



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 9V17 / pdb\_00009v17  
Title : Crystal structure of E. coli glycogen phosphorylase N185A/R267E mutant  
Authors : Takai, M.; Shobu, K.; Fukuda, Y.; Inoue, T.  
Deposited on : 2025-05-19  
Resolution : 3.70 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

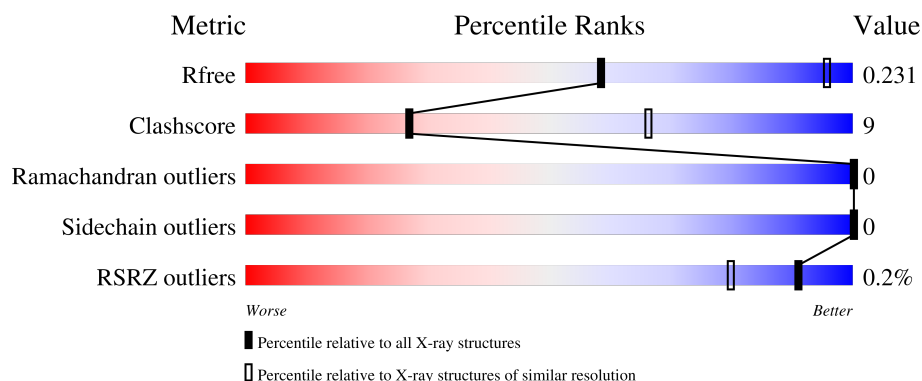
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.70 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))
$R_{free}$	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	817	 77% 21% .
1	B	817	 72% 24% .
1	C	817	 73% 25% .
1	D	817	 79% 18% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25758 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 Glycogen phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	P	S	0	0	0
			6478	4114	1121	1219	1	23			
1	B	791	Total	C	N	O	P	S	0	0	0
			6397	4058	1110	1205	1	23			
1	C	801	Total	C	N	O	P	S	0	0	0
			6478	4114	1121	1219	1	23			
1	D	792	Total	C	N	O	P	S	0	0	0
			6405	4064	1111	1206	1	23			

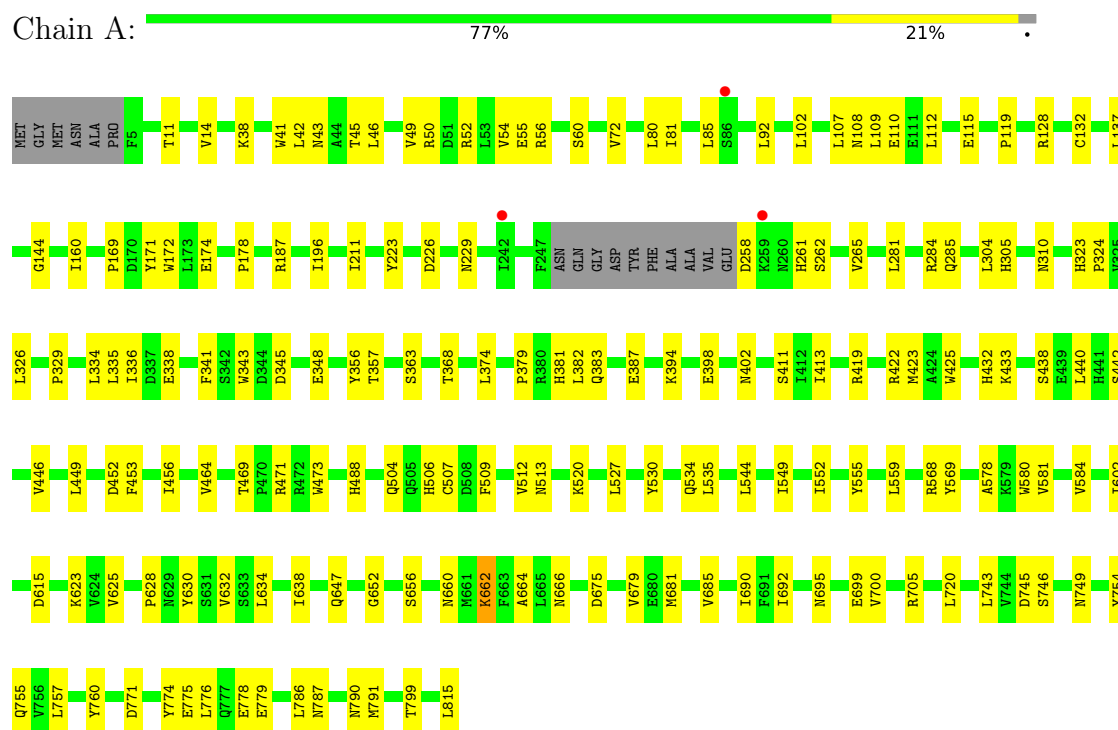
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P0AC86
A	0	GLY	-	expression tag	UNP P0AC86
A	185	ALA	ASN	engineered mutation	UNP P0AC86
A	267	GLU	ARG	engineered mutation	UNP P0AC86
B	-1	MET	-	initiating methionine	UNP P0AC86
B	0	GLY	-	expression tag	UNP P0AC86
B	185	ALA	ASN	engineered mutation	UNP P0AC86
B	267	GLU	ARG	engineered mutation	UNP P0AC86
C	-1	MET	-	initiating methionine	UNP P0AC86
C	0	GLY	-	expression tag	UNP P0AC86
C	185	ALA	ASN	engineered mutation	UNP P0AC86
C	267	GLU	ARG	engineered mutation	UNP P0AC86
D	-1	MET	-	initiating methionine	UNP P0AC86
D	0	GLY	-	expression tag	UNP P0AC86
D	185	ALA	ASN	engineered mutation	UNP P0AC86
D	267	GLU	ARG	engineered mutation	UNP P0AC86

### 3 Residue-property plots

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: Glycogen phosphorylase



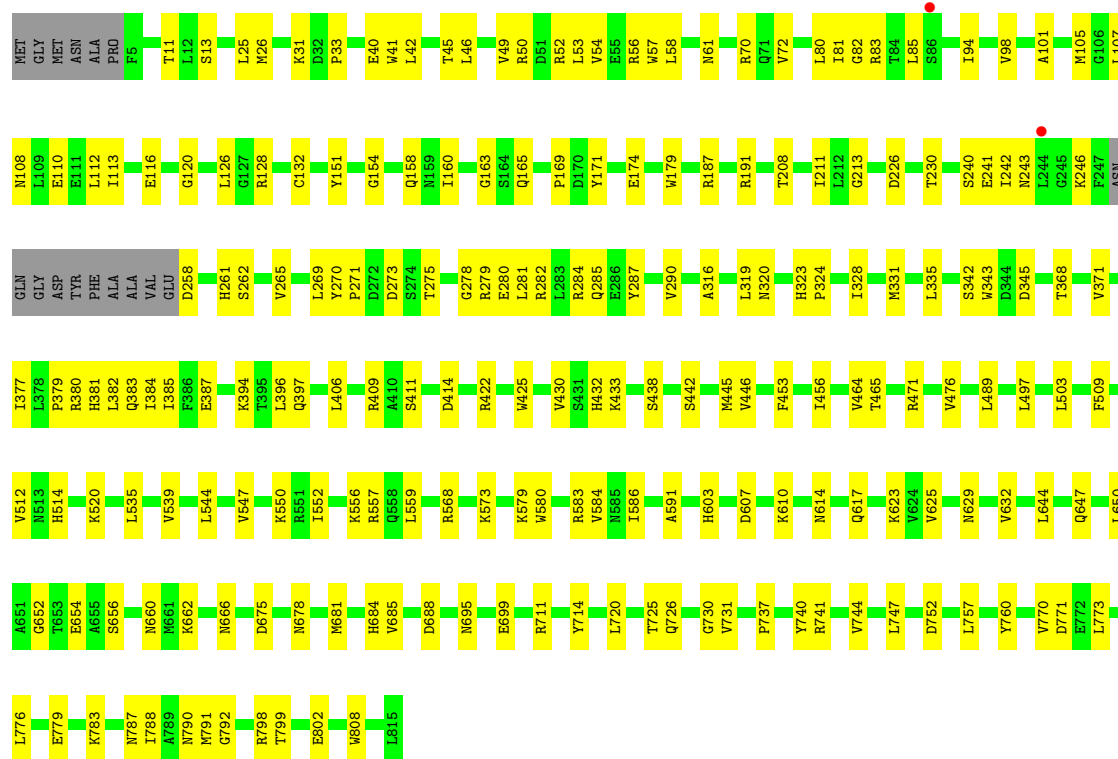
#### • Molecule 1: Glycogen phosphorylase





