



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 06:03 AM EDT

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

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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

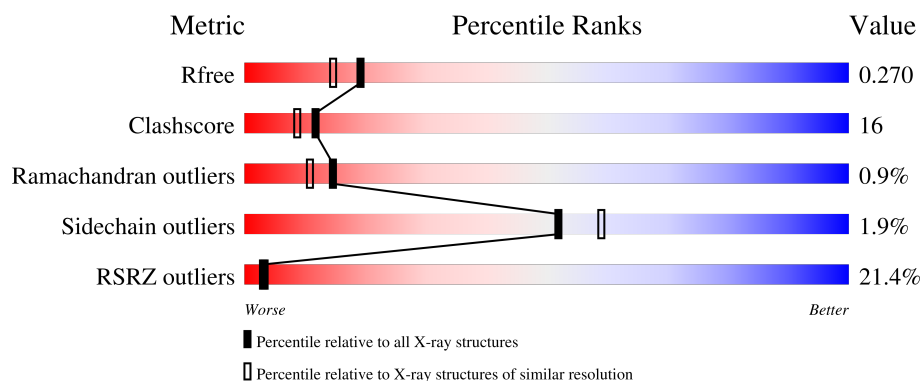
1 Overall quality at a glance

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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>28%</div> <div>60%</div> <div>31%</div> <div>8%</div> </div>
1	B	628	<div> <div>14%</div> <div>67%</div> <div>25%</div> <div>7%</div> </div>
1	C	628	<div> <div>18%</div> <div>67%</div> <div>23%</div> <div>8%</div> </div>

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	A	1	Total	Na	0	0
			1	1		
2	B	2	Total	Na	0	0
			2	2		
2	C	1	Total	Na	0	0
			1	1		

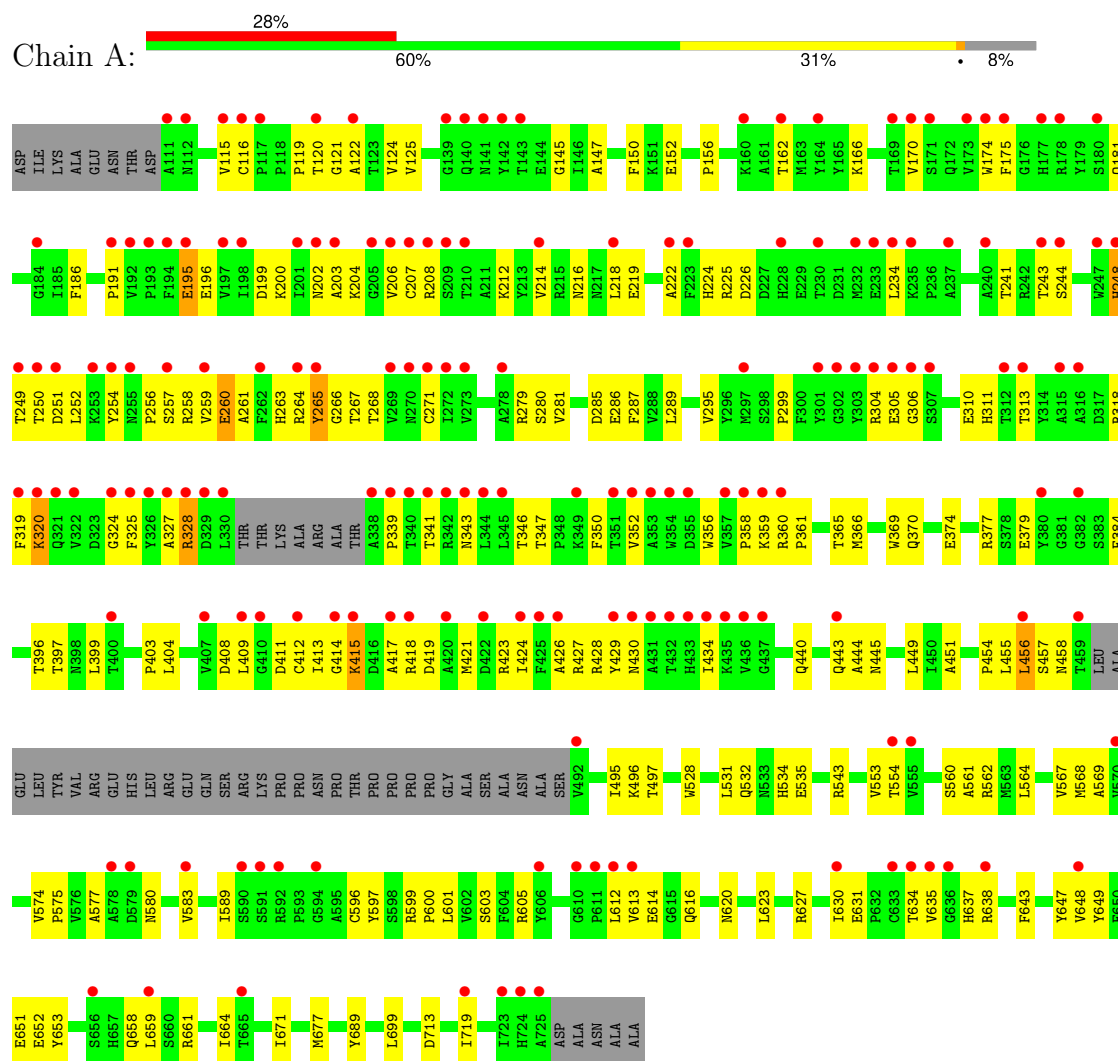
- Molecule 3 is water.

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, 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: Glycoprotein B



• Molecule 1: Glycoprotein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.96Å 100.04Å 100.13Å 67.04° 77.99° 70.31°	Depositor
Resolution (Å)	41.20 – 2.10 41.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.7 (41.20-2.10) 87.7 (41.20-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	7446 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14223	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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:A:202:ASN:OD1	1:A:328:ARG:HD2	1.89	0.72
1:C:543:ARG:HB2	1:C:568:MET:HE1	1.72	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:HD3	1:A:328:ARG:N	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:434:ILE:HD12	1:B:434:ILE:N	2.11	0.65
1:B:719:ILE:HG22	1:C:318:ARG:NH2	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:HA	1:A:443:GLN:NE2	2.12	0.64
1:B:224:HIS:HB2	1:B:269:VAL:HB	1.79	0.64
1:B:634:THR:HG22	1:B:635:VAL:N	2.12	0.64
1:B:630:ILE:HG22	1:B:631:GLU:N	2.13	0.64
1:A:328:ARG:HD3	1:A:328:ARG:H	1.62	0.63
1:B:109:THR:HG22	1:B:110:ASP:N	2.13	0.63
1:A:443:GLN:HA	1:A:443:GLN:HE21	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:256:PRO:HG3	1:C:265:TYR:C	2.20	0.62
1:C:434:ILE:N	1:C:434:ILE:HD12	2.14	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:119:PRO:HD2	1:C:562:ARG:HD3	1.81	0.61
1:C:637:HIS:CD2	1:C:653:TYR:H	2.19	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:170:VAL:HG12	1:B:186:PHE:HD2	1.66	0.60
