<b>F386</b> <b>F386</b> <b>1369</b> <b>1370</b> <b>1372</b> <b>1376</b> <b>1376</b> <b>1376</b> <b>1376</b> <b>1376</b> <b>1377</b> <b>1380</b>	P382 P382 P384 A384 A385 L385 T390 T391	R405 Y410 V411 V412 Y413 F413 E414
14.17 14.17 14.19 14.19 14.23 14.25 14.25 14.26 14.26 14.26 14.26 14.26 14.26 14.26 14.26 14.27 14.29	q432         q432           9433         9433           6LU         6LV           6LV         6LV           61         643           6440         7444           7444         7444           7445         7451           7451         7451	V457 (4465 (4465 (4468 (4468 (4480 (481) (	243 11 15 15 15 15 15 15 15 15 15	8524 1527 1528 1532 1532 1532 1532
L541 T542 G545 H548 B549 C550 C550 C550 S551 D557 V560	r563 D582 A599 A599 A599 A599 P80 P80 P80 P804 D604 B1615 B617 D618	6623 L641 K644 K652 V652 N653 N653 N653 L670	Q684 L687 R688 G691 M697	1702 4705 1709 1709
Y116 9715 7713 7713 7713 87723 87723 1719 87723 1725 1725 1725 1735	17 41 17 41 17 42 17 53 17 56 17 65 17 65 17 65 17 65 17 65 17 65	E 68 E769 1776 1777 1772 1773 1773 1775 1775 1775 1775 1775 1775	H8 04 18 07 18 07 18 14 H8 15 H8 15	1816 1817 7818 7818 1823 18224 18224 18225 1832
HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS	SIH			
• Molecule 2: MET	ſ-PRO			
Chain E:	50%	5	50%	
<mark>11232</mark> 12233				
• Molecule 2: MET	Γ-PRO			
Chain F:	50%	5	0%	
1233 1233 133				
• Molecule 2: MET	Г-PRO			
Chain G:	50%		50%	
1233 1233 133				
• Molecule 2: MET	Г-PRO			



Chain H:	50%	50%
283 233		



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	119.52Å 117.22Å 163.40Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $105.72^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{esolution}}(\mathbf{\hat{A}})$	43.47 - 3.00	Depositor
Resolution (A)	43.47 - 3.00	EDS
$\% { m Data \ completeness}$	88.1 (43.47-3.00)	Depositor
(in resolution range $)$	88.1(43.47-3.00)	EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.90 (at 3.01 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
D D .	0.286 , $0.345$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.287 , $0.344$	DCC
$R_{free}$ test set	3827 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.9	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 37.2	EDS
L-test for $twinning^2$	$ < L >=0.52, < L^2>=0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	26316	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 59.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6741e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	А	0.66	0/6759	0.70	0/9165
1	В	0.66	0/6733	0.70	0/9128
1	С	0.66	0/6754	0.70	0/9159
1	D	0.66	0/6779	0.70	0/9192
2	Е	0.87	0/16	1.31	0/19
2	F	0.66	0/16	0.61	0/19
2	G	0.68	0/16	0.68	0/19
2	Ĥ	0.65	0/16	0.68	0/19
All	All	0.66	0/27089	0.70	0/36720

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 (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	6563	0	6348	107	0
1	В	6540	0	6340	124	0
1	С	6560	0	6347	113	0
1	D	6585	0	6365	110	0
2	Ε	16	0	15	4	0
2	F	16	0	15	3	0
2	G	16	0	15	1	0
2	Н	16	0	15	3	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 9.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	1100111 2	distance (Å)	overlap (Å)
1:B:420:TRP:HZ3	1:B:694:LYS:HB2	1.26	0.97
1:A:307:ARG:O	1:A:310:SER:HB3	1.68	0.92
1:D:223:THR:HG21	1:D:239:ALA:HB3	1.54	0.87
1:B:420:TRP:CZ3	1:B:694:LYS:HB2	2.13	0.84
1:B:307:ARG:O	1:B:310:SER:HB3	1.78	0.81
1:A:729:TRP:CZ3	1:A:754:ALA:HB2	2.17	0.79
1:D:307:ARG:O	1:D:310:SER:HB3	1.83	0.77
1:D:697:MET:HG3	1:D:771:MET:SD	2.26	0.75
1:A:223:THR:HG21	1:A:239:ALA:HB3	1.69	0.74
1:B:371:ARG:NH1	1:B:768:GLU:OE2	2.20	0.74
1:B:362:LYS:HE3	1:B:432:GLN:HE22	1.53	0.72
1:C:307:ARG:O	1:C:310:SER:HB3	1.90	0.71
1:A:339:VAL:HG13	1:A:387:ILE:HG21	1.72	0.71
1:B:362:LYS:HG2	1:B:363:TYR:CD2	2.26	0.70
1:A:762:TYR:OH	2:E:233:PRO:HA	1.92	0.70
1:D:494:TRP:CG	1:D:519:LYS:HA	2.27	0.70
1:D:762:TYR:OH	2:H:233:PRO:HA	1.92	0.69
1:A:133:ARG:NH1	1:A:248:GLU:OE1	2.26	0.69
1:B:494:TRP:CG	1:B:519:LYS:HA	2.27	0.68
1:C:420:TRP:CZ3	1:C:694:LYS:HB2	2.29	0.68
1:C:371:ARG:NH1	1:C:768:GLU:OE2	2.25	0.68
1:C:641:LEU:HD13	1:C:709:LEU:HD13	1.75	0.67
1:A:367:MET:HE3	1:A:376:LEU:HD11	1.76	0.67
1:B:54:HIS:HE1	1:B:84:ASN:HD21	1.41	0.66
1:A:339:VAL:HG13	1:A:387:ILE:CG2	2.25	0.66
1:A:392:ASN:ND2	1:A:395:GLN:OE1	2.30	0.65
1:C:223:THR:HG21	1:C:239:ALA:HB3	1.79	0.64
1:C:373:GLN:NE2	1:C:769:ARG:HB2	2.12	0.64
1:B:810:ASN:C	1:B:810:ASN:HD22	1.99	0.63
1:A:371:ARG:CG	1:A:371:ARG:HH11	2.11	0.62
1:A:729:TRP:HZ3	1:A:754:ALA:HB2	1.63	0.62



Chain Non-H H(added) Clashes Symm-Clashes Mol H(model) 3 С 20 0 0 1 3 D 2 0 0 0 0 All All 263160 025460446

Continued from previous page...