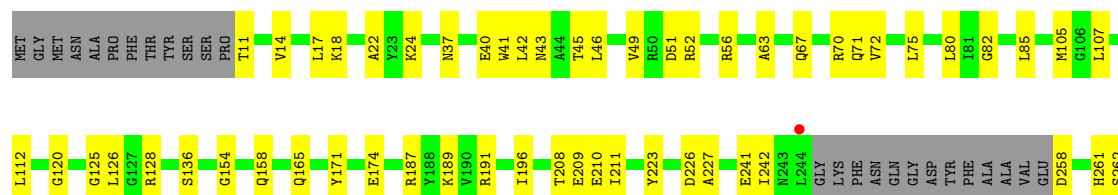
• Molecule 1: Glycogen phosphorylase

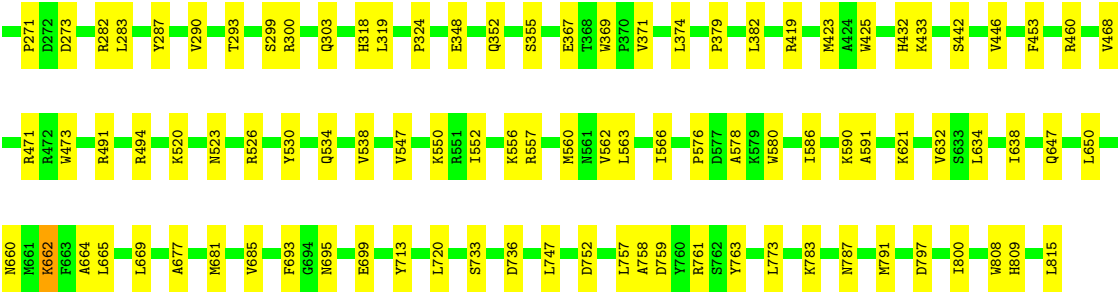
Chain C: 73% 25% .



• Molecule 1: Glycogen phosphorylase

Chain D: 79% 18% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.30Å 187.30Å 449.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.70 49.60 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.60-3.70) 98.3 (49.60-3.70)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.196 , 0.229 0.198 , 0.231	Depositor DCC
$R_{free}$ test set	4291 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.9	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 79.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: LLP

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	0.13	0/6598	0.36	0/8947
1	B	0.15	0/6513	0.36	0/8832
1	C	0.14	0/6598	0.37	0/8947
1	D	0.13	0/6521	0.36	0/8843
All	All	0.14	0/26230	0.36	0/35569

