



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:22 AM GMT

PDB ID : 2GUM  
Title : Crystal structure of the extracellular domain of glycoprotein B from Herpes Simplex Virus type I  
Authors : Heldwein, E.E.  
Deposited on : 2006-05-01  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

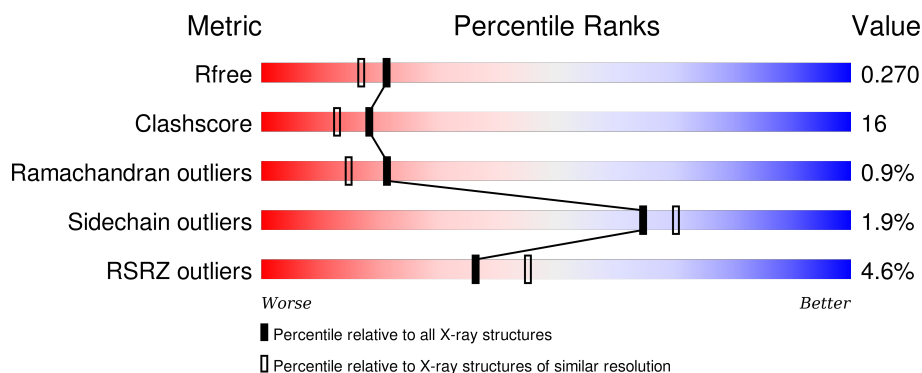
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	628	
1	B	628	
1	C	628	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	B	732	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14223 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 Glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4658	2941	819	876	22			
1	B	581	Total	C	N	O	S	0	0	0
			4694	2962	824	886	22			
1	C	575	Total	C	N	O	S	0	0	0
			4644	2931	813	878	22			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Na	0	0
			2	2		
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	82	Total	O	0	0
			82	82		
3	C	79	Total	O	0	0
			79	79		

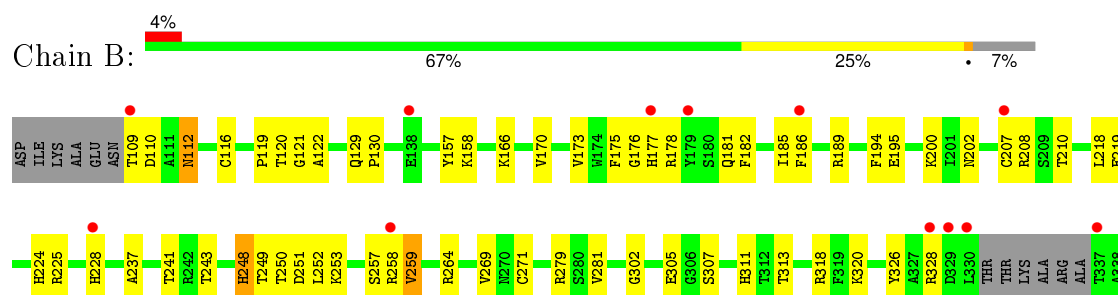
### 3 Residue-property plots

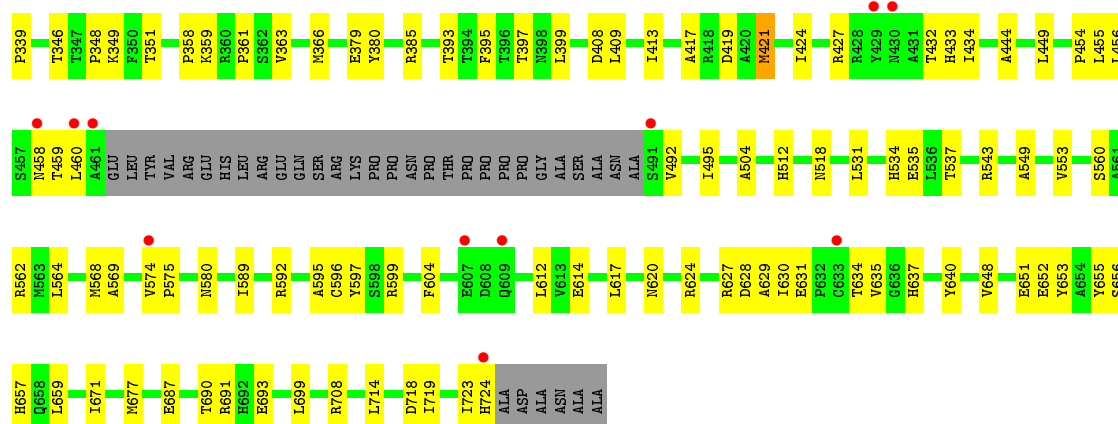
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Glycoprotein B