		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:339:VAL:HG23	1:D:385:LEU:O	2.00	0.62
1:A:233:LEU:HD11	1:A:287:VAL:HG11	1.82	0.62
1:D:494:TRP:CB	1:D:519:LYS:HA	2.29	0.62
1:C:209:LEU:H	1:C:223:THR:HG22	1.65	0.61
1:B:620:ARG:O	1:B:685:ARG:NH1	2.33	0.61
1:C:362:LYS:HD3	1:C:363:TYR:CE1	2.36	0.61
1:C:347:PRO:O	1:C:348:LYS:HB2	2.00	0.60
1:C:411:VAL:HG22	1:C:480:LYS:HA	1.84	0.60
1:C:420:TRP:HZ3	1:C:694:LYS:HB2	1.65	0.60
1:C:767:THR:HG22	1:C:771:MET:HB2	1.84	0.60
1:B:286:GLU:OE2	1:B:307:ARG:HD3	2.01	0.60
1:B:362:LYS:O	1:B:383:PRO:CD	2.50	0.59
1:C:644:TYR:HD2	1:C:646:GLY:H	1.49	0.59
1:C:712:VAL:HG12	1:C:719:ILE:HG13	1.84	0.59
1:C:60:GLN:NE2	1:C:557:ASP:OD2	2.36	0.59
1:A:379:VAL:HG12	1:A:411:VAL:HG22	1.83	0.59
1:B:709:LEU:HD21	1:B:724:VAL:HG11	1.85	0.59
1:B:762:TYR:OH	2:F:233:PRO:HA	2.02	0.59
1:C:413:TYR:OH	1:C:445:ASN:ND2	2.36	0.59
1:D:766:TYR:CE2	2:H:233:PRO:HD3	2.38	0.59
1:A:408:GLN:HE22	1:A:464:GLN:H	1.50	0.58
1:C:358:THR:HG23	3:C:902:HOH:O	2.02	0.58
1:A:232:VAL:HG13	1:A:233:LEU:H	1.68	0.58
1:A:371:ARG:HG2	1:A:371:ARG:HH11	1.68	0.58
1:B:369:LEU:HD12	1:B:375:TRP:O	2.03	0.58
1:B:233:LEU:HD12	1:B:287:VAL:HG11	1.85	0.58
1:A:494:TRP:CG	1:A:519:LYS:HA	2.39	0.58
1:D:362:LYS:HD2	1:D:432:GLN:HE22	1.69	0.58
1:B:357:TRP:HZ3	1:B:383:PRO:HG3	1.69	0.57
1:A:840:HIS:NE2	2:E:233:PRO:OXT	2.36	0.57
1:A:133:ARG:NH2	2:E:233:PRO:O	2.37	0.57
1:A:419:VAL:O	1:A:694:LYS:HE2	2.04	0.57
1:A:338:LEU:HD21	1:A:386:PHE:CZ	2.40	0.57
1:A:842:ILE:CG2	1:A:847:SER:HB2	2.35	0.57
1:B:362:LYS:HE3	1:B:432:GLN:NE2	2.19	0.57
1:D:451:PHE:CE1	1:D:493:GLU:HA	2.40	0.57
1:D:410:TYR:HB3	1:D:481:CYS:SG	2.45	0.57
1:B:440:CYS:SG	1:B:456:LYS:NZ	2.64	0.56
1:B:129:ARG:O	1:B:134:LEU:N	2.38	0.56
1:B:378:LEU:HD13	1:B:427:PHE:CD1	2.41	0.56
1:D:411:VAL:HG23	1:D:479:PHE:HB2	1.86	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:773:VAL:HG12	1:D:775:GLU:H	1.69	0.56
1:C:846:GLU:OE2	1:D:825:ARG:NH1	2.38	0.56
1:A:804:HIS:HD2	1:A:816:THR:OG1	1.88	0.56
1:A:287:VAL:O	1:B:299:LYS:HE2	2.06	0.56
1:C:359:ARG:NH2	1:C:508:GLU:OE2	2.38	0.56
1:C:243:THR:CG2	1:C:280:VAL:HG11	2.36	0.56
1:A:156:SER:OG	1:A:157:ASN:N	2.38	0.56
1:D:427:PHE:O	1:D:429:PRO:HD3	2.05	0.55
1:A:757:THR:HB	1:A:787:ALA:HB2	1.88	0.55
1:C:29:HIS:H	1:C:860:GLN:NE2	2.05	0.55
1:D:156:SER:OG	1:D:157:ASN:N	2.36	0.55
1:D:243:THR:CG2	1:D:280:VAL:HG11	2.36	0.55
1:B:201:PHE:CZ	1:B:212:ALA:HB3	2.41	0.55
1:B:376:LEU:HD13	1:B:376:LEU:C	2.27	0.55
1:A:489:LEU:HD22	1:A:532:TYR:HA	1.88	0.55
1:B:767:THR:HG22	1:B:771:MET:HB2	1.88	0.55
1:D:615:THR:HG1	1:D:617:SER:HG	1.55	0.55
1:D:511:LYS:HA	1:D:532:TYR:CE2	2.42	0.55
1:C:566:VAL:HG23	1:C:654:ASN:HA	1.89	0.55
1:C:208:ASP:OD1	1:C:223:THR:HG23	2.06	0.55
1:C:151:PHE:O	1:C:161:HIS:HA	2.07	0.55
1:A:249:GLU:OE1	1:A:249:GLU:HA	2.07	0.54
1:D:804:HIS:HD2	1:D:816:THR:OG1	1.89	0.54
1:B:412:VAL:HG21	1:B:439:LEU:CD2	2.37	0.54
1:D:417:THR:HG21	1:D:420:TRP:O	2.08	0.54
1:A:243:THR:CG2	1:A:280:VAL:HG11	2.38	0.54
1:C:234:ASP:O	1:C:236:PRO:HD3	2.08	0.54
1:B:380:LEU:HB2	1:B:410:TYR:HB2	1.90	0.54
1:A:825:ARG:HH22	1:B:837:ASN:HD22	1.56	0.54
1:D:354:ARG:NH1	1:D:425:ASP:OD1	2.41	0.54
1:D:133:ARG:NH2	1:D:248:GLU:OE2	2.41	0.54
1:D:412:VAL:CG1	1:D:441:PHE:CE2	2.90	0.54
1:D:641:LEU:HD21	1:D:705:GLN:HB3	1.90	0.54
1:A:277:TYR:CZ	1:A:318:LYS:HB2	2.43	0.53
1:D:712:VAL:HG12	1:D:719:ILE:HG13	1.90	0.53
1:B:645:GLY:HA3	1:B:735:LEU:HD12	1.89	0.53
1:A:55:ASP:HB3	1:A:142:TYR:HE1	1.73	0.53
1:A:155:ALA:HB3	1:A:160:PHE:CD1	2.42	0.53
1:B:243:THR:CG2	1:B:280:VAL:HG11	2.38	0.53
1:A:805:GLY:HA2	1:A:835:TYR:HB2	1.90	0.53
1:A:318:LYS:HD2	1:A:337:GLU:HB3	1.91	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:233:LEU:CD1	1:B:287:VAL:HG11	2.38	0.53
1:D:412:VAL:CG1	1:D:441:PHE:CZ	2.92	0.53
1:B:380:LEU:HD11	1:B:439:LEU:HD22	1.91	0.53
1:B:639:THR:OG1	1:B:719:ILE:HG23	2.09	0.53
1:C:201:PHE:CZ	1:C:212:ALA:HB3	2.43	0.53
1:D:377:GLN:NE2	1:D:414:GLU:OE2	2.42	0.53
1:D:339:VAL:HG11	1:D:468:TRP:HB3	1.90	0.52
1:C:460:VAL:HB	1:C:482:PRO:HG2	1.90	0.52
1:B:802:ILE:HG21	1:B:816:THR:HG23	1.90	0.52
1:C:419:VAL:HG21	1:C:687:LEU:HD23	1.92	0.52
1:B:409:PRO:HD2	1:B:479:PHE:CE1	2.45	0.52
1:A:790:VAL:HG11	1:A:823:LEU:HA	1.91	0.52
1:B:642:PHE:HB3	1:B:676:VAL:HG22	1.91	0.52
1:A:730:SER:OG	2:E:233:PRO:OXT	2.24	0.52
1:A:221:ARG:HH21	1:A:224:PHE:HA	1.73	0.52
1:A:611:PHE:CZ	1:A:623:GLY:HA3	2.44	0.52
1:B:376:LEU:HD13	1:B:377:GLN:N	2.24	0.52
1:B:54:HIS:CE1	1:B:84:ASN:HD21	2.25	0.52
1:B:379:VAL:HG12	1:B:411:VAL:HG22	1.92	0.52
1:D:131:ARG:HG3	1:D:247:GLN:HE21	1.75	0.52
1:D:756:VAL:HG11	1:D:759:TRP:CE3	2.44	0.52
1:B:370:ASP:HB3	1:B:375:TRP:CE3	2.45	0.52
1:B:652:VAL:HB	1:B:678:ASP:OD2	2.10	0.52
1:A:519:LYS:HB3	1:A:528:TYR:CZ	2.45	0.51
1:B:56:PHE:CD1	1:B:72:LEU:HD12	2.45	0.51
1:B:298:ARG:HH11	1:B:298:ARG:HB2	1.74	0.51
1:C:375:TRP:C	1:C:375:TRP:CD1	2.83	0.51
1:C:762:TYR:OH	2:G:233:PRO:HA	2.09	0.51
1:C:334:GLN:NE2	1:C:336:LYS:HE3	2.25	0.51
1:D:234:ASP:O	1:D:236:PRO:HD3	2.10	0.51
1:A:223:THR:CG2	1:A:239:ALA:HB3	2.39	0.51
1:A:250:PHE:O	1:A:354:ARG:NH1	2.35	0.51
1:A:339:VAL:HG22	1:A:385:LEU:O	2.10	0.51
1:D:371:ARG:HB2	1:D:372:PRO:HD3	1.92	0.51
1:A:133:ARG:HH12	1:A:248:GLU:CD	2.14	0.51
1:A:411:VAL:HB	1:A:480:LYS:HA	1.93	0.51
1:B:559:PHE:CZ	1:B:575:TYR:HB2	2.46	0.50
1:D:519:LYS:HB3	1:D:528:TYR:CZ	2.47	0.50
1:B:768:GLU:HA	1:B:772:ASP:O	2.12	0.50
1:D:201:PHE:CZ	1:D:212:ALA:HB3	2.47	0.50
1:D:623:GLY:HA2	1:D:652:VAL:HG21	1.92	0.50