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	491	ARG	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6478	0	6339	104	0
1	B	6397	0	6261	135	0
1	C	6478	0	6339	143	0
1	D	6405	0	6272	98	0
All	All	25758	0	25211	468	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 (468) 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:80:LEU:HD22	1:B:632:VAL:HG23	1.49	0.94
1:C:776:LEU:CD1	1:C:779:GLU:HB3	2.00	0.90
1:A:746:SER:HB3	1:C:741:ARG:HH21	1.48	0.77
1:B:422:ARG:HH21	1:B:425:TRP:CD1	2.02	0.77
1:D:56:ARG:HD3	1:D:226:ASP:HA	1.66	0.77
1:B:80:LEU:HD22	1:B:632:VAL:CG2	2.13	0.76
1:C:688:ASP:O	1:C:783:LYS:NZ	2.18	0.76
1:C:695:ASN:HB3	1:C:699:GLU:HB2	1.69	0.75
1:B:597:MET:HE1	1:B:743:LEU:HA	1.70	0.74
1:D:576:PRO:O	1:D:621:LYS:NZ	2.20	0.74
1:B:223:TYR:HB2	1:B:471:ARG:HD3	1.70	0.73
1:A:56:ARG:HD3	1:A:226:ASP:HA	1.70	0.73
1:D:660:ASN:HD22	1:D:677:ALA:HB3	1.55	0.71
1:A:535:LEU:HD13	1:A:625:VAL:HG13	1.70	0.71
1:C:240:SER:HA	1:D:171:TYR:HE2	1.56	0.71
1:C:371:VAL:HG13	1:C:382:LEU:HD11	1.74	0.69
1:B:657:GLY:H	1:B:677:ALA:HB2	1.55	0.69
1:B:196:ILE:HD11	1:B:379:PRO:HB2	1.73	0.69
1:C:56:ARG:HD3	1:C:226:ASP:HA	1.75	0.69
1:A:374:LEU:HD23	1:A:382:LEU:HD13	1.74	0.69
1:A:43:ASN:HA	1:A:46:LEU:HD12	1.74	0.69
1:B:411:SER:O	1:B:422:ARG:NH2	2.27	0.68
1:C:394:LYS:HA	1:C:397:GLN:HB2	1.76	0.68
1:C:343:TRP:NE1	1:C:387:GLU:OE1	2.25	0.68
1:D:550:LYS:NZ	1:D:662:LLP:OP1	2.26	0.68
1:C:776:LEU:HD12	1:C:779:GLU:HB3	1.77	0.67
1:B:695:ASN:HB3	1:B:699:GLU:HB2	1.77	0.66
1:A:411:SER:O	1:A:422:ARG:NH1	2.28	0.66
1:A:720:LEU:HD21	1:A:757:LEU:HD22	1.79	0.64
1:A:50:ARG:NH1	1:A:178:PRO:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:GLN:HG3	1:D:165:GLN:HG3	1.79	0.63
1:C:550:LYS:HD3	1:C:556:LYS:HD2	1.78	0.63
1:C:411:SER:O	1:C:422:ARG:NH2	2.32	0.62
1:B:386:PHE:HZ	1:B:419:ARG:HH12	1.48	0.62
1:C:211:ILE:HD11	1:C:262:SER:HB3	1.81	0.62
1:A:265:VAL:HG13	1:A:285:GLN:HA	1.81	0.62
1:D:733:SER:OG	1:D:736:ASP:O	2.17	0.62
1:B:80:LEU:CD2	1:B:632:VAL:HG23	2.28	0.61
1:C:465:THR:HB	1:C:798:ARG:HH22	1.64	0.61
1:B:279:ARG:HG2	1:B:369:TRP:HZ3	1.64	0.61
1:A:438:SER:HB3	1:A:656:SER:HB2	1.82	0.61
1:B:377:ILE:HG22	1:B:378:LEU:HG	1.83	0.60
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.66	0.60
1:C:720:LEU:HD21	1:C:757:LEU:HD22	1.83	0.60
1:D:550:LYS:HD3	1:D:556:LYS:HD2	1.83	0.60
1:A:520:LYS:NZ	1:A:666:ASN:O	2.23	0.60
1:C:11:THR:HG22	1:C:13:SER:H	1.67	0.59
1:C:52:ARG:HG3	1:C:52:ARG:HH11	1.67	0.59
1:A:368:THR:HG22	1:A:422:ARG:HA	1.85	0.59
1:C:776:LEU:HD12	1:C:776:LEU:O	2.03	0.59
1:B:726:GLN:HB3	1:B:731:VAL:HG11	1.84	0.59
1:A:488:HIS:CD2	1:A:512:VAL:HG22	2.36	0.59
1:A:776:LEU:HB2	1:A:779:GLU:HB2	1.84	0.59
1:A:749:ASN:ND2	1:C:714:TYR:OH	2.36	0.59
1:D:46:LEU:HD23	1:D:85:LEU:HD13	1.84	0.58
1:B:527:LEU:HD22	1:B:638:ILE:HA	1.84	0.58
1:C:368:THR:HG22	1:C:422:ARG:HA	1.85	0.58
1:B:552:ILE:HG13	1:B:602:ILE:HD11	1.85	0.58
1:D:318:HIS:ND1	1:D:355:SER:OG	2.31	0.58
1:C:383:GLN:O	1:C:387:GLU:HG3	2.04	0.58
1:A:187:ARG:HH22	1:B:174:GLU:HG2	1.69	0.57
1:B:134:LEU:HD11	1:B:231:LEU:HD13	1.86	0.57
1:C:243:ASN:HD21	1:C:246:LYS:HB3	1.69	0.57
1:C:539:VAL:HB	1:C:584:VAL:HG21	1.87	0.57
1:B:329:PRO:HB2	1:B:381:HIS:HD2	1.69	0.57
1:A:509:PHE:HB2	1:A:512:VAL:HG23	1.86	0.57
1:C:552:ILE:HB	1:C:591:ALA:HB2	1.87	0.57
1:C:678:ASN:HA	1:C:681:MET:HB2	1.87	0.57
1:C:273:ASP:HB2	1:C:279:ARG:HG2	1.86	0.56
1:A:440:LEU:HD22	1:A:679:VAL:HG21	1.86	0.56
1:B:726:GLN:HB3	1:B:731:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:MET:HE3	1:C:335:LEU:HD11	1.88	0.56
1:D:747:LEU:HA	1:D:752:ASP:HB2	1.87	0.56
1:A:473:TRP:CD2	1:A:662:LLP:HD2	2.40	0.56
1:C:83:ARG:HD3	1:C:113:ILE:HG22	1.88	0.56
1:D:557:ARG:HH21	1:D:650:LEU:HA	1.70	0.56
1:A:432:HIS:CD2	1:A:433:LYS:HG2	2.42	0.55
1:A:11:THR:HB	1:A:14:VAL:HG23	1.88	0.55
1:B:425:TRP:CD1	1:B:453:PHE:HZ	2.24	0.55
1:D:473:TRP:CE2	1:D:662:LLP:HD2	2.40	0.55
1:B:584:VAL:HG22	1:B:623:LYS:HB2	1.88	0.55
1:A:746:SER:HB3	1:C:741:ARG:NH2	2.19	0.55
1:C:281:LEU:HA	1:C:284:ARG:HD2	1.89	0.55
1:A:329:PRO:HB2	1:A:381:HIS:HD2	1.71	0.55
1:C:547:VAL:HG22	1:C:586:ILE:HB	1.88	0.55
1:D:287:TYR:HA	1:D:290:VAL:HG22	1.87	0.55
1:D:367:GLU:HB3	1:D:423:MET:HB2	1.88	0.55
1:A:56:ARG:HH22	1:A:92:LEU:HA	1.71	0.55
1:B:85:LEU:HG	1:B:89:MET:HE2	1.88	0.55
1:C:383:GLN:NE2	1:C:387:GLU:OE2	2.41	0.54
1:C:409:ARG:O	1:C:422:ARG:NH2	2.40	0.54
1:C:258:ASP:HA	1:C:261:HIS:HB3	1.88	0.54
1:C:603:HIS:CD2	1:C:607:ASP:OD2	2.60	0.54
1:B:568:ARG:NH2	1:B:581:VAL:O	2.40	0.54
1:A:647:GLN:CD	1:A:660:ASN:HB3	2.31	0.54
1:C:57:TRP:HE1	1:C:230:THR:HG22	1.72	0.54
1:C:158:GLN:HG3	1:C:165:GLN:HG3	1.89	0.54
1:C:174:GLU:HG2	1:D:187:ARG:HH22	1.73	0.54
1:D:45:THR:O	1:D:49:VAL:HG23	2.08	0.54
1:B:64:GLN:HG2	1:B:813:VAL:HG21	1.89	0.54
1:A:383:GLN:O	1:A:387:GLU:HG3	2.08	0.54
1:C:422:ARG:HB3	1:C:425:TRP:CE3	2.43	0.54
1:D:211:ILE:CG2	1:D:262:SER:HB3	2.38	0.54
1:A:506:HIS:HB3	1:A:512:VAL:HG21	1.89	0.53
1:B:42:LEU:HD13	1:B:112:LEU:HB3	1.90	0.53
1:C:568:ARG:HH22	1:C:771:ASP:CG	2.16	0.53
1:D:552:ILE:HB	1:D:591:ALA:HB2	1.89	0.53
1:A:56:ARG:NH2	1:A:92:LEU:HA	2.22	0.53
1:D:125:GLY:HA2	1:D:662:LLP:H5'2	1.90	0.53
1:D:550:LYS:HE2	1:D:647:GLN:OE1	2.08	0.53
1:A:363:SER:HB3	1:A:449:LEU:HD13	1.90	0.53
1:B:396:LEU:HD22	1:B:406:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:GLU:O	1:D:352:GLN:HG3	2.09	0.53
1:B:550:LYS:HE3	1:B:556:LYS:HD2	1.91	0.53