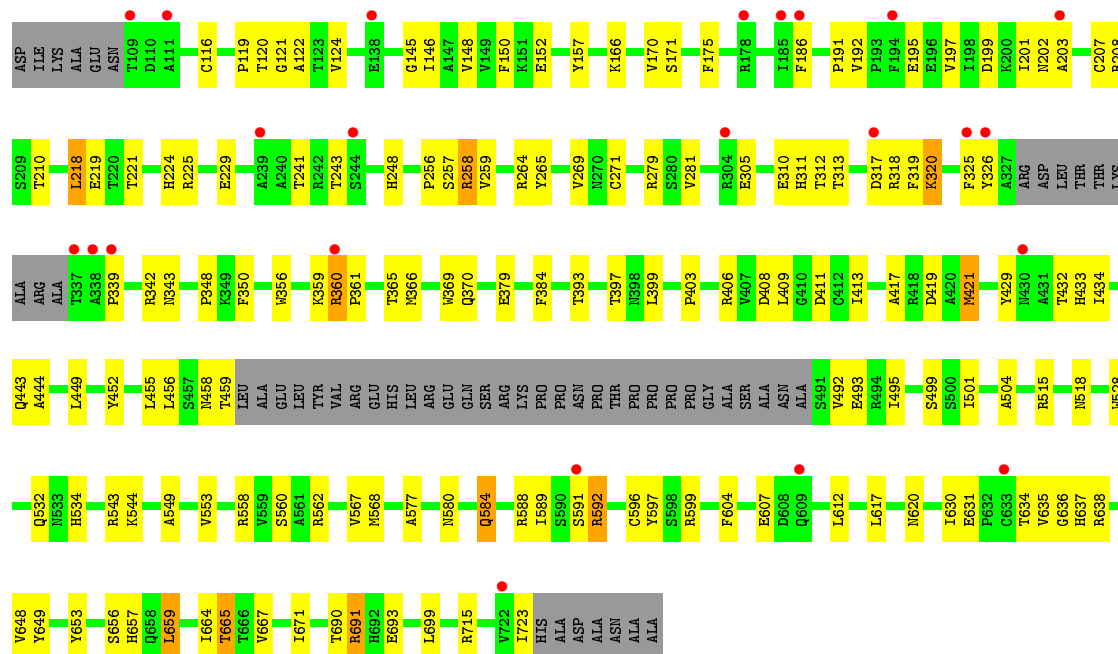


#### • Molecule 1: Glycoprotein B





• Molecule 1: Glycoprotein B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.96Å 100.04Å 100.13Å 67.04° 77.99° 70.31°	Depositor
Resolution (Å)	41.20 – 2.10 41.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.7 (41.20-2.10) 66.3 (41.10-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.275 0.245 , 0.270	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 164504 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/4775	0.62	0/6488
1	B	0.40	0/4811	0.62	0/6538
1	C	0.39	0/4760	0.61	0/6469
All	All	0.39	0/14346	0.61	0/19495

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4658	0	4467	182	0
1	B	4694	0	4501	150	0
1	C	4644	0	4450	136	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
3	A	62	0	0	1	0
3	B	82	0	0	2	0
3	C	79	0	0	1	0
All	All	14223	0	13418	427	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 16.