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:395:GLN:HE22	1:C:404:PRO:HD3	1.76	0.50
1:A:412:VAL:CG1	1:A:441:PHE:CE2	2.95	0.50
1:A:729:TRP:CZ3	1:A:754:ALA:CB	2.93	0.50
1:B:368:PHE:CE2	1:B:379:VAL:HG21	2.46	0.50
1:A:38:ILE:HD12	1:A:852:GLU:HB3	1.93	0.50
1:A:412:VAL:HG13	1:A:441:PHE:CE2	2.47	0.50
1:B:223:THR:HG21	1:B:239:ALA:HB3	1.94	0.50
1:C:319:LEU:O	1:C:336:LYS:HB2	2.12	0.50
1:D:709:LEU:HD21	1:D:724:VAL:HG11	1.94	0.50
1:B:801:LEU:HD12	1:B:831:GLN:HB2	1.94	0.50
1:A:274:ARG:HB3	1:A:319:LEU:HD21	1.94	0.49
1:B:201:PHE:CE1	1:B:214:ILE:HG23	2.47	0.49
1:B:362:LYS:CE	1:B:432:GLN:NE2	2.74	0.49
1:A:299:LYS:HE2	1:B:289:HIS:NE2	2.27	0.49
1:B:775:GLU:OE1	1:B:775:GLU:N	2.41	0.49
1:A:516:GLN:HA	1:A:526:HIS:O	2.12	0.49
1:A:362:LYS:HG2	1:A:363:TYR:CE1	2.47	0.49
1:C:613:PHE:CZ	1:C:621:LEU:HD12	2.48	0.49
1:C:768:GLU:HA	1:C:772:ASP:O	2.12	0.49
1:B:766:TYR:CZ	2:F:233:PRO:HD3	2.47	0.49
1:B:554:GLN:CD	1:B:554:GLN:H	2.16	0.49
1:B:807:LEU:O	1:B:839:ARG:NH1	2.45	0.49
1:B:362:LYS:O	1:B:383:PRO:HD3	2.12	0.49
1:C:410:TYR:HB3	1:C:481:CYS:SG	2.53	0.49
1:A:338:LEU:CD2	1:A:386:PHE:CZ	2.96	0.49
1:B:740:LEU:HD23	1:B:793:LEU:CD2	2.43	0.48
1:B:778:GLN:HA	1:B:778:GLN:HE21	1.78	0.48
1:D:363:TYR:HB2	1:D:380:LEU:HD22	1.94	0.48
1:B:131:ARG:HG3	1:B:247:GLN:HE21	1.77	0.48
1:C:681:GLY:HA2	1:C:690:GLU:HA	1.95	0.48
1:C:767:THR:O	1:C:771:MET:N	2.32	0.48
1:D:234:ASP:C	1:D:236:PRO:HD3	2.33	0.48
1:D:840:HIS:NE2	2:H:233:PRO:O	2.46	0.48
1:A:371:ARG:HB3	1:A:372:PRO:CD	2.44	0.48
1:A:626:TYR:HB2	1:A:674:VAL:HB	1.96	0.48
1:A:650:GLN:NE2	1:A:684:GLN:HG3	2.28	0.48
1:D:495:GLU:OE2	1:D:684:GLN:HA	2.14	0.48
1:D:29:HIS:H	1:D:860:GLN:NE2	2.11	0.48
1:A:448:LYS:HD3	1:A:455:TYR:CE2	2.49	0.48
1:B:357:TRP:CZ3	1:B:383:PRO:HG3	2.47	0.48
1:C:201:PHE:CD1	1:C:214:ILE:HG23	2.48	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:417:THR:HG21	1:C:420:TRP:C	2.33	0.48
1:D:516:GLN:NE2	1:D:550:CYS:SG	2.87	0.48
1:C:511:LYS:HA	1:C:532:TYR:CE2	2.49	0.48
1:A:390:THR:HG21	1:A:395:GLN:NE2	2.29	0.47
1:B:307:ARG:O	1:B:310:SER:CB	2.57	0.47
1:A:372:PRO:O	1:A:373:GLN:HB2	2.14	0.47
1:B:240:GLY:HA2	1:B:255:GLY:O	2.14	0.47
1:B:340:GLN:HB3	1:B:345:LEU:HG	1.96	0.47
1:D:373:GLN:OE1	1:D:769:ARG:HD3	2.14	0.47
1:D:494:TRP:HB2	1:D:519:LYS:HA	1.96	0.47
1:D:540:ARG:NH1	1:D:542:THR:O	2.47	0.47
1:D:542:THR:HB	1:D:548:HIS:CD2	2.49	0.47
1:C:410:TYR:CB	1:C:461:LEU:HD22	2.45	0.47
1:A:183:GLN:HA	1:A:183:GLN:HE21	1.78	0.47
1:B:809:GLU:HG3	1:B:839:ARG:NH1	2.29	0.47
1:C:339:VAL:CG1	1:C:403:VAL:HG21	2.45	0.47
1:D:209:LEU:H	1:D:223:THR:HG22	1.79	0.47
1:B:757:THR:HA	1:B:786:VAL:HG22	1.97	0.47
1:D:548:HIS:ND1	1:D:563:TYR:HB3	2.29	0.47
1:D:367:MET:HE1	1:D:423:VAL:HG13	1.97	0.47
1:C:605:TYR:CE1	1:C:658:GLY:HA2	2.50	0.47
1:D:223:THR:CG2	1:D:239:ALA:HB3	2.37	0.47
1:A:543:THR:O	1:A:548:HIS:HE1	1.98	0.47
1:B:362:LYS:O	1:B:383:PRO:HD2	2.13	0.47
1:C:494:TRP:CG	1:C:519:LYS:HA	2.49	0.47
1:C:58:PHE:CD1	1:C:553:SER:HA	2.50	0.47
1:A:679:GLY:O	1:A:682:SER:HB2	2.15	0.47
1:A:716:TYR:HB3	1:A:718:PHE:CE2	2.50	0.47
1:C:773:VAL:HG13	1:C:775:GLU:CD	2.35	0.47
1:D:494:TRP:CD2	1:D:519:LYS:HB2	2.50	0.47
1:C:405:ARG:HA	1:C:466:TYR:O	2.15	0.46
1:D:223:THR:HG21	1:D:239:ALA:CB	2.37	0.46
1:D:716:TYR:HB3	1:D:718:PHE:CE2	2.50	0.46
1:B:362:LYS:HG2	1:B:363:TYR:CE2	2.49	0.46
1:C:681:GLY:O	1:C:690:GLU:HG3	2.15	0.46