1:B:714:LEU:HD23	1:B:719:ILE:HD12	1.83	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:HE21	1:C:584:GLN:HA	1.66	0.59
1:A:195:GLU:OE1	1:A:196:GLU:N	2.36	0.59
1:A:634:THR:HG22	1:A:635:VAL:N	2.16	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:HG13	1:B:170:VAL:O	2.03	0.59
1:B:250:THR:HG22	1:B:251:ASP:N	2.17	0.59
1:A:319:PHE:O	1:A:320:LYS:HE3	2.03	0.59
1:C:492:VAL:HG12	1:C:493:GLU:N	2.17	0.59
1:A:404:LEU:HD11	1:A:413:ILE:HG21	1.85	0.58
1:B:241:THR:O	1:B:243:THR:HG23	2.03	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: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:N	1:C:659:LEU:HD23	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:A:204:LYS:HB2	1:A:206:VAL:HG22	1.86	0.57
1:B:549:ALA:O	1:B:553:VAL:HG23	2.05	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:A:554:THR:HG22	1:C:667:VAL:HB	1.87	0.56
1:C:218:LEU:HD22	1:C:219:GLU:H	1.70	0.56
1:C:664:ILE:N	1:C:664:ILE:HD12	2.21	0.56
1:B:380:TYR:O	1:B:385:ARG:NH1	2.39	0.56
1:C:166:LYS:HE2	1:C:207:CYS:SG	2.45	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:241:THR:O	1:C:243:THR:HG23	2.06	0.56
1:C:360:ARG:CD	1:C:411:ASP:OD2	2.53	0.56
1:A:531:LEU:O	1:A:535:GLU:HG2	2.05	0.55
1:C:218:LEU:HD22	1:C:219:GLU:N	2.21	0.55
1:A:601:LEU:HD23	1:A:616:GLN:HB3	1.88	0.55
1:C:599:ARG:NH1	1:C:617:LEU:O	2.39	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:N	1:A:434:ILE:HD12	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:A:346:THR:HG23	1:A:346:THR:O	2.07	0.54
1:C:175:PHE:HB3	1:C:258:ARG:NH1	2.22	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:A:225:ARG:HD2	1:A:254:TYR:HB2	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: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:A:423:ARG:HH11	1:A:423:ARG:HB2	1.73	0.53
1:C:325:PHE:CD2	1:C:342:ARG:HB2	2.44	0.53
1:C:577:ALA:HB3	1:C:580:ASN:ND2	2.23	0.53
1:A:120:THR:C	1:A:122:ALA:H	2.12	0.52
1:A:222:ALA:HB1	1:A:267:THR:HG21	1.89	0.52
1:B:434:ILE:HD11	1:B:458:ASN:OD1	2.08	0.52
1:A:318:ARG:O	1:A:346:THR:HG22	2.09	0.52
1:A:597:TYR:CE1	1:A:601:LEU:HD11	2.44	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:A:659:LEU:HD12	1:A:659:LEU:N	2.25	0.52
1:C:671:ILE:HD12	1:C:671:ILE:N	2.24	0.52
1:C:515:ARG:NH2	3:C:790:HOH:O	2.40	0.52
1:B:166:LYS:HG2	1:B:271:CYS:HA	1.91	0.52
1:B:630:ILE:CG2	1:B:631:GLU:N	2.72	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:H	1:A:328:ARG:CD	2.22	0.51