1:C:584:VAL:HG22	1:C:623:LYS:HB2	1.90	0.53
1:A:584:VAL:HG22	1:A:623:LYS:HB2	1.90	0.53
1:C:726:GLN:HB3	1:C:731:VAL:HG11	1.90	0.53
1:B:46:LEU:HD23	1:B:85:LEU:HD13	1.89	0.53
1:D:318:HIS:HD1	1:D:355:SER:HG	1.43	0.53
1:D:557:ARG:NH2	1:D:650:LEU:HA	2.24	0.53
1:B:371:VAL:HG23	1:B:419:ARG:O	2.09	0.53
1:D:43:ASN:HA	1:D:46:LEU:HD12	1.91	0.53
1:A:119:PRO:HA	1:A:172:TRP:CE3	2.44	0.52
1:A:281:LEU:HA	1:A:284:ARG:HD2	1.90	0.52
1:D:733:SER:OG	1:D:733:SER:O	2.27	0.52
1:A:771:ASP:O	1:A:775:GLU:HG3	2.09	0.52
1:C:41:TRP:CD2	1:C:107:LEU:HD11	2.44	0.52
1:B:325:VAL:HB	1:B:423:MET:HE3	1.90	0.52
1:D:37:ASN:OD1	1:D:40:GLU:N	2.29	0.52
1:B:11:THR:HG22	1:B:12:LEU:HD12	1.90	0.52
1:B:691:PHE:CE2	1:B:770:VAL:HG22	2.44	0.52
1:D:374:LEU:HD23	1:D:382:LEU:HD13	1.92	0.52
1:A:132:CYS:SG	1:A:469:THR:HG22	2.50	0.52
1:A:413:ILE:HG21	1:A:419:ARG:HH21	1.75	0.52
1:B:128:ARG:NH2	1:B:132:CYS:SG	2.76	0.52
1:C:647:GLN:CD	1:C:660:ASN:HB3	2.35	0.51
1:A:211:ILE:HD11	1:A:262:SER:HB3	1.92	0.51
1:C:535:LEU:HD12	1:C:625:VAL:HG13	1.90	0.51
1:D:547:VAL:HG22	1:D:586:ILE:HB	1.93	0.51
1:C:42:LEU:HB2	1:C:112:LEU:HD22	1.92	0.51
1:C:45:THR:O	1:C:49:VAL:HG23	2.10	0.51
1:C:80:LEU:CD2	1:C:632:VAL:HG22	2.40	0.51
1:C:163:GLY:O	1:C:603:HIS:HA	2.11	0.51
1:C:275:THR:OG1	1:C:278:GLY:N	2.44	0.51
1:D:319:LEU:HB3	1:D:324:PRO:HG2	1.92	0.51
1:D:720:LEU:HD21	1:D:757:LEU:HD22	1.91	0.51
1:C:747:LEU:HA	1:C:752:ASP:HB2	1.92	0.51
1:D:223:TYR:HB2	1:D:471:ARG:HD3	1.91	0.51
1:D:557:ARG:HH12	1:D:759:ASP:HB2	1.76	0.51
1:C:442:SER:O	1:C:446:VAL:HG23	2.10	0.51
1:A:336:ILE:HD11	1:A:343:TRP:HA	1.93	0.51
1:B:473:TRP:CE2	1:B:662:LLP:HD2	2.45	0.51
1:B:559:LEU:HD21	1:B:747:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ILE:HG13	1:D:379:PRO:HB2	1.91	0.51
1:A:329:PRO:HB2	1:A:381:HIS:CD2	2.46	0.51
1:C:720:LEU:HB2	1:C:760:TYR:CE2	2.45	0.51
1:A:60:SER:OG	1:A:226:ASP:O	2.28	0.50
1:B:43:ASN:HA	1:B:46:LEU:HD12	1.93	0.50
1:B:59:ARG:HH21	1:B:226:ASP:CG	2.19	0.50
1:B:374:LEU:HD23	1:B:382:LEU:HD13	1.93	0.50
1:B:778:GLU:O	1:B:782:ALA:N	2.41	0.50
1:A:334:LEU:HD23	1:A:338:GLU:HG3	1.93	0.50
1:B:714:TYR:O	1:B:721:HIS:HB2	2.11	0.50
1:C:544:LEU:HB3	1:C:583:ARG:HG2	1.93	0.50
1:B:50:ARG:O	1:B:54:VAL:HG23	2.10	0.50
1:D:211:ILE:HG23	1:D:262:SER:HB3	1.92	0.50
1:B:196:ILE:CD1	1:B:379:PRO:HB2	2.42	0.50
1:D:664:ALA:HB3	1:D:791:MET:HE2	1.94	0.50
1:B:60:SER:OG	1:B:226:ASP:O	2.29	0.50
1:A:535:LEU:O	1:A:535:LEU:HD23	2.11	0.50
1:B:321:ASP:O	1:B:324:PRO:HD2	2.11	0.50
1:B:329:PRO:HB2	1:B:381:HIS:CD2	2.46	0.50
1:C:787:ASN:O	1:C:791:MET:HG2	2.11	0.50
1:D:530:TYR:CE1	1:D:534:GLN:HG3	2.46	0.50
1:A:681:MET:O	1:A:685:VAL:HG22	2.12	0.50
1:C:57:TRP:O	1:C:61:ASN:HB2	2.12	0.50
1:D:425:TRP:CD1	1:D:453:PHE:HZ	2.30	0.50
1:A:452:ASP:O	1:A:456:ILE:HG13	2.12	0.49
1:B:334:LEU:HD23	1:B:338:GLU:HG3	1.93	0.49
1:C:442:SER:HA	1:C:445:MET:HE2	1.94	0.49
1:D:258:ASP:OD1	1:D:258:ASP:N	2.43	0.49
1:D:634:LEU:O	1:D:638:ILE:HG13	2.12	0.49
1:A:568:ARG:NH2	1:A:581:VAL:O	2.44	0.49
1:B:331:MET:HE3	1:B:335:LEU:HD11	1.94	0.49
1:C:287:TYR:HA	1:C:290:VAL:HG22	1.95	0.49
1:C:509:PHE:HB2	1:C:512:VAL:HG23	1.94	0.49
1:B:63:ALA:HB1	1:B:813:VAL:HG11	1.95	0.49
1:B:681:MET:O	1:B:685:VAL:HG22	2.13	0.49
1:C:46:LEU:HD22	1:C:179:TRP:NE1	2.27	0.49
1:D:80:LEU:HD22	1:D:632:VAL:HG23	1.93	0.49
1:B:120:GLY:O	1:B:154:GLY:HA2	2.13	0.49
1:B:279:ARG:HG2	1:B:369:TRP:CZ3	2.46	0.49
1:A:720:LEU:HB2	1:A:760:TYR:CE2	2.47	0.49
1:B:478:ASN:OD1	1:B:523:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD11	1:D:293:THR:HG21	1.95	0.49
1:B:417:ASN:HD22	1:B:420:ARG:HD2	1.77	0.49
1:B:601:ILE:O	1:B:605:ILE:HG13	2.12	0.49
1:A:196:ILE:HD11	1:A:379:PRO:C	2.37	0.49
1:D:681:MET:O	1:D:685:VAL:HG22	2.13	0.49
1:A:345:ASP:O	1:A:348:GLU:HB3	2.13	0.48
1:C:471:ARG:O	1:C:476:VAL:HG23	2.13	0.48
1:B:281:LEU:HA	1:B:284:ARG:HD2	1.95	0.48
1:C:342:SER:OG	1:C:345:ASP:OD2	2.31	0.48
1:C:57:TRP:HE1	1:C:230:THR:CG2	2.26	0.48
1:B:323:HIS:HB2	1:B:324:PRO:HD3	1.94	0.48
1:B:524:LYS:HE2	1:B:541:PRO:O	2.13	0.48
1:B:773:LEU:HG	1:B:780:TRP:HE3	1.78	0.48
1:B:787:ASN:O	1:B:791:MET:HG2	2.13	0.48
1:D:562:VAL:O	1:D:566:ILE:HG13	2.14	0.48
1:D:665:LEU:HD13	1:D:791:MET:HB2	1.95	0.48
1:B:137:LEU:HB3	1:B:229:ASN:HD21	1.77	0.48
1:B:191:ARG:HD3	1:B:208:THR:OG1	2.13	0.48
1:B:328:ILE:HD13	1:B:430:VAL:HB	1.94	0.48
1:C:559:LEU:HD21	1:C:747:LEU:HD11	1.96	0.48
1:B:368:THR:HG22	1:B:422:ARG:HA	1.96	0.48
1:A:326:LEU:HG	1:A:423:MET:HE1	1.96	0.48
1:D:52:ARG:HG3	1:D:52:ARG:NH1	2.25	0.48
1:C:776:LEU:HD13	1:C:779:GLU:HB3	1.91	0.48
1:A:695:ASN:HB3	1:A:699:GLU:HB2	1.95	0.48
1:B:557:ARG:HH12	1:B:759:ASP:HB2	1.77	0.48
1:C:80:LEU:HD23	1:C:632:VAL:HG22	1.96	0.48
1:B:25:LEU:HD23	1:B:33:PRO:HG3	1.95	0.47
1:B:713:TYR:CE2	1:B:758:ALA:HA	2.49	0.47
1:B:664:ALA:HB3	1:B:791:MET:HE2	1.95	0.47
1:C:50:ARG:O	1:C:54:VAL:HG23	2.15	0.47
1:C:46:LEU:HD22	1:C:179:TRP:HE1	1.79	0.47
1:A:46:LEU:HD23	1:A:85:LEU:HD13	1.96	0.47
1:D:787:ASN:O	1:D:791:MET:HG2	2.14	0.47
1:A:60:SER:HA	1:A:815:LEU:HD11	1.96	0.47
1:B:569:TYR:CD2	1:B:612:ILE:HG12	2.50	0.47
1:C:191:ARG:HH11	1:C:208:THR:HG21	1.78	0.47
1:C:730:GLY:HA3	1:C:737:PRO:HA	1.97	0.47
1:A:552:ILE:HG13	1:A:602:ILE:HD11	1.97	0.47
1:C:557:ARG:NH2	1:C:650:LEU:HA	2.30	0.47
1:D:41:TRP:CD2	1:D:107:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:ASN:HB3	1:D:699:GLU:HB2	1.96	0.47
1:C:280:GLU:HG3	1:C:377:ILE:HD11	1.95	0.47