1:D:617:SER:O	1:D:618:ASP:HB2	2.16	0.46
1:B:151:PHE:O	1:B:161:HIS:HA	2.15	0.46
1:C:24:PHE:O	1:C:723:ARG:NH1	2.46	0.46
1:B:201:PHE:CD1	1:B:214:ILE:HG23	2.51	0.46
1:B:643:VAL:HG21	1:B:726:ILE:CG1	2.46	0.46
1:C:203:PHE:CE1	1:C:210:TRP:HB2	2.50	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:412:VAL:HG21	1:B:439:LEU:HD23	1.97	0.46
1:B:68:HIS:CE1	1:B:90:GLU:HB3	2.50	0.46
1:D:412:VAL:HG11	1:D:441:PHE:CE2	2.50	0.46
1:C:188:ARG:HG2	1:C:203:PHE:CD1	2.51	0.46
1:C:751:ILE:HD13	1:C:855:LEU:HD13	1.98	0.46
1:B:773:VAL:HG12	1:B:775:GLU:HB2	1.98	0.46
1:C:124:GLU:HB3	1:C:189:MET:SD	2.56	0.46
1:C:729:TRP:CZ3	1:C:754:ALA:HB2	2.51	0.46
1:B:646:GLY:N	1:B:731:TYR:CD1	2.84	0.46
1:C:367:MET:HE1	1:C:423:VAL:HG13	1.97	0.46
1:C:643:VAL:HG12	1:C:644:TYR:N	2.31	0.46
1:D:371:ARG:CB	1:D:372:PRO:HD3	2.46	0.46
1:A:211:VAL:HG11	1:A:322:PHE:CZ	2.51	0.46
1:A:540:ARG:NH1	1:A:542:THR:O	2.47	0.46
1:B:263:SER:O	1:B:272:THR:HG22	2.16	0.46
1:B:494:TRP:CB	1:B:519:LYS:HA	2.45	0.46
1:B:227:GLN:N	1:B:235:ASP:OD2	2.45	0.46
1:D:131:ARG:NE	1:D:248:GLU:OE1	2.30	0.46
1:B:209:LEU:H	1:B:223:THR:HG22	1.82	0.45
1:B:371:ARG:C	1:B:373:GLN:H	2.20	0.45
1:B:804:HIS:CD2	1:B:816:THR:OG1	2.70	0.45
1:C:548:HIS:CD2	1:C:563:TYR:HB3	2.51	0.45
1:C:651:LEU:HA	1:C:651:LEU:HD23	1.83	0.45
1:D:741:ILE:HG22	1:D:742:HIS:CD2	2.52	0.45
1:D:807:LEU:HB2	1:D:839:ARG:HG2	1.97	0.45
1:D:814:PHE:O	1:D:818:PHE:N	2.46	0.45
1:A:797:PRO:O	1:A:798:ASN:HB2	2.17	0.45
1:D:545:GLY:O	1:D:654:ASN:ND2	2.47	0.45
1:B:432:GLN:HB2	1:B:432:GLN:HE21	1.63	0.45
1:B:42:ARG:NH1	1:B:852:GLU:OE2	2.41	0.45
1:A:773:VAL:HG12	1:A:775:GLU:CD	2.37	0.45
1:D:687:LEU:O	1:D:691:GLY:N	2.44	0.45
1:A:238:SER:O	1:A:280:VAL:N	2.41	0.45
1:B:629:HIS:NE2	1:B:665:ASN:ND2	2.65	0.45
1:C:359:ARG:HH22	1:C:508:GLU:CD	2.20	0.45
1:A:631:LEU:O	1:A:633:PRO:HD3	2.17	0.45
1:A:645:GLY:HA3	1:A:735:LEU:HD11	1.97	0.45
1:D:702:ILE:O	1:D:706:VAL:HG23	2.17	0.45
1:A:299:LYS:HE3	1:B:287:VAL:HB	1.99	0.45
1:C:641:LEU:HD21	1:C:705:GLN:HE21	1.82	0.45
1:D:200:PHE:CZ	1:D:324:THR:HG21	2.52	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:307:ARG:O	1:D:310:SER:CB	2.61	0.45
1:D:363:TYR:CB	1:D:380:LEU:HD22	2.47	0.45
1:D:429:PRO:HA	1:D:441:PHE:CB	2.47	0.45
1:B:766:TYR:CE1	2:F:233:PRO:HD3	2.51	0.45
1:D:362:LYS:CD	1:D:432:GLN:HE22	2.30	0.44
1:B:716:TYR:HB3	1:B:718:PHE:CE2	2.52	0.44
1:C:84:ASN:ND2	1:C:139:ILE:O	2.45	0.44
1:D:382:PRO:HA	1:D:383:PRO:HD3	1.88	0.44
1:D:444:ALA:HB1	1:D:452:CYS:SG	2.57	0.44
1:D:58:PHE:CZ	1:D:560:VAL:HG23	2.52	0.44
1:A:207:SER:HB3	1:A:238:SER:HB2	2.00	0.44
1:B:773:VAL:HG13	1:B:775:GLU:CD	2.38	0.44
1:C:432:GLN:O	1:C:433:SER:CB	2.66	0.44
1:C:757:THR:HA	1:C:786:VAL:HG22	2.00	0.44
1:D:308:THR:HG21	1:D:781:TYR:HE2	1.83	0.44
1:A:367:MET:CE	1:A:376:LEU:HD11	2.47	0.44
1:B:118:HIS:HB3	1:B:120:VAL:HG23	1.99	0.44
1:B:72:LEU:O	1:B:88:TYR:HA	2.17	0.44
1:C:773:VAL:CG1	1:C:775:GLU:HG2	2.48	0.44
1:C:834:ILE:HD12	1:D:832:LEU:HD21	2.00	0.44
1:B:740:LEU:HD23	1:B:793:LEU:HD22	2.00	0.44
1:C:540:ARG:NH1	1:C:544:PRO:HD3	2.32	0.44
1:D:226:HIS:HA	1:D:235:ASP:OD1	2.18	0.44
1:D:371:ARG:NH1	1:D:768:GLU:OE2	2.49	0.44
1:D:56:PHE:HA	1:D:73:TYR:O	2.18	0.44
1:A:158:SER:HB2	1:A:188:ARG:HH21	1.82	0.44
1:A:56:PHE:HE1	1:A:595:MET:HE1	1.82	0.44
1:B:236:PRO:HD2	1:B:237:LYS:H	1.83	0.44
1:C:420:TRP:HZ3	1:C:694:LYS:CB	2.29	0.44