All (427) 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:366:MET:CE	1:B:495:ILE:HB	1.70	1.21
1:B:366:MET:HE1	1:B:495:ILE:CB	1.91	0.99
1:B:366:MET:HE1	1:B:495:ILE:HB	0.95	0.95
1:A:699:LEU:HD13	1:C:281:VAL:HG13	1.51	0.91
1:B:202:ASN:O	1:B:328:ARG:HG3	1.78	0.84
1:A:250:THR:HG22	1:A:251:ASP:H	1.42	0.83
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.64	0.79
1:B:592:ARG:HG3	1:B:595:ALA:HB3	1.65	0.78
1:A:343:ASN:OD1	1:A:356:TRP:HB2	1.86	0.76
1:A:713:ASP:HB3	1:A:719:ILE:HD11	1.67	0.76
1:A:412:CYS:HA	1:A:415:LYS:HD2	1.68	0.75
1:B:417:ALA:O	1:B:421:MET:HB2	1.86	0.75
1:A:121:GLY:HA3	1:C:638:ARG:HH11	1.53	0.74
1:A:241:THR:O	1:A:243:THR:HG23	1.89	0.73
1:A:671:ILE:HD11	1:C:534:HIS:CD2	2.23	0.72
1:C:591:SER:O	1:C:592:ARG:HB2	1.88	0.72
1:C:543:ARG:HB2	1:C:568:MET:HE1	1.72	0.72
1:A:202:ASN:OD1	1:A:328:ARG:HD2	1.89	0.72
1:A:397:THR:HG22	1:A:444:ALA:HA	1.72	0.71
1:B:512:HIS:ND1	3:B:787:HOH:O	2.23	0.71
1:C:634:THR:HG22	1:C:635:VAL:H	1.54	0.71
1:B:326:TYR:CZ	1:B:339:PRO:HG3	2.26	0.70
1:C:634:THR:HG22	1:C:635:VAL:N	2.06	0.70
1:B:531:LEU:O	1:B:535:GLU:HG2	1.91	0.70
1:C:543:ARG:HB2	1:C:568:MET:CE	2.22	0.70
1:A:328:ARG:N	1:A:328:ARG:HD3	2.06	0.69
1:A:156:PRO:HG2	1:A:279:ARG:NH2	2.06	0.69
1:C:116:CYS:HB3	1:C:560:SER:HB2	1.74	0.69
1:B:119:PRO:HD2	1:B:562:ARG:HD3	1.75	0.69
1:A:166:LYS:HE2	1:A:207:CYS:SG	2.33	0.68
1:B:719:ILE:HG22	1:C:318:ARG:HH21	1.56	0.68
1:A:202:ASN:HA	1:A:328:ARG:HG3	1.75	0.68
1:C:429:TYR:HB3	1:C:433:HIS:HB2	1.75	0.68
1:B:109:THR:HG22	1:B:110:ASP:H	1.60	0.67
1:B:628:ASP:O	1:B:630:ILE:HG13	1.94	0.67
1:A:250:THR:HG22	1:A:251:ASP:N	2.10	0.66
1:A:638:ARG:HH11	1:B:121:GLY:HA3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:HIS:HA	1:C:271:CYS:O	1.94	0.66
1:C:365:THR:O	1:C:366:MET:HE2	1.95	0.66
1:C:199:ASP:O	1:C:203:ALA:HB3	1.96	0.66
1:A:424:ILE:HG12	1:A:427:ARG:NH2	2.11	0.66
1:B:719:ILE:HG22	1:C:318:ARG:NH2	2.11	0.65
1:B:434:ILE:HD12	1:B:434:ILE:N	2.11	0.65
1:C:434:ILE:HD11	1:C:458:ASN:OD1	1.96	0.65
1:B:346:THR:HG22	1:B:351:THR:OG1	1.95	0.65
1:A:377:ARG:HD3	1:A:384:PHE:CE1	2.32	0.65
1:A:250:THR:HG22	1:A:252:LEU:H	1.62	0.65
1:A:304:ARG:HD2	1:A:341:THR:HG21	1.79	0.65
1:B:589:ILE:HG12	1:B:597:TYR:CE1	2.32	0.65
1:A:443:GLN:NE2	1:A:443:GLN:HA	2.12	0.64
1:B:634:THR:HG22	1:B:635:VAL:N	2.12	0.64
1:B:224:HIS:HB2	1:B:269:VAL:HB	1.79	0.64
1:B:630:ILE:HG22	1:B:631:GLU:N	2.13	0.64
1:A:328:ARG:H	1:A:328:ARG:HD3	1.62	0.63
1:B:109:THR:HG22	1:B:110:ASP:N	2.13	0.63
1:A:443:GLN:HE21	1:A:443:GLN:HA	1.62	0.63
1:B:166:LYS:HE2	1:B:207:CYS:SG	2.38	0.63
1:C:360:ARG:CB	1:C:361:PRO:HD3	2.29	0.63
1:A:719:ILE:HG22	1:B:318:ARG:HH21	1.64	0.63
1:C:326:TYR:CE1	1:C:339:PRO:HG3	2.35	0.62
1:C:637:HIS:HD2	1:C:653:TYR:H	1.47	0.62
1:C:434:ILE:N	1:C:434:ILE:HD12	2.14	0.62
1:C:256:PRO:HG3	1:C:265:TYR:C	2.20	0.62
1:B:252:LEU:HD23	1:C:723:ILE:HD11	1.82	0.61
1:C:146:ILE:HG13	1:C:455:LEU:HD11	1.83	0.61
1:C:152:GLU:HA	1:C:366:MET:CE	2.30	0.61
1:B:614:GLU:HB2	1:B:627:ARG:NH2	2.16	0.61
1:C:637:HIS:CD2	1:C:653:TYR:H	2.19	0.61
1:C:119:PRO:HD2	1:C:562:ARG:HD3	1.81	0.61
1:A:199:ASP:O	1:A:203:ALA:HB3	2.01	0.61
1:A:170:VAL:HG13	1:A:186:PHE:HB3	1.83	0.60
1:C:406:ARG:O	1:C:492:VAL:HG13	2.01	0.60
1:A:191:PRO:HA	1:A:350:PHE:HA	1.84	0.60
1:B:714:LEU:HD23	1:B:719:ILE:HD12	1.83	0.60
1:B:170:VAL:HG12	1:B:186:PHE:HD2	1.66	0.60
1:A:596:CYS:O	1:A:630:ILE:HG23	2.01	0.60
1:B:177:HIS:O	1:B:178:ARG:HB2	2.01	0.60
1:A:259:VAL:HG23	1:A:264:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:HIS:HD2	1:B:653:TYR:H	1.49	0.59
1:C:170:VAL:CG1	1:C:186:PHE:HB3	2.32	0.59
1:A:162:THR:HG21	1:A:328:ARG:HH22	1.68	0.59
1:C:584:GLN:HA	1:C:584:GLN:HE21	1.66	0.59
1:A:634:THR:HG22	1:A:635:VAL:N	2.16	0.59
1:A:195:GLU:OE1	1:A:196:GLU:N	2.36	0.59
1:B:637:HIS:CD2	1:B:653:TYR:H	2.21	0.59
1:B:359:LYS:HE2	1:B:409:LEU:HD11	1.85	0.59