1:B:200:LYS:NZ	1:B:208:ARG:NH1	2.59	0.51
1:B:637:HIS:O	1:B:651:GLU:HA	2.10	0.51
1:C:413:ILE:HD13	1:C:449:LEU:CD2	2.39	0.51
1:C:656:SER:OG	1:C:657:HIS:HD2	1.92	0.51
1:A:671:ILE:HD12	1:A:671:ILE:N	2.25	0.51
1:A:648:VAL:HG13	1:A:648:VAL:O	2.11	0.51
1:A:719:ILE:HG22	1:B:318:ARG:NH2	2.25	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:A:374:GLU:HG2	1:A:429:TYR:OH	2.12	0.50
1:B:250:THR:HG22	1:B:252:LEU:H	1.77	0.50
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.77	0.50
1:A:366:MET:CE	1:A:495:ILE:HB	2.42	0.50
1:B:194:PHE:HZ	1:B:318:ARG:O	1.95	0.50
1:A:583:VAL:HG23	1:A:643:PHE:CZ	2.47	0.49
1:A:170:VAL:HG13	1:A:170:VAL:O	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:HG13	1:C:648:VAL:O	2.12	0.49
1:A:267:THR:HG22	1:A:268:THR:N	2.26	0.49
1:A:397:THR:HG22	1:A:444:ALA:CA	2.41	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: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:C:634:THR:CG2	1:C:635:VAL:N	2.75	0.49
1:B:648:VAL:HG13	1:B:648:VAL:O	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:319:PHE:O	1:C:320:LYS:HE3	2.13	0.48
1:C:492:VAL:HG12	1:C:493:GLU:H	1.76	0.48
1:A:671:ILE:HD11	1:C:534:HIS:CG	2.48	0.48
1:B:677:MET:CE	1:C:518:ASN:HB3	2.44	0.48
1:C:170:VAL:HG13	1:C:170:VAL:O	2.14	0.48
1:A:214:VAL:HG13	1:A:214:VAL:O	2.14	0.48
1:A:265:TYR:CD1	1:A:265:TYR:N	2.81	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:311:HIS:HE2	1:A:313:THR:HG1	1.61	0.47
1:A:358:PRO:HG2	1:A:361:PRO:HG2	1.96	0.47
1:A:601:LEU:HD22	1:A:627:ARG:HD3	1.96	0.47
1:A:310:GLU:OE2	1:A:359:LYS:HD2	2.15	0.47
1:C:634:THR:CG2	1:C:635:VAL:H	2.22	0.47
1:A:124:VAL:O	1:C:665:THR:CG2	2.62	0.47
1:C:434:ILE:HD12	1:C:456:LEU:O	2.15	0.47
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.96	0.47
1:A:638:ARG:NH1	1:B:121:GLY:HA3	2.26	0.47
1:A:661:ARG:NH1	1:B:129:GLN:HG2	2.29	0.47
1:C:310:GLU:OE2	1:C:359:LYS:HD2	2.15	0.47
1:C:313:THR:HG22	1:C:313:THR:O	2.15	0.47
1:A:396:THR:HB	1:A:445:ASN:HD22	1.80	0.47
1:B:248:HIS:HA	1:B:271:CYS:O	2.14	0.47
1:B:630:ILE:CG2	1:B:631:GLU:H	2.28	0.47
1:C:588:ARG:HG2	1:C:588:ARG:HH11	1.79	0.47
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.97	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:C:406:ARG:O	1:C:406:ARG:HG2	2.14	0.47
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.80	0.47
1:C:501:ILE:HG13	1:C:501:ILE:O	2.14	0.47