1:C:308:THR:HG21	1:C:781:TYR:HE2	1.81	0.44
1:B:192:LYS:NZ	1:B:256:TYR:O	2.50	0.43
1:B:57:GLN:HB2	1:B:73:TYR:HB2	2.00	0.43
1:C:444:ALA:HB1	1:C:452:CYS:SG	2.57	0.43
1:A:400:ALA:O	1:A:403:VAL:HG23	2.18	0.43
1:A:807:LEU:HB2	1:A:839:ARG:HG2	1.99	0.43
1:B:29:HIS:CE1	1:B:37:ILE:HD11	2.53	0.43
1:B:308:THR:HG21	1:B:781:TYR:HE2	1.83	0.43
1:A:412:VAL:CG1	1:A:441:PHE:CZ	3.02	0.43
1:A:426:ILE:HD12	1:A:498:ALA:HB2	2.01	0.43
1:D:375:TRP:CD1	1:D:375:TRP:O	2.71	0.43
1:D:413:TYR:CE1	1:D:457:VAL:HG21	2.54	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:380:LEU:HD11	1:A:439:LEU:HD22	2.00	0.43
1:B:806:PHE:HB2	1:B:834:ILE:HG23	2.00	0.43
1:C:442:LEU:HD23	1:C:456:LYS:HA	1.99	0.43
1:C:307:ARG:HA	1:C:763:ASP:HA	2.00	0.43
1:A:339:VAL:CG2	1:A:385:LEU:O	2.67	0.43
1:D:432:GLN:CG	1:D:439:LEU:HD13	2.49	0.43
1:A:741:ILE:HD13	1:A:789:HIS:HB2	2.00	0.43
1:C:709:LEU:HD21	1:C:724:VAL:HG21	2.01	0.43
1:D:77:MET:HB3	1:D:78:PRO:HD2	2.00	0.43
1:C:272:THR:HG22	1:C:323:GLN:HE21	1.82	0.43
1:D:790:VAL:HG11	1:D:823:LEU:HA	2.00	0.43
1:A:814:PHE:O	1:A:818:PHE:N	2.45	0.43
1:C:319:LEU:HD12	1:C:386:PHE:CG	2.54	0.43
1:D:764:THR:HA	1:D:768:GLU:HG3	2.01	0.43
1:A:231:ASN:N	1:A:231:ASN:OD1	2.52	0.43
1:B:373:GLN:NE2	1:B:765:GLY:O	2.48	0.43
1:B:738:MET:SD	1:B:786:VAL:HG12	2.58	0.43
1:C:445:ASN:HB3	1:C:455:TYR:CE1	2.54	0.43
1:C:783:ALA:HA	1:C:789:HIS:HE2	1.84	0.43
1:D:188:ARG:HG2	1:D:203:PHE:CE1	2.54	0.43
1:B:209:LEU:HD11	1:B:275:ILE:HG21	2.01	0.42
1:B:528:TYR:CE1	1:B:540:ARG:HB2	2.54	0.42
1:C:439:LEU:HD23	1:C:441:PHE:CD2	2.54	0.42
1:C:757:THR:HB	1:C:787:ALA:HB2	2.01	0.42
1:D:355:ALA:HA	1:D:366:ALA:HA	2.01	0.42
1:B:354:ARG:NH2	1:B:425:ASP:OD1	2.53	0.42
1:C:397:LEU:HA	1:C:400:ALA:HB3	2.00	0.42
1:C:417:THR:HG22	1:C:421:ILE:HG12	2.00	0.42
1:C:483:ILE:HG22	1:C:485:GLU:O	2.19	0.42
1:C:807:LEU:O	1:C:839:ARG:NH1	2.52	0.42
1:D:165:GLY:HA2	1:D:170:PHE:CE1	2.54	0.42
1:A:445:ASN:HB3	1:A:455:TYR:CE1	2.54	0.42
1:C:419:VAL:HB	1:C:420:TRP:H	1.66	0.42
1:C:563:TYR:CZ	1:C:571:CYS:HB2	2.54	0.42
1:C:758:VAL:HG12	1:C:761:ALA:H	1.85	0.42
1:D:527:LEU:HB3	1:D:542:THR:HG23	2.02	0.42
1:B:376:LEU:O	1:B:414:GLU:HA	2.19	0.42
1:D:155:ALA:HB3	1:D:160:PHE:CD1	2.53	0.42
1:A:811:VAL:HG13	1:A:815:HIS:ND1	2.34	0.42
1:C:737:LEU:HD12	1:C:786:VAL:HG21	2.00	0.42
1:C:724:VAL:CG1	1:C:746:VAL:O	2.68	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:C:319:LEU:HD12	1:C:386:PHE:CD1	2.55	0.42
1:C:520:ASP:HB2	1:C:528:TYR:OH	2.20	0.42
1:B:54:HIS:CE1	1:B:75:LEU:HB2	2.55	0.42
1:D:243:THR:HG21	1:D:280:VAL:HG11	2.00	0.42
1:D:730:SER:N	1:D:753:GLY:O	2.53	0.42
1:D:82:ARG:HD2	1:D:83:GLU:HB3	2.02	0.42
1:C:208:ASP:OD1	1:C:223:THR:CG2	2.67	0.42
1:C:319:LEU:HD21	1:C:357:TRP:HH2	1.85	0.42
1:C:520:ASP:OD2	1:C:540:ARG:NE	2.47	0.42
1:A:625:ILE:HD12	1:A:675:VAL:HG22	2.02	0.41
1:A:766:TYR:O	1:A:770:TYR:CD2	2.73	0.41
1:B:88:TYR:OH	1:B:172:VAL:O	2.38	0.41
1:B:805:GLY:HA2	1:B:835:TYR:HB2	2.01	0.41
1:C:318:LYS:HD2	1:C:337:GLU:HA	2.02	0.41
1:D:405:ARG:O	1:D:465:GLY:HA2	2.20	0.41
1:D:417:THR:HG21	1:D:420:TRP:C	2.40	0.41
1:B:58:PHE:CE2	1:B:72:LEU:HD11	2.55	0.41
1:C:243:THR:HG21	1:C:280:VAL:HG11	2.02	0.41
1:C:448:LYS:HD3	1:C:455:TYR:CE2	2.54	0.41
1:C:527:LEU:HB3	1:C:542:THR:HG23	2.01	0.41
1:C:528:TYR:CD1	1:C:540:ARG:HB2	2.56	0.41
1:D:359:ARG:NE	1:D:431:PRO:HD3	2.35	0.41
1:A:145:HIS:O	1:A:149:GLY:N	2.53	0.41