1:D:71:GLN:HE22	1:D:300:ARG:HH21	1.61	0.47
1:A:334:LEU:O	1:A:338:GLU:HB2	2.15	0.47
1:D:271:PRO:HG2	1:D:282:ARG:HG2	1.96	0.47
1:D:191:ARG:HD3	1:D:208:THR:HG21	1.96	0.46
1:D:538:VAL:HG23	1:D:538:VAL:O	2.14	0.46
1:A:42:LEU:HB2	1:A:112:LEU:HD22	1.98	0.46
1:C:438:SER:HB3	1:C:656:SER:HB2	1.97	0.46
1:D:713:TYR:CD2	1:D:758:ALA:HA	2.50	0.46
1:B:657:GLY:HA3	1:B:660:ASN:OD1	2.14	0.46
1:A:787:ASN:O	1:A:791:MET:HG2	2.15	0.46
1:B:94:ILE:O	1:B:98:VAL:HG23	2.15	0.46
1:B:441:HIS:C	1:B:441:HIS:CD2	2.93	0.46
1:B:558:GLN:O	1:B:562:VAL:HG23	2.15	0.46
1:B:659:SER:O	1:B:663:PHE:HD2	1.99	0.46
1:C:265:VAL:HG13	1:C:285:GLN:HA	1.96	0.46
1:B:425:TRP:CD1	1:B:453:PHE:CZ	3.03	0.46
1:C:489:LEU:HD11	1:C:503:LEU:HB2	1.97	0.46
1:B:662:LLP:NZ	1:B:662:LLP:O3	2.37	0.46
1:C:94:ILE:O	1:C:98:VAL:HG23	2.16	0.46
1:C:53:LEU:HD12	1:C:179:TRP:HZ3	1.80	0.46
1:C:240:SER:HA	1:D:171:TYR:CE2	2.43	0.46
1:B:447:GLN:OE1	1:B:447:GLN:HA	2.15	0.46
1:C:377:ILE:C	1:C:379:PRO:HD3	2.41	0.46
1:C:158:GLN:HB3	1:C:629:ASN:HA	1.96	0.46
1:A:102:LEU:HD12	1:A:109:LEU:HB2	1.97	0.45
1:A:504:GLN:HA	1:A:507:CYS:SG	2.56	0.45
1:B:557:ARG:NH2	1:B:650:LEU:HA	2.31	0.45
1:C:726:GLN:HB3	1:C:731:VAL:CG1	2.45	0.45
1:D:273:ASP:HB3	1:D:282:ARG:HG3	1.98	0.45
1:A:81:ILE:HD11	1:A:119:PRO:HG2	1.98	0.45
1:A:647:GLN:HG3	1:A:660:ASN:HB3	1.98	0.45
1:C:151:TYR:CE1	1:C:269:LEU:HD12	2.51	0.45
1:C:323:HIS:HB2	1:C:324:PRO:HD3	1.98	0.45
1:C:169:PRO:HG2	1:C:171:TYR:CZ	2.50	0.45
1:C:497:LEU:HD23	1:C:792:GLY:HA2	1.98	0.45
1:B:506:HIS:HB3	1:B:512:VAL:HG21	1.98	0.45
1:A:128:ARG:HA	1:A:128:ARG:HD2	1.64	0.45
1:A:41:TRP:CD2	1:A:107:LEU:HD11	2.52	0.45
1:B:399:GLN:O	1:B:401:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:VAL:O	1:B:727:ILE:HG13	2.16	0.45
1:C:556:LYS:NZ	1:C:654:GLU:OE1	2.47	0.45
1:D:560:MET:HA	1:D:563:LEU:HD12	1.98	0.45
1:B:735:GLU:OE1	1:B:735:GLU:N	2.42	0.45
1:C:187:ARG:HH22	1:D:174:GLU:HG3	1.82	0.45
1:D:227:ALA:HB2	1:D:815:LEU:HD21	1.99	0.45
1:D:442:SER:O	1:D:446:VAL:HG23	2.16	0.45
1:B:70:ARG:NH1	1:B:313:ASP:O	2.40	0.45
1:B:462:THR:OG1	1:B:463:ASN:N	2.50	0.45
1:B:705:ARG:HE	1:B:705:ARG:HB2	1.59	0.45
1:C:380:ARG:O	1:C:384:ILE:HG13	2.17	0.45
1:D:189:LYS:HD2	1:D:210:GLU:OE1	2.17	0.45
1:A:786:LEU:O	1:A:790:ASN:ND2	2.50	0.45
1:D:773:LEU:HD21	1:D:783:LYS:HD2	1.99	0.45
1:A:652:GLY:H	1:A:675:ASP:CG	2.25	0.45
1:A:690:ILE:HG23	1:A:692:ILE:HG12	1.98	0.45
1:B:90:LEU:O	1:B:90:LEU:HD23	2.17	0.45
1:C:573:LYS:HD2	1:C:617:GLN:OE1	2.17	0.45
1:D:22:ALA:HB2	1:D:105:MET:HE1	1.98	0.45
1:A:50:ARG:O	1:A:54:VAL:HG23	2.17	0.44
1:B:328:ILE:HG21	1:B:430:VAL:HG21	1.99	0.44
1:B:645:SER:HB3	1:B:670:THR:HA	1.98	0.44
1:C:647:GLN:HG3	1:C:660:ASN:HB3	1.98	0.44
1:D:209:GLU:OE1	1:D:261:HIS:NE2	2.47	0.44
1:B:485:LEU:O	1:B:489:LEU:HB2	2.18	0.44
1:A:169:PRO:HG2	1:A:171:TYR:CZ	2.52	0.44
1:B:595:TYR:HE1	1:B:597:MET:HB2	1.82	0.44
1:C:414:ASP:HB2	1:C:422:ARG:HH11	1.82	0.44
1:C:422:ARG:HH21	1:C:425:TRP:CD1	2.34	0.44
1:B:568:ARG:HH22	1:B:581:VAL:HB	1.83	0.44
1:D:37:ASN:OD1	1:D:37:ASN:C	2.61	0.44
1:A:80:LEU:HD22	1:A:632:VAL:HG23	2.00	0.44
1:C:120:GLY:O	1:C:154:GLY:HA2	2.17	0.44
1:A:335:LEU:HB3	1:A:341:PHE:CD2	2.53	0.44
1:C:81:ILE:HG13	1:C:82:GLY:N	2.33	0.44
1:C:381:HIS:O	1:C:385:ILE:HG13	2.17	0.44
1:D:299:SER:O	1:D:303:GLN:HG2	2.18	0.44
1:A:137:LEU:HB3	1:A:229:ASN:ND2	2.33	0.44
1:C:128:ARG:NH1	1:C:132:CYS:SG	2.86	0.44
1:C:328:ILE:HD13	1:C:430:VAL:HB	1.99	0.44
1:D:520:LYS:HB2	1:D:520:LYS:HE2	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HD12	1:A:774:TYR:CG	2.52	0.44
1:A:559:LEU:HD11	1:A:743:LEU:HD21	1.98	0.44
1:B:432:HIS:CD2	1:B:433:LYS:HG2	2.52	0.44
1:B:503:LEU:HD21	1:B:785:MET:HG2	1.98	0.44
1:C:126:LEU:HD22	1:C:320:ASN:ND2	2.32	0.44
1:A:323:HIS:HB2	1:A:324:PRO:HD3	2.00	0.44
1:C:191:ARG:HD2	1:C:208:THR:HG21	2.00	0.44
1:C:319:LEU:HD22	1:C:324:PRO:HB2	1.99	0.44
1:D:241:GLU:H	1:D:241:GLU:CD	2.25	0.44
1:B:330:GLU:OE1	1:B:381:HIS:NE2	2.38	0.43
1:C:520:LYS:NZ	1:C:666:ASN:O	2.28	0.43
1:D:63:ALA:O	1:D:67:GLN:HG3	2.18	0.43
1:B:375:GLY:O	1:B:379:PRO:HB3	2.18	0.43
1:C:187:ARG:HH22	1:D:174:GLU:CG	2.31	0.43
1:D:523:ASN:O	1:D:526:ARG:HB3	2.18	0.43
1:B:276:TYR:CE2	1:B:373:MET:HE2	2.54	0.43
1:C:432:HIS:O	1:C:433:LYS:HD3	2.18	0.43
1:B:80:LEU:HB2	1:B:127:GLY:HA3	2.00	0.43
1:B:473:TRP:CD2	1:B:662:LLP:HD2	2.53	0.43
1:C:52:ARG:HG3	1:C:52:ARG:NH1	2.32	0.43
1:D:11:THR:HA	1:D:14:VAL:HB	1.99	0.43
1:A:45:THR:O	1:A:49:VAL:HG23	2.17	0.43
1:A:52:ARG:HA	1:A:55:GLU:HG3	1.99	0.43
1:D:468:VAL:HG11	1:D:662:LLP:HG2	2.00	0.43
1:A:634:LEU:HD23	1:A:634:LEU:HA	1.77	0.43
1:B:265:VAL:HG13	1:B:285:GLN:HA	2.00	0.43
1:C:269:LEU:HD23	1:C:270:TYR:HB2	2.00	0.43
1:C:271:PRO:HD2	1:C:282:ARG:HG2	2.00	0.43
1:D:283:LEU:HD12	1:D:369:TRP:CE2	2.53	0.43
1:A:664:ALA:HB3	1:A:791:MET:HE2	2.00	0.43
1:C:42:LEU:HD21	1:C:116:GLU:HB2	1.99	0.43
1:C:610:LYS:O	1:C:614:ASN:ND2	2.41	0.43
1:D:371:VAL:HG23	1:D:419:ARG:O	2.18	0.43
1:B:196:ILE:CG2	1:B:203:THR:HG22	2.48	0.43
1:C:108:ASN:HD21	1:C:110:GLU:HG2	1.83	0.43
1:A:749:ASN:O	1:C:725:THR:HG23	2.19	0.43
1:B:471:ARG:HG3	1:B:471:ARG:HH11	1.84	0.43
1:C:171:TYR:O	1:C:174:GLU:HB2	2.19	0.43
1:A:310:ASN:OD1	1:A:310:ASN:N	2.49	0.42
1:B:471:ARG:O	1:B:476:VAL:HG23	2.19	0.42
1:B:720:LEU:HD21	1:B:757:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:HD22	1:C:128:ARG:HG2	2.01	0.42
1:A:160:ILE:HG12	1:A:628:PRO:HB3	2.01	0.42
1:A:258:ASP:HA	1:A:261:HIS:HB3	2.01	0.42