1:B:170:VAL:O	1:B:170:VAL:HG13	2.03	0.59
1:B:250:THR:HG22	1:B:251:ASP:N	2.17	0.59
1:C:492:VAL:HG12	1:C:493:GLU:N	2.17	0.59
1:A:319:PHE:O	1:A:320:LYS:HE3	2.03	0.59
1:A:404:LEU:HD11	1:A:413:ILE:HG21	1.85	0.58
1:B:250:THR:HG22	1:B:251:ASP:H	1.67	0.58
1:C:577:ALA:HB3	1:C:580:ASN:HD22	1.67	0.58
1:B:241:THR:O	1:B:243:THR:HG23	2.03	0.58
1:B:535:GLU:HB2	3:B:735:HOH:O	2.03	0.58
1:B:723:ILE:O	1:B:724:HIS:HB2	2.02	0.58
1:A:216:ASN:HD22	1:B:185:ILE:HD13	1.69	0.58
1:B:170:VAL:CG1	1:B:186:PHE:HB3	2.33	0.58
1:A:408:ASP:OD1	1:A:409:LEU:HG	2.02	0.58
1:C:659:LEU:HD23	1:C:659:LEU:N	2.19	0.58
1:B:534:HIS:CD2	1:C:671:ILE:HD11	2.38	0.57
1:C:417:ALA:O	1:C:421:MET:HB2	2.04	0.57
1:C:170:VAL:HG13	1:C:186:PHE:HB3	1.86	0.57
1:C:630:ILE:HG22	1:C:631:GLU:N	2.19	0.57
1:B:687:GLU:OE2	1:C:499:SER:HB2	2.04	0.57
1:B:549:ALA:O	1:B:553:VAL:HG23	2.05	0.57
1:A:204:LYS:HB2	1:A:206:VAL:HG22	1.86	0.57
1:A:216:ASN:ND2	1:B:185:ILE:HD13	2.19	0.57
1:A:577:ALA:HB3	1:A:580:ASN:HD22	1.70	0.57
1:C:413:ILE:HD13	1:C:449:LEU:HD23	1.87	0.57
1:B:194:PHE:CE2	1:B:346:THR:HG23	2.40	0.56
1:C:443:GLN:OE1	1:C:495:ILE:HD12	2.04	0.56
1:A:377:ARG:HD3	1:A:384:PHE:CD1	2.40	0.56
1:C:218:LEU:HD22	1:C:219:GLU:H	1.70	0.56
1:A:554:THR:HG22	1:C:667:VAL:HB	1.87	0.56
1:C:664:ILE:N	1:C:664:ILE:HD12	2.21	0.56
1:C:166:LYS:HE2	1:C:207:CYS:SG	2.45	0.56
1:B:380:TYR:O	1:B:385:ARG:NH1	2.39	0.56
1:B:596:CYS:O	1:B:630:ILE:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ARG:HD3	1:C:411:ASP:OD2	2.05	0.56
1:C:360:ARG:CD	1:C:411:ASP:OD2	2.53	0.56
1:C:241:THR:O	1:C:243:THR:HG23	2.06	0.56
1:C:218:LEU:HD22	1:C:219:GLU:N	2.21	0.55
1:A:531:LEU:O	1:A:535:GLU:HG2	2.05	0.55
1:C:599:ARG:NH1	1:C:617:LEU:O	2.39	0.55
1:A:601:LEU:HD23	1:A:616:GLN:HB3	1.88	0.55
1:A:434:ILE:HD11	1:A:458:ASN:OD1	2.07	0.55
1:B:257:SER:O	1:B:264:ARG:NH1	2.37	0.55
1:C:360:ARG:HB3	1:C:361:PRO:HD3	1.89	0.55
1:A:637:HIS:HB3	1:A:652:GLU:HA	1.90	0.54
1:A:152:GLU:HA	1:A:366:MET:HE2	1.89	0.54
1:A:145:GLY:HA2	1:A:455:LEU:HG	1.88	0.54
1:A:281:VAL:HG13	1:B:699:LEU:HD13	1.88	0.54
1:A:287:PHE:CD2	1:A:299:PRO:HG3	2.41	0.54
1:A:170:VAL:HG12	1:A:186:PHE:HD2	1.73	0.54
1:C:191:PRO:HA	1:C:350:PHE:HA	1.90	0.54
1:A:170:VAL:CG1	1:A:186:PHE:HB3	2.38	0.54
1:A:434:ILE:HD12	1:A:434:ILE:N	2.23	0.54
1:B:397:THR:HG22	1:B:444:ALA:HA	1.90	0.54
1:B:366:MET:CE	1:B:495:ILE:CB	2.65	0.54
1:C:397:THR:HG22	1:C:444:ALA:HA	1.90	0.54
1:C:175:PHE:HB3	1:C:258:ARG:NH1	2.22	0.54
1:A:346:THR:O	1:A:346:THR:HG23	2.07	0.54
1:A:202:ASN:O	1:A:328:ARG:HB3	2.08	0.53
1:A:426:ALA:HA	1:A:430:ASN:HB3	1.91	0.53
1:A:434:ILE:HD11	1:A:458:ASN:HA	1.90	0.53
1:B:176:GLY:O	1:B:258:ARG:NH2	2.41	0.53
1:C:393:THR:HG23	1:C:504:ALA:HB1	1.91	0.53
1:A:225:ARG:HD2	1:A:254:TYR:HB2	1.90	0.53
1:B:358:PRO:HG2	1:B:361:PRO:HG2	1.91	0.53
1:B:456:LEU:HD21	1:B:460:LEU:CD2	2.39	0.53
1:A:630:ILE:HG22	1:A:631:GLU:N	2.24	0.53
1:C:577:ALA:HB3	1:C:580:ASN:ND2	2.23	0.53
1:A:423:ARG:HB2	1:A:423:ARG:HH11	1.73	0.53
1:C:325:PHE:CD2	1:C:342:ARG:HB2	2.44	0.53
1:B:434:ILE:HD11	1:B:458:ASN:OD1	2.08	0.52
1:A:222:ALA:HB1	1:A:267:THR:HG21	1.89	0.52
1:A:120:THR:C	1:A:122:ALA:H	2.12	0.52
1:A:597:TYR:CE1	1:A:601:LEU:HD11	2.44	0.52
1:A:318:ARG:O	1:A:346:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:VAL:HG13	1:C:699:LEU:HD13	1.90	0.52
1:C:343:ASN:OD1	1:C:356:TRP:HB2	2.10	0.52
1:A:358:PRO:HG2	1:A:361:PRO:CG	2.39	0.52
1:A:424:ILE:HG12	1:A:427:ARG:HH21	1.73	0.52
1:C:671:ILE:HD12	1:C:671:ILE:N	2.24	0.52
1:A:659:LEU:HD12	1:A:659:LEU:N	2.25	0.52
1:C:515:ARG:NH2	3:C:790:HOH:O	2.40	0.52
1:B:630:ILE:CG2	1:B:631:GLU:N	2.72	0.52
1:B:166:LYS:HG2	1:B:271:CYS:HA	1.91	0.52
1:C:403:PRO:HG2	1:C:406:ARG:HH21	1.75	0.52
1:B:170:VAL:HG13	1:B:186:PHE:HB3	1.92	0.52
1:B:677:MET:HE3	1:C:518:ASN:HB3	1.92	0.52
1:B:257:SER:HB3	1:B:264:ARG:HH12	1.75	0.52
1:A:328:ARG:CD	1:A:328:ARG:H	2.22	0.51