1:C:580:ASN:O	1:C:604:PHE:HA	2.15	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:A:677:MET:CE	1:B:518:ASN:HB3	2.46	0.46
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.97	0.46
1:A:124:VAL:O	1:C:665:THR:HG22	2.15	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:B:119:PRO:HG3	1:B:560:SER:HB3	1.98	0.46
1:B:433:HIS:C	1:B:434:ILE:HD12	2.36	0.46
1:C:366:MET:HG3	1:C:413:ILE:HD11	1.97	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: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:328:ARG:N	1:A:328:ARG:CD	2.78	0.46
1:A:411:ASP:O	1:A:415:LYS:HG3	2.16	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:A:369:TRP:CD2	1:A:370:GLN:HG2	2.52	0.45
1:B:393:THR:HG23	1:B:504:ALA:HB1	1.97	0.45
1:A:647:TYR:CE1	1:A:664:ILE:HD12	2.52	0.45
1:B:359:LYS:O	1:B:363:VAL:HG22	2.16	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: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:B:366:MET:HG3	1:B:413:ILE:HD11	1.97	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:HG2	1:C:208:ARG:HH11	1.81	0.45
1:C:311:HIS:CG	1:C:312:THR:N	2.84	0.45
1:A:224:HIS:C	1:A:226:ASP:H	2.19	0.45
1:A:535:GLU:HB2	3:A:732:HOH:O	2.17	0.45
1:A:649:TYR:CE2	1:A:651:GLU:HG3	2.51	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: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:B:313:THR:HG22	1:B:313:THR:O	2.16	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:A:119:PRO:HD2	1:A:562:ARG:HD3	1.99	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:B:166:LYS:NZ	1:B:210:THR:O	2.46	0.45
1:C:166:LYS:HG2	1:C:271:CYS:HA	1.98	0.45
1:C:257:SER:OG	1:C:264:ARG:NH1	2.47	0.45
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: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: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:120:THR:C	1:B:122:ALA:N	2.70	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: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: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:A:417:ALA:O	1:A:421:MET:HG3	2.17	0.44
1:B:121:GLY:O	1:B:122:ALA:C	2.56	0.44
1:C:145:GLY:HA3	1:C:452:TYR:CZ	2.53	0.44
1:C:197:VAL:HA	1:C:201:ILE:HD12	2.00	0.44
1:A:256:PRO:HD3	1:A:266:GLY:HA3	2.00	0.44
1:A:150:PHE:HB2	1:A:449:LEU:HB3	1.99	0.44
1:B:109:THR:CG2	1:B:110:ASP:N	2.81	0.44
1:A:170:VAL:CG1	1:A:186:PHE:HD2	2.31	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:GLU:HG3	1:C:399:LEU:HD21	1.99	0.43