1:A:337:GLU:HG2	1:A:389:SER:OG	2.20	0.41
1:A:357:TRP:CE3	1:A:364:ALA:HB2	2.55	0.41
1:A:639:THR:HA	1:A:673:ALA:O	2.20	0.41
1:C:641:LEU:HD22	1:C:747:PHE:CE1	2.56	0.41
1:D:212:ALA:HA	1:D:218:GLU:O	2.21	0.41
1:D:236:PRO:HB2	1:D:283:SER:OG	2.19	0.41
1:A:457:VAL:HG22	1:A:486:GLU:HG3	2.02	0.41
1:D:725:ALA:HB2	1:D:863:LEU:HD22	2.03	0.41
1:D:771:MET:O	1:D:772:ASP:CB	2.69	0.41
1:A:548:HIS:HB3	1:A:561:SER:HG	1.86	0.41
1:B:60:GLN:HG3	1:B:70:HIS:CE1	2.56	0.41
1:B:645:GLY:HA3	1:B:735:LEU:CD1	2.49	0.41
1:B:751:ILE:HG23	1:B:801:LEU:HD23	2.02	0.41
1:B:243:THR:HG21	1:B:280:VAL:HG11	2.02	0.41
1:B:797:PRO:O	1:B:798:ASN:HB2	2.19	0.41
1:C:764:THR:HB	1:C:768:GLU:OE1	2.20	0.41
1:D:350:GLU:HG2	1:D:371:ARG:HG2	2.02	0.41
1:D:644:TYR:O	1:D:735:LEU:HD12	2.21	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:131:ARG:NE	1:A:248:GLU:HG2	2.35	0.41
1:A:239:ALA:HB1	1:A:277:TYR:CE1	2.55	0.41
1:B:426:ILE:HD12	1:B:498:ALA:HB2	2.01	0.41
1:C:623:GLY:HA2	1:C:652:VAL:HG21	2.02	0.41
1:C:801:LEU:HD12	1:C:831:GLN:CB	2.51	0.41
1:A:392:ASN:HD22	1:A:395:GLN:CD	2.24	0.41
1:A:609:GLU:HB3	1:A:625:ILE:CG2	2.50	0.41
1:C:464:GLN:O	1:C:464:GLN:HG3	2.20	0.41
1:C:58:PHE:CZ	1:C:560:VAL:HG23	2.56	0.41
1:D:705:GLN:O	1:D:709:LEU:HB2	2.21	0.41
1:B:371:ARG:HB3	1:B:372:PRO:HD3	2.01	0.41
1:C:191:PRO:HA	1:C:202:SER:O	2.21	0.41
1:C:740:LEU:HD23	1:C:793:LEU:HD22	2.03	0.41
1:D:670:LEU:HD12	1:D:856:LEU:HD22	2.03	0.41
1:A:158:SER:HB2	1:A:188:ARG:NH2	2.35	0.41
1:A:527:LEU:HB3	1:A:542:THR:HG23	2.03	0.41
1:B:644:TYR:CZ	1:B:649:VAL:HG21	2.56	0.41
1:C:735:LEU:HD23	1:C:735:LEU:HA	1.81	0.41
1:D:60:GLN:NE2	1:D:557:ASP:OD2	2.52	0.41
1:B:512:LEU:HD23	1:B:531:SER:HA	2.04	0.40
1:A:371:ARG:CG	1:A:371:ARG:NH1	2.77	0.40
1:A:368:PHE:CE2	1:A:379:VAL:HG21	2.57	0.40
1:B:131:ARG:HG3	1:B:247:GLN:NE2	2.35	0.40
1:B:405:ARG:O	1:B:465:GLY:HA2	2.22	0.40
1:C:801:LEU:HD12	1:C:831:GLN:HB2	2.02	0.40
1:D:151:PHE:O	1:D:161:HIS:HA	2.21	0.40
1:A:339:VAL:HG13	1:A:387:ILE:HG23	2.03	0.40
1:A:369:LEU:HG	1:A:376:LEU:HD12	2.03	0.40
1:B:519:LYS:HB3	1:B:528:TYR:CZ	2.56	0.40
1:B:680:ARG:NH2	1:B:704:ASP:OD1	2.55	0.40
1:A:825:ARG:NH2	1:B:837:ASN:HD22	2.17	0.40
1:C:319:LEU:O	1:C:336:LYS:N	2.54	0.40
1:D:160:PHE:CE2	1:D:179:GLU:HG2	2.55	0.40
1:D:412:VAL:HG13	1:D:441:PHE:CE2	2.56	0.40
1:B:412:VAL:HG21	1:B:439:LEU:HD22	2.04	0.40
1:B:785:SER:HB2	1:B:788:LEU:HD12	2.03	0.40
1:C:751:ILE:HG23	1:C:801:LEU:HD23	2.02	0.40
1:C:308:THR:HB	1:C:763:ASP:O	2.21	0.40
1:D:369:LEU:HD21	1:D:376:LEU:HB2	2.03	0.40
1:D:350:GLU:CD	1:D:371:ARG:HG2	2.41	0.40
1:D:521:THR:CG2	1:D:524:GLU:HB2	2.51	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD23	1:D:651:LEU:HA	1.85	0.40
1:B:376:LEU:HB2	1:B:421:ILE:HG21	2.03	0.40
1:B:806:PHE:HB3	1:B:836:PRO:HA	2.03	0.40
1:C:192:LYS:NZ	1:C:256:TYR:O	2.49	0.40
1:C:494:TRP:CE3	1:C:519:LYS:HB2	2.57	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	$\mathbf{ntiles}$
1	А	790/898~(88%)	735~(93%)	52 (7%)	3~(0%)	34	72
1	В	785/898~(87%)	729~(93%)	55 (7%)	1 (0%)	51	85
1	С	790/898~(88%)	735~(93%)	50~(6%)	5(1%)	25	64
1	D	794/898~(88%)	730~(92%)	61 (8%)	3~(0%)	34	72
All	All	3159/3592 (88%)	2929 (93%)	218(7%)	12 (0%)	34	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	232	VAL
1	А	465	GLY
1	D	772	ASP
1	С	207	SER
1	С	348	LYS
1	С	814	PHE
1	А	772	ASP
1	В	236	PRO
1	С	419	VAL
1	С	839	ARG