1:A:527:LEU:HD22	1:A:638:ILE:HA	2.01	0.42
1:B:57:TRP:NE1	1:B:61:ASN:HD21	2.16	0.42
1:B:644:LEU:HD12	1:B:644:LEU:HA	1.90	0.42
1:B:721:HIS:O	1:B:725:THR:OG1	2.25	0.42
1:C:773:LEU:HD21	1:C:783:LYS:HD2	2.00	0.42
1:B:125:GLY:HA2	1:B:662:LLP:H5'2	2.01	0.42
1:B:171:TYR:O	1:B:174:GLU:HB2	2.19	0.42
1:A:402:ASN:OD1	1:A:402:ASN:N	2.52	0.42
1:A:569:TYR:OH	1:A:615:ASP:OD2	2.29	0.42
1:B:132:CYS:SG	1:B:469:THR:HG22	2.59	0.42
1:B:489:LEU:HD11	1:B:503:LEU:HB2	2.01	0.42
1:D:42:LEU:HD22	1:D:112:LEU:O	2.19	0.42
1:D:223:TYR:CZ	1:D:494:ARG:HD3	2.55	0.42
1:D:432:HIS:O	1:D:460:ARG:HG2	2.19	0.42
1:C:25:LEU:HD23	1:C:33:PRO:HG3	2.01	0.42
1:C:464:VAL:HG12	1:C:799:THR:HG23	2.01	0.42
1:C:580:TRP:HA	1:C:580:TRP:CE3	2.55	0.42
1:D:432:HIS:ND1	1:D:433:LYS:HG2	2.35	0.42
1:A:108:ASN:HD21	1:A:110:GLU:HG2	1.84	0.42
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.77	0.42
1:A:442:SER:O	1:A:446:VAL:HG23	2.20	0.42
1:C:101:ALA:O	1:C:105:MET:HG3	2.19	0.42
1:D:17:LEU:HD23	1:D:17:LEU:HA	1.88	0.42
1:D:695:ASN:HB3	1:D:699:GLU:CB	2.50	0.42
1:B:287:TYR:HA	1:B:290:VAL:HG22	2.02	0.42
1:B:784:ALA:O	1:B:788:ILE:HG13	2.20	0.42
1:C:241:GLU:HG2	1:C:242:ILE:O	2.19	0.42
1:C:681:MET:O	1:C:685:VAL:HG22	2.18	0.42
1:C:773:LEU:HD23	1:C:773:LEU:O	2.19	0.42
1:D:18:LYS:HG3	1:D:105:MET:SD	2.60	0.42
1:A:223:TYR:HB2	1:A:471:ARG:HD2	2.02	0.42
1:A:304:LEU:HB3	1:A:305:HIS:ND1	2.34	0.42
1:B:275:THR:OG1	1:B:278:GLY:N	2.47	0.42
1:B:557:ARG:HB2	1:B:648:ILE:O	2.19	0.42
1:B:689:ASN:ND2	1:B:786:LEU:HD13	2.35	0.42
1:C:26:MET:HE2	1:C:26:MET:HB3	1.86	0.42
1:C:46:LEU:HD23	1:C:85:LEU:HD13	2.00	0.42
1:A:174:GLU:CG	1:B:187:ARG:HH22	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HG3	1:B:471:ARG:NH1	2.34	0.42
1:B:555:TYR:HB3	1:B:754:TYR:CZ	2.54	0.42
1:D:120:GLY:O	1:D:154:GLY:HA2	2.20	0.42
1:D:578:ALA:HB3	1:D:580:TRP:NE1	2.35	0.42
1:B:21:ILE:HD11	1:B:45:THR:HG23	2.01	0.41
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.90	0.41
1:B:405:ASP:HB3	1:B:409:ARG:HH12	1.85	0.41
1:C:160:ILE:HD13	1:C:160:ILE:HA	1.92	0.41
1:D:82:GLY:HA3	1:D:632:VAL:HG11	2.02	0.41
1:D:158:GLN:NE2	1:D:590:LYS:HA	2.35	0.41
1:A:513:ASN:ND2	1:A:778:GLU:HG2	2.35	0.41
1:B:32:ASP:OD1	1:B:34:VAL:HG23	2.21	0.41
1:B:755:GLN:HB3	1:B:758:ALA:HB3	2.03	0.41
1:C:396:LEU:HD21	1:C:456:ILE:HD13	2.02	0.41
1:B:396:LEU:HD21	1:B:456:ILE:HD13	2.02	0.41
1:C:31:LYS:HG2	1:C:40:GLU:OE1	2.21	0.41
1:C:644:LEU:HD22	1:C:770:VAL:HG11	2.01	0.41
1:C:652:GLY:H	1:C:675:ASP:CG	2.28	0.41
1:D:471:ARG:HH22	1:D:797:ASP:CG	2.29	0.41
1:D:693:PHE:CZ	1:D:763:TYR:HD1	2.38	0.41
1:B:273:ASP:HB3	1:B:282:ARG:HG3	2.02	0.41
1:C:425:TRP:HD1	1:C:453:PHE:HZ	1.67	0.41
1:C:684:HIS:O	1:C:790:ASN:HB2	2.21	0.41
1:D:24:LYS:HE3	1:D:51:ASP:OD2	2.20	0.41
1:D:669:LEU:HD23	1:D:669:LEU:HA	1.89	0.41
1:A:700:VAL:HG13	1:A:755:GLN:NE2	2.36	0.41
1:B:298:LEU:HD21	1:B:331:MET:HE1	2.02	0.41
1:C:579:LYS:HE2	1:C:579:LYS:HB3	1.91	0.41
1:C:740:TYR:O	1:C:744:VAL:HG23	2.21	0.41
1:C:798:ARG:NH1	1:C:802:GLU:OE2	2.46	0.41
1:A:394:LYS:O	1:A:398:GLU:HG3	2.21	0.41
1:C:57:TRP:HE3	1:C:58:LEU:HD23	1.86	0.41
1:D:761:ARG:HA	1:D:761:ARG:HD3	1.65	0.41
1:A:578:ALA:HB3	1:A:580:TRP:NE1	2.36	0.41
1:A:705:ARG:HE	1:A:705:ARG:HB2	1.51	0.41
1:A:745:ASP:CG	1:C:711:ARG:HH22	2.29	0.41
1:B:72:VAL:HG21	1:B:808:TRP:CD2	2.56	0.41
1:B:437:VAL:HG22	1:B:441:HIS:ND1	2.35	0.41
1:C:187:ARG:HA	1:C:213:GLY:O	2.20	0.41
1:C:514:HIS:O	1:C:514:HIS:ND1	2.54	0.41
1:D:72:VAL:HG21	1:D:808:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:SER:HB2	1:D:800:ILE:HG13	2.03	0.41
1:A:38:LYS:HD3	1:A:115:GLU:OE1	2.21	0.41
1:A:72:VAL:O	1:A:144:GLY:HA2	2.20	0.41
1:A:530:TYR:CE1	1:A:534:GLN:HG3	2.56	0.41
1:B:211:ILE:HG21	1:B:262:SER:HB2	2.03	0.41
1:C:11:THR:HG22	1:C:13:SER:N	2.34	0.41
1:C:70:ARG:NH2	1:C:316:ALA:HB2	2.36	0.41
1:C:72:VAL:HG21	1:C:808:TRP:CD2	2.56	0.41
1:D:128:ARG:HD3	1:D:473:TRP:HZ2	1.85	0.41
1:B:158:GLN:NE2	1:B:590:LYS:HA	2.35	0.40
1:C:211:ILE:CD1	1:C:262:SER:HB3	2.50	0.40
1:C:788:ILE:H	1:C:788:ILE:HG13	1.61	0.40
1:D:242:ILE:O	1:D:242:ILE:HG13	2.20	0.40
1:A:425:TRP:CD1	1:A:453:PHE:HZ	2.40	0.40
1:B:433:LYS:HD3	1:B:433:LYS:HA	1.84	0.40
1:A:211:ILE:CD1	1:A:262:SER:HB3	2.50	0.40
1:B:742:ASP:OD1	1:B:742:ASP:N	2.54	0.40
1:A:356:TYR:CD1	1:A:357:THR:N	2.90	0.40
1:B:527:LEU:HD13	1:B:637:LEU:HG	2.04	0.40
1:B:695:ASN:HB3	1:B:699:GLU:CB	2.48	0.40
1:C:151:TYR:CZ	1:C:269:LEU:HD12	2.57	0.40
1:D:70:ARG:HD3	1:D:809:HIS:O	2.22	0.40
1:A:464:VAL:HG12	1:A:799:THR:HG23	2.03	0.40
1:A:549:ILE:HD12	1:A:630:TYR:HE1	1.86	0.40
1:A:555:TYR:HB3	1:A:754:TYR:CZ	2.57	0.40
1:B:119:PRO:HA	1:B:172:TRP:CE3	2.57	0.40
1:B:587:PHE:O	1:B:626:PHE:HA	2.22	0.40
1:C:396:LEU:HD13	1:C:406:LEU:HD23	2.03	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	796/817 (97%)	766 (96%)	30 (4%)	0	100	100
1	B	786/817 (96%)	746 (95%)	40 (5%)	0	100	100
1	C	796/817 (97%)	763 (96%)	33 (4%)	0	100	100
1	D	787/817 (96%)	759 (96%)	28 (4%)	0	100	100
All	All	3165/3268 (97%)	3034 (96%)	131 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	697/708 (98%)	697 (100%)	0	100	100
1	B	688/708 (97%)	688 (100%)	0	100	100
1	C	697/708 (98%)	697 (100%)	0	100	100
1	D	689/708 (97%)	689 (100%)	0	100	100
All	All	2771/2832 (98%)	2771 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	61	ASN
1	A	198	GLN
1	A	229	ASN
1	A	260	ASN
1	A	261	HIS
1	A	339	HIS
1	A	514	HIS
1	A	523	ASN
1	A	585	ASN