1:C:656:SER:OG	1:C:657:HIS:CD2	2.70	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:A:260:GLU:O	1:A:261:ALA:HB3	2.19	0.43
1:A:543:ARG:HB2	1:A:568:MET:CE	2.48	0.43
1:C:192:VAL:HG11	1:C:201:ILE:HD11	2.00	0.43
1:A:325:PHE:CE2	1:A:327:ALA:HA	2.53	0.43
1:A:434:ILE:HD12	1:A:456:LEU:O	2.18	0.43
1:B:170:VAL:HG12	1:B:186:PHE:CD2	2.51	0.43
1:C:607:GLU:HA	1:C:607:GLU:OE2	2.18	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:B:592:ARG:HG3	1:B:595:ALA:CB	2.44	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: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: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:A:256:PRO:HG3	1:A:265:TYR:C	2.39	0.43
1:B:116:CYS:HB3	1:B:560:SER:HB2	2.01	0.43
1:B:454:PRO:O	1:B:455:LEU:HD23	2.17	0.43
1:C:120:THR:C	1:C:122:ALA:N	2.72	0.43
1:A:313:THR:O	1:A:313:THR:HG22	2.19	0.43
1:A:254:TYR:HB3	1:A:267:THR:O	2.19	0.42
1:C:543:ARG:HG3	1:C:544:LYS:N	2.34	0.42
1:B:302:GLY:N	1:B:307:SER:HB3	2.35	0.42
1:B:326:TYR:OH	1:B:339:PRO:HG3	2.18	0.42
1:B:580:ASN:O	1:B:604:PHE:HA	2.19	0.42
1:C:630:ILE:CG2	1:C:631:GLU:N	2.81	0.42
1:A:534:HIS:CD2	1:B:671:ILE:HD11	2.54	0.42
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.90	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:175:PHE:CE2	1:A:258:ARG:HA	2.55	0.42
1:A:414:GLY:O	1:A:418:ARG:HG3	2.19	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:A:599:ARG:HA	1:A:600:PRO:HD3	1.89	0.42
1:B:564:LEU:CD1	1:B:569:ALA:HB2	2.50	0.42
1:B:624:ARG:NH2	1:B:628:ASP:OD2	2.42	0.42
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.18	0.42
1:A:147:ALA:HA	1:A:451:ALA:O	2.20	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:634:THR:HG22	1:A:635:VAL:H	1.81	0.42
1:A:658:GLN:C	1:A:659:LEU:HD12	2.40	0.42
1:B:175:PHE:CE2	1:B:258:ARG:HA	2.55	0.42
1:A:603:SER:HA	1:A:613:VAL:O	2.20	0.42
1:C:120:THR:O	1:C:122:ALA:N	2.53	0.42
1:A:677:MET:HE1	1:B:518:ASN:HB3	2.00	0.42
1:B:637:HIS:HB3	1:B:652:GLU:HA	2.01	0.42
1:A:216:ASN:OD1	1:B:253:LYS:HG3	2.20	0.41
1:A:377:ARG:NH2	1:A:440:GLN:OE1	2.53	0.41
1:A:360:ARG:NH1	1:A:409:LEU:HD23	2.35	0.41
1:C:152:GLU:HA	1:C:366:MET:HE1	2.00	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: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:224:HIS:CD2	1:C:225:ARG:HG3	2.55	0.41
1:C:432:THR:HB	1:C:433:HIS:HD2	1.85	0.41
1:C:612:LEU:HD12	1:C:612:LEU:HA	1.95	0.41
1:C:671:ILE:N	1:C:671:ILE:CD1	2.82	0.41
1:A:234:LEU:HD23	1:A:249:THR:HG23	2.02	0.41