1:C:413:ILE:HD13	1:C:449:LEU:CD2	2.39	0.51
1:B:637:HIS:O	1:B:651:GLU:HA	2.10	0.51
1:B:200:LYS:NZ	1:B:208:ARG:NH1	2.59	0.51
1:C:656:SER:OG	1:C:657:HIS:HD2	1.92	0.51
1:A:671:ILE:N	1:A:671:ILE:HD12	2.25	0.51
1:A:719:ILE:HG22	1:B:318:ARG:NH2	2.25	0.51
1:A:648:VAL:HG13	1:A:648:VAL:O	2.11	0.51
1:C:152:GLU:HA	1:C:366:MET:HE2	1.93	0.51
1:C:408:ASP:O	1:C:409:LEU:HB2	2.11	0.51
1:A:365:THR:O	1:A:366:MET:HE2	2.11	0.50
1:C:202:ASN:ND2	1:C:325:PHE:HE1	2.09	0.50
1:C:379:GLU:HG3	1:C:399:LEU:CD2	2.42	0.50
1:A:125:VAL:HG12	1:C:665:THR:HG23	1.94	0.50
1:B:250:THR:HG22	1:B:252:LEU:H	1.77	0.50
1:A:374:GLU:HG2	1:A:429:TYR:OH	2.12	0.50
1:B:194:PHE:HZ	1:B:318:ARG:O	1.95	0.50
1:A:366:MET:CE	1:A:495:ILE:HB	2.42	0.50
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.77	0.50
1:A:583:VAL:HG23	1:A:643:PHE:CZ	2.47	0.49
1:A:170:VAL:O	1:A:170:VAL:HG13	2.12	0.49
1:B:358:PRO:HG2	1:B:361:PRO:CG	2.42	0.49
1:B:719:ILE:HG21	1:C:348:PRO:HG3	1.93	0.49
1:B:110:ASP:OD1	1:B:112:ASN:HB3	2.13	0.49
1:C:648:VAL:O	1:C:648:VAL:HG13	2.12	0.49
1:A:397:THR:HG22	1:A:444:ALA:CA	2.41	0.49
1:A:267:THR:HG22	1:A:268:THR:N	2.26	0.49
1:A:121:GLY:HA3	1:C:638:ARG:NH1	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HE2	1:A:219:GLU:CD	2.33	0.49
1:C:634:THR:CG2	1:C:635:VAL:N	2.75	0.49
1:B:432:THR:HB	1:B:433:HIS:HD2	1.78	0.49
1:B:543:ARG:HB2	1:B:568:MET:CE	2.43	0.49
1:B:648:VAL:O	1:B:648:VAL:HG13	2.12	0.49
1:B:110:ASP:C	1:B:112:ASN:H	2.14	0.49
1:B:634:THR:HG22	1:B:635:VAL:H	1.78	0.49
1:A:423:ARG:HB2	1:A:423:ARG:NH1	2.28	0.48
1:B:456:LEU:HD21	1:B:460:LEU:HD22	1.95	0.48
1:C:121:GLY:O	1:C:122:ALA:C	2.51	0.48
1:A:637:HIS:HD2	1:A:653:TYR:H	1.62	0.48
1:B:543:ARG:HB2	1:B:568:MET:HE1	1.94	0.48
1:C:492:VAL:HG12	1:C:493:GLU:H	1.76	0.48
1:C:319:PHE:O	1:C:320:LYS:HE3	2.13	0.48
1:A:671:ILE:HD11	1:C:534:HIS:CG	2.48	0.48
1:C:170:VAL:O	1:C:170:VAL:HG13	2.14	0.48
1:B:677:MET:CE	1:C:518:ASN:HB3	2.44	0.48
1:A:265:TYR:N	1:A:265:TYR:CD1	2.81	0.48
1:A:214:VAL:HG13	1:A:214:VAL:O	2.14	0.48
1:C:210:THR:HG21	1:C:229:GLU:HB2	1.96	0.48
1:C:175:PHE:HB3	1:C:258:ARG:HH11	1.78	0.48
1:B:258:ARG:HG3	1:B:259:VAL:N	2.27	0.48
1:A:202:ASN:HA	1:A:328:ARG:CG	2.43	0.47
1:A:601:LEU:HD22	1:A:627:ARG:CD	2.43	0.47
1:A:601:LEU:HD22	1:A:627:ARG:HD3	1.96	0.47
1:A:358:PRO:HG2	1:A:361:PRO:HG2	1.96	0.47
1:A:311:HIS:HE2	1:A:313:THR:HG1	1.61	0.47
1:C:634:THR:CG2	1:C:635:VAL:H	2.22	0.47
1:A:310:GLU:OE2	1:A:359:LYS:HD2	2.15	0.47
1:C:434:ILE:HD12	1:C:456:LEU:O	2.15	0.47
1:A:124:VAL:O	1:C:665:THR:CG2	2.62	0.47
1:A:638:ARG:NH1	1:B:121:GLY:HA3	2.26	0.47
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.96	0.47
1:C:310:GLU:OE2	1:C:359:LYS:HD2	2.15	0.47
1:C:313:THR:O	1:C:313:THR:HG22	2.15	0.47
1:A:661:ARG:NH1	1:B:129:GLN:HG2	2.29	0.47
1:B:630:ILE:CG2	1:B:631:GLU:H	2.28	0.47
1:B:248:HIS:HA	1:B:271:CYS:O	2.14	0.47
1:C:588:ARG:HH11	1:C:588:ARG:HG2	1.79	0.47
1:A:396:THR:HB	1:A:445:ASN:HD22	1.80	0.47
1:C:406:ARG:HG2	1:C:406:ARG:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:HG21	1:B:395:PHE:CZ	2.49	0.47
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.97	0.47
1:C:580:ASN:O	1:C:604:PHE:HA	2.15	0.47
1:B:208:ARG:HH11	1:B:208:ARG:HG2	1.80	0.47
1:C:501:ILE:O	1:C:501:ILE:HG13	2.14	0.47
1:A:152:GLU:OE1	1:A:496:LYS:HA	2.14	0.47
1:C:589:ILE:HG12	1:C:597:TYR:CE1	2.49	0.47
1:A:120:THR:O	1:A:122:ALA:N	2.48	0.46
1:C:690:THR:OG1	1:C:693:GLU:HG3	2.15	0.46
1:A:577:ALA:HB3	1:A:580:ASN:ND2	2.30	0.46
1:A:637:HIS:CD2	1:A:653:TYR:H	2.32	0.46
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.97	0.46
1:A:677:MET:CE	1:B:518:ASN:HB3	2.46	0.46
1:A:124:VAL:O	1:C:665:THR:HG22	2.15	0.46
1:B:119:PRO:HG3	1:B:560:SER:HB3	1.98	0.46
1:C:366:MET:HG3	1:C:413:ILE:HD11	1.97	0.46
1:B:433:HIS:C	1:B:434:ILE:HD12	2.36	0.46
1:A:120:THR:C	1:A:122:ALA:N	2.67	0.46
1:A:689:TYR:CE1	1:B:691:ARG:NH2	2.83	0.46