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Mol	Chain	Res	Type
1	D	419	VAL
1	D	339	VAL

### 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	Perce	entiles
1	А	712/785~(91%)	675~(95%)	37~(5%)	23	59
1	В	712/785~(91%)	673~(94%)	39~(6%)	21	57
1	С	714/785~(91%)	677~(95%)	37~(5%)	23	59
1	D	715/785~(91%)	682~(95%)	33~(5%)	27	64
2	Ε	2/2~(100%)	2~(100%)	0	100	100
2	F	2/2~(100%)	2~(100%)	0	100	100
2	G	2/2~(100%)	2~(100%)	0	100	100
2	Η	2/2~(100%)	2(100%)	0	100	100
All	All	2861/3148~(91%)	2715 (95%)	146 (5%)	24	60

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	55	ASP
1	А	60	GLN
1	А	130	GLU
1	А	147	GLU
1	А	150	LEU
1	А	183	GLN
1	А	209	LEU
1	А	223	THR
1	А	226	HIS
1	А	231	ASN
1	A	287	VAL
1	А	288	ILE
1	A	319	LEU



Mol	Chain	Res	Type
1	А	326	SER
1	А	339	VAL
1	А	371	ARG
1	А	389	SER
1	А	403	VAL
1	А	447	CYS
1	А	469	SER
1	А	520	ASP
1	А	551	SER
1	А	590	ARG
1	А	632	GLN
1	А	682	SER
1	А	683	CYS
1	А	688	ARG
1	А	697	MET
1	А	700	VAL
1	А	701	GLU
1	А	764	THR
1	А	778	GLN
1	А	810	ASN
1	А	821	SER
1	А	843	ARG
1	А	846	GLU
1	А	847	SER
1	В	104	SER
1	В	108	MET
1	В	123	ARG
1	В	128	LEU
1	В	130	GLU
1	В	147	GLU
1	В	150	LEU
1	B	187	PRO
1	В	189	MET
1	В	209	LEU
1	В	226	HIS
1	В	232	VAL
1	В	233	LEU
1	В	235	ASP
1	B	238	SER
1	B	251	ASP
1	В	300	THR
1	В	307	ARG