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Mol	Chain	Res	Type
1	A	600	HIS
1	A	749	ASN
1	B	61	ASN
1	B	159	ASN
1	B	198	GLN
1	B	305	HIS
1	B	358	ASN
1	B	417	ASN
1	B	585	ASN
1	B	603	HIS
1	B	629	ASN
1	B	689	ASN
1	C	39	HIS
1	C	64	GLN
1	C	184	HIS
1	C	285	GLN
1	C	777	GLN
1	C	809	HIS
1	D	198	GLN
1	D	264	ASN
1	D	488	HIS
1	D	501	ASN
1	D	504	GLN
1	D	636	GLN
1	D	753	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	D	662	1	23,24,25	2.53	6 (26%)	25,32,34	1.26	3 (12%)
1	LLP	B	662	1	23,24,25	2.54	6 (26%)	25,32,34	1.34	4 (16%)
1	LLP	C	662	1	23,24,25	2.51	6 (26%)	25,32,34	1.35	3 (12%)
1	LLP	A	662	1	23,24,25	2.50	6 (26%)	25,32,34	1.31	4 (16%)

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
1	LLP	D	662	1	-	2/16/17/19	0/1/1/1
1	LLP	B	662	1	-	4/16/17/19	0/1/1/1
1	LLP	C	662	1	-	8/16/17/19	0/1/1/1
1	LLP	A	662	1	-	4/16/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	662	LLP	C4-C4'	7.42	1.62	1.46
1	B	662	LLP	C4-C4'	7.24	1.62	1.46
1	C	662	LLP	C4-C4'	7.18	1.61	1.46
1	A	662	LLP	C4-C4'	7.14	1.61	1.46
1	D	662	LLP	C4'-NZ	5.01	1.44	1.27
1	B	662	LLP	C4'-NZ	4.97	1.43	1.27
1	C	662	LLP	C4'-NZ	4.94	1.43	1.27
1	A	662	LLP	C4'-NZ	4.88	1.43	1.27
1	B	662	LLP	C4-C5	-4.04	1.36	1.42
1	C	662	LLP	C4-C5	-4.01	1.36	1.42
1	A	662	LLP	C4-C5	-3.90	1.36	1.42
1	B	662	LLP	C2'-C2	3.82	1.56	1.50
1	C	662	LLP	C2'-C2	3.78	1.56	1.50
1	D	662	LLP	C4-C5	-3.77	1.36	1.42
1	D	662	LLP	C2'-C2	3.68	1.56	1.50
1	A	662	LLP	C2'-C2	3.65	1.56	1.50
1	B	662	LLP	C6-N1	3.30	1.41	1.34
1	C	662	LLP	C6-N1	3.19	1.40	1.34
1	A	662	LLP	C6-N1	3.17	1.40	1.34
1	D	662	LLP	C6-N1	3.11	1.40	1.34
1	B	662	LLP	C5'-C5	2.24	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	LLP	C5'-C5	2.18	1.56	1.50
1	C	662	LLP	C5'-C5	2.15	1.56	1.50
1	D	662	LLP	C5'-C5	2.12	1.56	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	662	LLP	C4-C4'-NZ	-3.26	108.98	124.04
1	A	662	LLP	CE-NZ-C4'	-3.15	108.63	118.72
1	B	662	LLP	C4-C4'-NZ	-3.10	109.73	124.04
1	A	662	LLP	C4-C4'-NZ	-3.07	109.89	124.04
1	D	662	LLP	CE-NZ-C4'	-3.02	109.04	118.72
1	C	662	LLP	CE-NZ-C4'	-2.80	109.75	118.72
1	B	662	LLP	CE-NZ-C4'	-2.77	109.84	118.72
1	D	662	LLP	C4-C4'-NZ	-2.66	111.76	124.04
1	C	662	LLP	C5-C6-N1	-2.36	120.00	123.83
1	A	662	LLP	C5-C6-N1	-2.32	120.06	123.83
1	D	662	LLP	C5-C6-N1	-2.29	120.11	123.83
1	B	662	LLP	C5-C6-N1	-2.11	120.41	123.83
1	A	662	LLP	C3-C4-C5	2.08	119.95	118.28
1	B	662	LLP	C3-C4-C5	2.06	119.93	118.28