1:A:224:HIS:CD2	1:A:225:ARG:HG2	2.55	0.41
1:A:454:PRO:O	1:A:455:LEU:HD23	2.20	0.41
1:B:723:ILE:O	1:B:724:HIS:CB	2.65	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:C:591:SER:O	1:C:592:ARG:CB	2.62	0.41
1:A:174:TRP:HB2	1:A:263:HIS:CE1	2.56	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:432:THR:HG22	1:B:432:THR:O	2.21	0.41
1:B:655:TYR:C	1:B:655:TYR:CD2	2.93	0.41
1:C:649:TYR:O	1:C:656:SER:HB3	2.20	0.41
1:A:456:LEU:HD12	1:A:457:SER:N	2.36	0.41
1:B:237:ALA:HB1	1:C:715:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:THR:HG23	1:B:271:CYS:HB3	2.03	0.41
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: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:543:ARG:HB2	1:C:568:MET:HE3	2.02	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:HD12	1:B:612:LEU:HA	1.89	0.40
1:A:564:LEU:HD12	1:A:569:ALA:HB2	2.03	0.40
1:B:458:ASN:O	1:B:460:LEU:N	2.54	0.40
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.56	0.40
1:A:543:ARG:HD2	1:A:568:MET:CE	2.51	0.40
1:A:589:ILE:HG12	1:A:597:TYR:CE1	2.56	0.40
1:B:181:GLN:HE21	1:B:181:GLN:HB3	1.62	0.40
1:B:424:ILE:HG12	1:B:427:ARG:NH2	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
1:C:635:VAL:HG12	1:C:636:GLY:N	2.37	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%)	12	8
1	B	575/628 (92%)	538 (94%)	32 (6%)	5 (1%)	14	11
1	C	569/628 (91%)	533 (94%)	32 (6%)	4 (1%)	19	16
All	All	1714/1884 (91%)	1602 (94%)	97 (6%)	15 (1%)	14	11

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%)	58	65
1	B	507/543 (93%)	499 (98%)	8 (2%)	58	65
1	C	502/543 (92%)	490 (98%)	12 (2%)	44	49
All	All	1511/1629 (93%)	1483 (98%)	28 (2%)	52	59

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

Sometimes 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th 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 ²)	Q<0.9
1	A	576/628 (91%)	1.42	173 (30%) 1 1	24, 62, 87, 113	0
1	B	581/628 (92%)	0.86	86 (14%) 7 7	22, 50, 82, 109	0
1	C	575/628 (91%)	1.10	112 (19%) 4 4	21, 56, 82, 95	0
All	All	1732/1884 (91%)	1.13	371 (21%) 3 3	21, 56, 85, 113	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	CYS	8.7
1	B	330	LEU	6.7
1	A	330	LEU	6.5
1	B	460	LEU	5.7
1	A	234	LEU	5.4
1	A	725	ALA	5.1
1	B	174	TRP	5.0
1	C	194	PHE	4.9
1	A	322	VAL	4.8
1	B	111	ALA	4.7
1	C	327	ALA	4.7
1	A	303	TYR	4.7
1	B	361	PRO	4.6
1	A	232	MET	4.6
1	B	173	VAL	4.5
1	A	192	VAL	4.5
1	A	230	THR	4.5
1	A	328	ARG	4.5