Mol	Chain	Res	Type
1	В	351	TYR
1	В	389	SER
1	В	390	THR
1	В	408	GLN
1	В	412	VAL
1	В	432	GLN
1	В	447	CYS
1	В	469	SER
1	В	473	SER
1	В	499	ARG
1	В	503	LYS
1	В	549	SER
1	В	567	SER
1	В	604	ASP
1	В	696	GLN
1	В	719	ILE
1	В	773	VAL
1	В	778	GLN
1	В	809	GLU
1	В	810	ASN
1	В	847	SER
1	С	23	ARG
1	С	102	LEU
1	С	104	SER
1	С	115	THR
1	С	130	GLU
1	С	141	SER
1	С	147	GLU
1	C	171	MET
1	С	172	VAL
1	С	194	CYS
1	C	209	LEU
1	С	221	ARG
1	C	223	THR
1	С	248	GLU
1	C	272	THR
1	С	279	GLU
1	С	342	PHE
1	C	343	SER
1	С	345	LEU
1	C	351	TYR
1	С	392	ASN



Mol	Chain	Res	Type
1	С	411	VAL
1	С	433	SER
1	С	447	CYS
1	С	464	GLN
1	С	491	SER
1	С	557	ASP
1	С	558	MET
1	С	597	GLU
1	С	604	ASP
1	С	609	GLU
1	С	662	LEU
1	С	703	GLU
1	С	734	PHE
1	С	773	VAL
1	С	809	GLU
1	С	810	ASN
1	D	20	PRO
1	D	27	GLN
1	D	101	LEU
1	D	125	GLU
1	D	158	SER
1	D	168	ASN
1	D	184	CYS
1	D	189	MET
1	D	209	LEU
1	D	220	ARG
1	D	223	THR
1	D	233	LEU
1	D	238	SER
1	D	259	CYS
1	D	263	SER
1	D	313	PRO
1	D	319	LEU
1	D	324	THR
1	D	334	GLN
1	D	343	SER
1	D	345	LEU
1	D	351	TYR
1	D	371	ARG
1	D	390	THR
1	D	392	ASN
1	D	520	ASP



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Mol	Chain	$\mathbf{Res}$	Type
1	D	551	SER
1	D	582	ASP
1	D	688	ARG
1	D	712	VAL
1	D	722	SER
1	D	764	THR
1	D	810	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	107	GLN
1	А	113	GLN
1	А	183	GLN
1	А	205	ASN
1	А	206	ASN
1	А	231	ASN
1	А	247	GLN
1	А	374	GLN
1	А	377	GLN
1	А	392	ASN
1	А	395	GLN
1	А	406	ASN
1	А	408	GLN
1	А	432	GLN
1	А	525	HIS
1	А	548	HIS
1	А	650	GLN
1	А	705	GLN
1	А	778	GLN
1	А	804	HIS
1	А	817	ASN
1	А	831	GLN
1	А	833	GLN
1	В	29	HIS
1	В	54	HIS
1	В	70	HIS
1	В	247	GLN
1	В	323	GLN
1	В	334	GLN
1	В	340	GLN
1	В	432	GLN



$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type
1	В	507	ASN
1	В	548	HIS
1	В	562	HIS
1	В	650	GLN
1	В	665	ASN
1	В	705	GLN
1	В	778	GLN
1	В	804	HIS
1	В	810	ASN
1	В	822	GLN
1	В	831	GLN
1	В	837	ASN
1	С	70	HIS
1	С	154	GLN
1	С	206	ASN
1	С	247	GLN
1	С	323	GLN
1	С	340	GLN
1	С	406	ASN
1	С	432	GLN
1	С	445	ASN
1	С	464	GLN
1	С	507	ASN
1	С	548	HIS
1	С	612	HIS
1	С	665	ASN
1	С	684	GLN
1	С	705	GLN
1	С	710	GLN
1	С	804	HIS
1	С	810	ASN
1	С	860	GLN
1	D	183	GLN
1	D	247	GLN
1	D	334	GLN
1	D	340	GLN
1	D	377	GLN
1	D	392	ASN
1	D	408	GLN
1	D	424	HIS
1	D	432	GLN
1	D	516	GLN



Mol	Chain	Res	Type
1	D	562	HIS
1	D	650	GLN
1	D	684	GLN
1	D	705	GLN
1	D	742	HIS
1	D	804	HIS
1	D	810	ASN
1	D	831	GLN
1	D	860	GLN

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#### 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)

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)

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<sup>th</sup> 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>	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	808/898 (89%)	-0.21	8 (0%) 82 59	10,  26,  60,  83	0
1	В	805/898~(89%)	-0.20	10 (1%) 79 54	8, 24, 53, 81	0
1	С	808/898 (89%)	-0.23	5 (0%) 89 72	9, 23, 54, 80	0
1	D	812/898~(90%)	-0.23	5 (0%) 89 72	9, 23, 55, 77	0
2	Ε	2/2~(100%)	0.62	0 100 100	43,  43,  43,  44	0
2	F	2/2~(100%)	0.56	0 100 100	30,30,30,31	0
2	G	2/2~(100%)	1.23	0 100 100	38,  38,  38,  38	0
2	Η	2/2~(100%)	1.49	0 100 100	42, 42, 42, 45	0
All	All	3241/3600 (90%)	-0.21	28 (0%) 84 63	8, 24, 56, 83	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	111	HIS	4.6
1	В	118	HIS	4.2
1	А	118	HIS	3.7
1	С	118	HIS	3.5
1	В	327	GLN	3.3
1	А	111	HIS	3.3
1	D	118	HIS	3.3
1	А	113	GLN	2.9
1	С	65	SER	2.8
1	А	93	LYS	2.8
1	D	62	THR	2.8
1	А	79	TYR	2.8
1	В	117	HIS	2.7
1	С	94	LYS	2.7
1	В	82	ARG	2.6
1	A	469	SER	2.6



Mol	Chain	Res	Type	RSRZ
1	D	64	GLU	2.6
1	С	168	ASN	2.3
1	В	391	GLU	2.3
1	В	113	GLN	2.3
1	А	472	PHE	2.3
1	D	437	ASP	2.2
1	D	185	SER	2.2
1	В	535	ALA	2.2
1	А	166	GLY	2.2
1	В	112	PHE	2.2
1	С	64	GLU	2.2
1	В	110	ASP	2.2

## 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 monosaccharides 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.