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	662	LLP	C5'-OP4-P-OP2
1	C	662	LLP	C5'-OP4-P-OP3
1	B	662	LLP	C4-C4'-NZ-CE
1	C	662	LLP	C4-C4'-NZ-CE
1	D	662	LLP	CE-CD-CG-CB
1	C	662	LLP	CE-CD-CG-CB
1	A	662	LLP	CE-CD-CG-CB
1	B	662	LLP	CD-CE-NZ-C4'
1	C	662	LLP	CD-CE-NZ-C4'
1	D	662	LLP	CD-CE-NZ-C4'
1	A	662	LLP	CG-CD-CE-NZ
1	B	662	LLP	CE-CD-CG-CB
1	A	662	LLP	CD-CE-NZ-C4'
1	C	662	LLP	C5'-OP4-P-OP1
1	A	662	LLP	C3-C4-C4'-NZ
1	C	662	LLP	C4-C5-C5'-OP4

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Mol	Chain	Res	Type	Atoms
1	B	662	LLP	C-CA-CB-CG
1	C	662	LLP	C3-C4-C4'-NZ

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	662	LLP	4	0
1	B	662	LLP	4	0
1	A	662	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	800/817 (97%)	-0.38	3 (0%) 88 72	106, 139, 177, 242	0
1	B	790/817 (96%)	-0.45	0 100 100	100, 132, 170, 247	0
1	C	800/817 (97%)	-0.38	2 (0%) 90 76	101, 138, 178, 264	0
1	D	791/817 (96%)	-0.43	1 (0%) 92 86	97, 130, 166, 255	0
All	All	3181/3268 (97%)	-0.41	6 (0%) 91 80	97, 135, 175, 264	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	LEU	3.3
1	A	259	LYS	2.8
1	A	86	SER	2.8
1	D	244	LEU	2.5
1	C	86	SER	2.5
1	A	242	ILE	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	A	662	24/25	0.96	0.11	121,131,140,143	0
1	LLP	B	662	24/25	0.96	0.10	106,116,128,142	0
1	LLP	D	662	24/25	0.96	0.10	105,118,132,153	0
1	LLP	C	662	24/25	0.97	0.09	112,128,137,149	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.