1:A:614:GLU:HB3	1:A:627:ARG:CZ	2.45	0.46
1:B:640:TYR:HB2	1:C:567:VAL:HG22	1.97	0.46
1:B:380:TYR:HB3	1:B:385:ARG:NH1	2.31	0.46
1:A:411:ASP:O	1:A:415:LYS:HG3	2.16	0.46
1:A:328:ARG:CD	1:A:328:ARG:N	2.78	0.46
1:A:181:GLN:HB2	1:C:221:THR:O	2.15	0.46
1:A:324:GLY:HA2	1:A:339:PRO:HB3	1.97	0.46
1:A:244:SER:OG	1:B:708:ARG:NH2	2.46	0.46
1:A:561:ALA:HA	1:A:569:ALA:O	2.16	0.46
1:A:689:TYR:HE1	1:B:691:ARG:NH2	2.13	0.45
1:B:656:SER:OG	1:B:657:HIS:HD2	1.98	0.45
1:B:393:THR:HG23	1:B:504:ALA:HB1	1.97	0.45
1:A:369:TRP:CD2	1:A:370:GLN:HG2	2.52	0.45
1:B:432:THR:HB	1:B:433:HIS:CD2	2.52	0.45
1:C:360:ARG:HD2	1:C:411:ASP:OD2	2.17	0.45
1:B:359:LYS:O	1:B:363:VAL:HG22	2.16	0.45
1:A:647:TYR:CE1	1:A:664:ILE:HD12	2.52	0.45
1:B:366:MET:HG3	1:B:413:ILE:HD11	1.97	0.45
1:B:109:THR:CG2	1:B:110:ASP:H	2.29	0.45
1:B:120:THR:C	1:B:122:ALA:H	2.19	0.45
1:B:224:HIS:O	1:B:225:ARG:HB2	2.16	0.45
1:A:152:GLU:HA	1:A:366:MET:CE	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ARG:HH11	1:C:208:ARG:HG2	1.81	0.45
1:C:311:HIS:CG	1:C:312:THR:N	2.84	0.45
1:B:413:ILE:HD13	1:B:449:LEU:HD23	1.99	0.45
1:C:458:ASN:O	1:C:459:THR:C	2.55	0.45
1:A:535:GLU:HB2	3:A:732:HOH:O	2.17	0.45
1:A:224:HIS:C	1:A:226:ASP:H	2.19	0.45
1:A:649:TYR:CE2	1:A:651:GLU:HG3	2.51	0.45
1:C:403:PRO:HG2	1:C:406:ARG:NH2	2.30	0.45
1:C:549:ALA:O	1:C:553:VAL:HG23	2.16	0.45
1:B:313:THR:O	1:B:313:THR:HG22	2.16	0.45
1:A:528:TRP:O	1:A:532:GLN:HG2	2.17	0.45
1:B:173:VAL:HG12	1:B:182:PHE:CD1	2.52	0.45
1:C:166:LYS:HG2	1:C:271:CYS:HA	1.98	0.45
1:B:166:LYS:NZ	1:B:210:THR:O	2.46	0.45
1:A:256:PRO:HB3	1:A:264:ARG:HB3	1.98	0.45
1:A:366:MET:HE1	1:A:495:ILE:HB	1.98	0.45
1:A:119:PRO:HD2	1:A:562:ARG:HD3	1.99	0.45
1:C:257:SER:OG	1:C:264:ARG:NH1	2.47	0.45
1:B:630:ILE:HG22	1:B:631:GLU:H	1.81	0.44
1:C:384:PHE:CD2	1:C:399:LEU:HA	2.53	0.44
1:A:374:GLU:OE2	1:A:428:ARG:NH2	2.50	0.44
1:A:497:THR:O	1:C:691:ARG:NH2	2.49	0.44
1:B:120:THR:C	1:B:122:ALA:N	2.70	0.44
1:A:257:SER:O	1:A:264:ARG:NH1	2.49	0.44
1:A:289:LEU:HD11	1:A:352:VAL:HG11	1.98	0.44
1:B:432:THR:HA	1:B:458:ASN:ND2	2.32	0.44
1:C:596:CYS:HB3	1:C:653:TYR:CE2	2.52	0.44
1:A:218:LEU:HD23	1:B:182:PHE:CZ	2.53	0.44
1:B:157:TYR:O	1:B:279:ARG:HA	2.18	0.44
1:B:634:THR:CG2	1:B:635:VAL:N	2.78	0.44
1:B:311:HIS:HE2	1:B:313:THR:HG1	1.66	0.44
1:B:121:GLY:O	1:B:122:ALA:C	2.56	0.44
1:C:197:VAL:HA	1:C:201:ILE:HD12	2.00	0.44
1:A:417:ALA:O	1:A:421:MET:HG3	2.17	0.44
1:C:145:GLY:HA3	1:C:452:TYR:CZ	2.53	0.44
1:A:256:PRO:HD3	1:A:266:GLY:HA3	2.00	0.44
1:B:109:THR:CG2	1:B:110:ASP:N	2.81	0.44
1:A:150:PHE:HB2	1:A:449:LEU:HB3	1.99	0.44
1:A:170:VAL:CG1	1:A:186:PHE:HD2	2.31	0.43
1:C:656:SER:OG	1:C:657:HIS:CD2	2.70	0.43
1:C:379:GLU:HG3	1:C:399:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASP:O	1:A:286:GLU:HB3	2.18	0.43
1:B:218:LEU:C	1:B:218:LEU:HD23	2.39	0.43
1:A:166:LYS:HG2	1:A:271:CYS:HA	2.00	0.43
1:A:196:GLU:O	1:A:200:LYS:HB2	2.17	0.43
1:C:192:VAL:HG11	1:C:201:ILE:HD11	2.00	0.43
1:A:543:ARG:HB2	1:A:568:MET:CE	2.48	0.43
1:A:260:GLU:O	1:A:261:ALA:HB3	2.19	0.43
1:A:434:ILE:HD12	1:A:456:LEU:O	2.18	0.43
1:A:325:PHE:CE2	1:A:327:ALA:HA	2.53	0.43
1:B:170:VAL:HG12	1:B:186:PHE:CD2	2.51	0.43
1:C:607:GLU:OE2	1:C:607:GLU:HA	2.18	0.43
1:B:592:ARG:HG3	1:B:595:ALA:CB	2.44	0.43
1:B:379:GLU:HG3	1:B:399:LEU:HD21	2.00	0.43
1:B:408:ASP:HA	1:B:492:VAL:CG1	2.48	0.43
1:A:411:ASP:O	1:A:415:LYS:HE3	2.18	0.43
1:C:256:PRO:HB3	1:C:264:ARG:HB3	2.00	0.43
1:A:212:LYS:HE2	1:A:219:GLU:OE1	2.18	0.43
1:A:379:GLU:HG3	1:A:399:LEU:HD21	2.00	0.43
1:C:208:ARG:C	1:C:210:THR:H	2.21	0.43
1:A:250:THR:CG2	1:A:251:ASP:H	2.22	0.43
1:A:252:LEU:HD23	1:B:718:ASP:HB3	2.01	0.43
1:B:116:CYS:HB3	1:B:560:SER:HB2	2.01	0.43
1:A:256:PRO:HG3	1:A:265:TYR:C	2.39	0.43
1:C:120:THR:C	1:C:122:ALA:N	2.72	0.43
1:B:454:PRO:O	1:B:455:LEU:HD23	2.17	0.43
1:A:313:THR:HG22	1:A:313:THR:O	2.19	0.43
1:C:543:ARG:HG3	1:C:544:LYS:N	2.34	0.42
1:A:254:TYR:HB3	1:A:267:THR:O	2.19	0.42
1:B:326:TYR:OH	1:B:339:PRO:HG3	2.18	0.42
1:C:630:ILE:CG2	1:C:631:GLU:N	2.81	0.42
1:B:580:ASN:O	1:B:604:PHE:HA	2.19	0.42
1:B:302:GLY:N	1:B:307:SER:HB3	2.35	0.42
1:C:171:SER:O	1:C:265:TYR:HA	2.19	0.42
1:C:224:HIS:HB2	1:C:269:VAL:HB	2.01	0.42
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.90	0.42
1:A:534:HIS:CD2	1:B:671:ILE:HD11	2.54	0.42
1:A:414:GLY:O	1:A:418:ARG:HG3	2.19	0.42
1:A:175:PHE:CE2	1:A:258:ARG:HA	2.55	0.42
1:A:248:HIS:HA	1:A:271:CYS:O	2.19	0.42
1:A:616:GLN:HG2	1:A:627:ARG:HA	2.00	0.42
1:B:218:LEU:HD23	1:B:219:GLU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:ARG:NH2	1:B:628:ASP:OD2	2.42	0.42
1:B:564:LEU:CD1	1:B:569:ALA:HB2	2.50	0.42
1:A:599:ARG:HA	1:A:600:PRO:HD3	1.89	0.42
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.18	0.42
1:A:719:ILE:HG23	1:B:348:PRO:HG3	2.02	0.42
1:B:200:LYS:HZ1	1:B:208:ARG:NH1	2.18	0.42
1:A:147:ALA:HA	1:A:451:ALA:O	2.20	0.42
1:A:634:THR:HG22	1:A:635:VAL:H	1.81	0.42
1:B:175:PHE:CE2	1:B:258:ARG:HA	2.55	0.42
1:A:658:GLN:C	1:A:659:LEU:HD12	2.40	0.42
1:C:120:THR:O	1:C:122:ALA:N	2.53	0.42
1:A:603:SER:HA	1:A:613:VAL:O	2.20	0.42
1:B:637:HIS:HB3	1:B:652:GLU:HA	2.01	0.42
1:A:677:MET:HE1	1:B:518:ASN:HB3	2.00	0.42
1:A:377:ARG:NH2	1:A:440:GLN:OE1	2.53	0.41
1:A:216:ASN:OD1	1:B:253:LYS:HG3	2.20	0.41
1:C:152:GLU:HA	1:C:366:MET:HE1	2.00	0.41
1:A:360:ARG:NH1	1:A:409:LEU:HD23	2.35	0.41
1:A:347:THR:N	1:A:350:PHE:O	2.44	0.41
1:A:634:THR:CG2	1:A:635:VAL:N	2.81	0.41
1:C:432:THR:HB	1:C:433:HIS:HD2	1.85	0.41
1:A:191:PRO:HB3	1:A:350:PHE:CA	2.50	0.41
1:A:259:VAL:CG2	1:A:264:ARG:HH11	2.33	0.41
1:C:671:ILE:CD1	1:C:671:ILE:N	2.82	0.41
1:C:224:HIS:CD2	1:C:225:ARG:HG3	2.55	0.41
1:C:612:LEU:HA	1:C:612:LEU:HD12	1.95	0.41
1:A:234:LEU:HD23	1:A:249:THR:HG23	2.02	0.41
1:C:591:SER:O	1:C:592:ARG:CB	2.62	0.41
1:B:723:ILE:O	1:B:724:HIS:CB	2.65	0.41
1:A:454:PRO:O	1:A:455:LEU:HD23	2.20	0.41
1:A:224:HIS:CD2	1:A:225:ARG:HG2	2.55	0.41
1:C:124:VAL:HG11	1:C:567:VAL:HG21	2.03	0.41
1:C:148:VAL:HG12	1:C:150:PHE:CE1	2.54	0.41
1:B:432:THR:HG22	1:B:432:THR:O	2.21	0.41
1:C:649:TYR:O	1:C:656:SER:HB3	2.20	0.41
1:A:208:ARG:HG2	1:A:208:ARG:NH1	2.35	0.41
1:A:553:VAL:HG21	1:B:537:THR:OG1	2.21	0.41
1:B:655:TYR:CD2	1:B:655:TYR:C	2.93	0.41
1:A:174:TRP:HB2	1:A:263:HIS:CE1	2.56	0.41
1:B:249:THR:HG23	1:B:271:CYS:HB3	2.03	0.41
1:A:456:LEU:HD12	1:A:457:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ARG:NH1	1:B:617:LEU:O	2.51	0.41
1:C:157:TYR:O	1:C:279:ARG:HA	2.21	0.41
1:B:237:ALA:HB1	1:C:715:ARG:O	2.21	0.41
1:C:543:ARG:HB2	1:C:568:MET:HE3	2.02	0.41
1:A:287:PHE:CZ	1:A:295:VAL:HG11	2.56	0.41
1:C:528:TRP:O	1:C:532:GLN:HG2	2.20	0.41
1:C:558:ARG:HD2	1:C:558:ARG:HA	1.90	0.41
1:A:605:ARG:HH21	1:A:612:LEU:HD13	1.85	0.41
1:B:574:VAL:HA	1:B:575:PRO:HD3	1.85	0.41
1:B:612:LEU:HA	1:B:612:LEU:HD12	1.89	0.40
1:B:458:ASN:O	1:B:460:LEU:N	2.54	0.40
1:A:564:LEU:HD12	1:A:569:ALA:HB2	2.03	0.40
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.56	0.40
1:A:589:ILE:HG12	1:A:597:TYR:CE1	2.56	0.40
1:A:543:ARG:HD2	1:A:568:MET:CE	2.51	0.40
1:B:181:GLN:HB3	1:B:181:GLN:HE21	1.62	0.40
1:B:424:ILE:HG12	1:B:427:ARG:NH2	2.37	0.40
1:C:635:VAL:HG12	1:C:636:GLY:N	2.37	0.40
1:A:649:TYR:HB2	1:A:659:LEU:HD11	2.03	0.40
1:B:129:GLN:HB3	1:B:130:PRO:HD2	2.04	0.40
1:B:158:LYS:HE3	1:B:279:ARG:NH1	2.36	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	570/628 (91%)	531 (93%)	33 (6%)	6 (1%)	17	11
1	B	575/628 (92%)	538 (94%)	32 (6%)	5 (1%)	21	15
1	C	569/628 (91%)	533 (94%)	32 (6%)	4 (1%)	26	21
All	All	1714/1884 (91%)	1602 (94%)	97 (6%)	15 (1%)	21	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	B	305	GLU
1	C	305	GLU
1	C	592	ARG
1	A	306	GLY
1	B	629	ALA
1	A	260	GLU
1	B	228	HIS
1	B	459	THR
1	A	415	LYS
1	A	456	LEU
1	C	259	VAL
1	C	360	ARG
1	B	259	VAL
1	A	403	PRO

### 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	502/543 (92%)	494 (98%)	8 (2%)	70	76
1	B	507/543 (93%)	499 (98%)	8 (2%)	70	76
1	C	502/543 (92%)	490 (98%)	12 (2%)	57	61
All	All	1511/1629 (93%)	1483 (98%)	28 (2%)	65	70

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

Mol	Chain	Res	Type
1	A	195	GLU
1	A	248	HIS
1	A	265	TYR
1	A	320	LYS
1	A	328	ARG
1	A	419	ASP

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Mol	Chain	Res	Type
1	A	567	VAL
1	A	620	ASN
1	B	112	ASN
1	B	195	GLU
1	B	248	HIS
1	B	320	LYS
1	B	419	ASP
1	B	421	MET
1	B	620	ASN
1	B	659	LEU
1	C	195	GLU
1	C	218	LEU
1	C	258	ARG
1	C	317	ASP
1	C	320	LYS
1	C	419	ASP
1	C	421	MET
1	C	584	GLN
1	C	620	ASN
1	C	659	LEU
1	C	665	THR
1	C	691	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	172	GLN
1	A	181	GLN
1	A	248	HIS
1	A	370	GLN
1	A	443	GLN
1	A	445	ASN
1	A	534	HIS
1	A	580	ASN
1	A	620	ASN
1	A	637	HIS
1	A	658	GLN
1	B	112	ASN
1	B	181	GLN
1	B	433	HIS
1	B	584	GLN

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Mol	Chain	Res	Type
1	B	620	ASN
1	B	637	HIS
1	B	657	HIS
1	C	140	GLN
1	C	181	GLN
1	C	370	GLN
1	C	433	HIS
1	C	580	ASN
1	C	620	ASN
1	C	637	HIS
1	C	657	HIS
1	C	658	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	576/628 (91%)	0.38	33 (5%)	27 35	24, 62, 87, 113	0
1	B	581/628 (92%)	0.16	23 (3%)	42 51	22, 50, 82, 109	0
1	C	575/628 (91%)	0.25	23 (4%)	42 51	21, 56, 82, 95	0
All	All	1732/1884 (91%)	0.26	79 (4%)	36 45	21, 56, 85, 113	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	461	ALA	6.2
1	A	329	ASP	6.1
1	A	247	TRP	5.5
1	A	725	ALA	5.5
1	A	326	TYR	5.3
1	A	328	ARG	5.2
1	B	724	HIS	5.0
1	A	207	CYS	4.5
1	A	178	ARG	4.5
1	B	138	GLU	4.5
1	A	724	HIS	4.4
1	C	194	PHE	4.4
1	A	609	GLN	4.2
1	B	460	LEU	4.2
1	B	609	GLN	4.1
1	A	330	LEU	4.1
1	A	612	LEU	3.9
1	C	337	THR	3.9
1	C	325	PHE	3.8
1	A	438	GLN	3.5
1	C	109	THR	3.5
1	C	326	TYR	3.5
1	A	415	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	430	ASN	3.4
1	C	138	GLU	3.4
1	C	591	SER	3.4
1	C	339	PRO	3.4
1	A	305	GLU	3.3
1	B	330	LEU	3.2
1	A	239	ALA	3.0
1	A	304	ARG	3.0
1	C	609	GLN	3.0
1	A	170	VAL	3.0
1	A	430	ASN	3.0
1	C	178	ARG	3.0
1	C	722	VAL	2.9
1	C	338	ALA	2.9
1	B	177	HIS	2.8
1	C	633	CYS	2.8
1	B	429	TYR	2.8
1	A	228	HIS	2.7
1	B	258	ARG	2.7
1	C	430	ASN	2.6
1	C	185	ILE	2.6
1	B	574	VAL	2.6
1	A	177	HIS	2.6
1	A	233	GLU	2.5
1	B	337	THR	2.5
1	C	186	PHE	2.5
1	A	185	ILE	2.5
1	C	239	ALA	2.5
1	A	230	THR	2.5
1	A	203	ALA	2.4
1	C	244	SER	2.4
1	B	186	PHE	2.4
1	B	491	SER	2.4
1	C	203	ALA	2.3
1	B	458	ASN	2.3
1	B	179	TYR	2.3
1	B	329	ASP	2.3
1	A	195	GLU	2.3
1	B	328	ARG	2.3
1	B	633	CYS	2.3
1	A	262	PHE	2.2
1	B	607	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	303	TYR	2.2
1	C	317	ASP	2.2
1	B	207	CYS	2.2
1	A	338	ALA	2.2
1	A	111	ALA	2.1
1	A	122	ALA	2.1
1	C	304	ARG	2.1
1	A	582	ILE	2.1
1	B	228	HIS	2.1
1	A	169	THR	2.0
1	B	109	THR	2.0
1	A	138	GLU	2.0
1	C	111	ALA	2.0
1	C	360	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	B	732	1/1	0.78	0.21	7.04	52,52,52,52	0
2	NA	B	731	1/1	0.96	0.14	0.38	50,50,50,50	0
2	NA	A	731	1/1	0.98	0.06	-2.83	42,42,42,42	0
2	NA	C	731	1/1	0.96	0.07	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.