1	A	116	CYS	4.4
1	B	724	HIS	4.4
1	C	303	TYR	4.4
1	A	160	LYS	4.4
1	B	461	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	344	LEU	4.3
1	B	491	SER	4.3
1	C	244	SER	4.3
1	C	322	VAL	4.3
1	A	249	THR	4.3
1	A	247	TRP	4.2
1	B	138	GLU	4.2
1	A	326	TYR	4.2
1	C	360	ARG	4.2
1	A	206	VAL	4.2
1	A	724	HIS	4.2
1	B	429	TYR	4.2
1	C	300	PHE	4.1
1	C	722	VAL	4.1
1	A	194	PHE	4.0
1	B	177	HIS	4.0
1	A	319	PHE	4.0
1	B	633	CYS	4.0
1	C	443	GLN	4.0
1	A	164	TYR	3.9
1	B	360	ARG	3.9
1	A	316	ALA	3.9
1	B	431	ALA	3.9
1	A	415	LYS	3.9
1	B	207	CYS	3.9
1	B	723	ILE	3.8
1	B	337	THR	3.8
1	C	717	ALA	3.8
1	C	723	ILE	3.8
1	A	343	ASN	3.7
1	A	170	VAL	3.7
1	A	250	THR	3.7
1	A	265	TYR	3.7
1	A	139	GLY	3.7
1	A	218	LEU	3.6
1	C	109	THR	3.6
1	A	254	TYR	3.6
1	A	162	THR	3.6
1	C	359	LYS	3.6
1	C	633	CYS	3.6
1	A	203	ALA	3.6
1	A	578	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	380	TYR	3.5
1	C	410	GLY	3.5
1	A	611	PRO	3.5
1	A	329	ASP	3.5
1	A	169	THR	3.4
1	A	459	THR	3.4
1	B	634	THR	3.4
1	C	341	THR	3.4
1	A	723	ILE	3.4
1	C	174	TRP	3.4
1	A	353	ALA	3.4
1	B	139	GLY	3.4
1	C	492	VAL	3.3
1	B	430	ASN	3.3
1	A	590	SER	3.3
1	A	431	ALA	3.3
1	C	419	ASP	3.3
1	C	380	TYR	3.3
1	C	635	VAL	3.3
1	A	235	LYS	3.3
1	C	412	CYS	3.3
1	A	228	HIS	3.3
1	A	262	PHE	3.2
1	B	611	PRO	3.2
1	A	178	ARG	3.2
1	A	357	VAL	3.2
1	C	314	TYR	3.2
1	C	302	GLY	3.2
1	A	342	ARG	3.2
1	A	248	HIS	3.2
1	A	613	VAL	3.2
1	C	361	PRO	3.2
1	C	409	LEU	3.2
1	A	271	CYS	3.2
1	A	420	ALA	3.2
1	A	426	ALA	3.2
1	A	341	THR	3.1
1	B	492	VAL	3.1
1	B	434	ILE	3.1
1	A	173	VAL	3.1
1	C	363	VAL	3.1
1	C	319	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	179	TYR	3.1
1	C	207	CYS	3.1
1	A	659	LEU	3.1
1	B	109	THR	3.1
1	A	425	PHE	3.0
1	A	205	GLY	3.0
1	C	228	HIS	3.0
1	C	234	LEU	3.0
1	A	174	TRP	3.0
1	A	142	TYR	3.0
1	A	429	TYR	3.0
1	A	251	ASP	3.0
1	C	317	ASP	3.0
1	A	320	LYS	3.0
1	A	634	THR	3.0
1	A	273	VAL	3.0
1	A	338	ALA	3.0
1	B	589	ILE	3.0
1	C	301	TYR	3.0
1	B	428	ARG	3.0
1	A	209	SER	3.0
1	C	192	VAL	3.0
1	A	327	ALA	3.0
1	C	589	ILE	3.0
1	A	436	VAL	3.0
1	A	633	CYS	2.9
1	A	141	ASN	2.9
1	A	339	PRO	2.9
1	A	492	VAL	2.9
1	A	272	ILE	2.9
1	B	180	SER	2.9
1	A	255	ASN	2.9
1	C	597	TYR	2.9
1	A	360	ARG	2.9
1	B	304	ARG	2.9
1	A	325	PHE	2.9
1	C	491	SER	2.9
1	A	410	GLY	2.9
1	C	320	LYS	2.9
1	A	214	VAL	2.8
1	A	304	ARG	2.8
1	A	430	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	352	VAL	2.8
1	A	120	THR	2.8
1	B	210	THR	2.8
1	A	301	TYR	2.8
1	A	358	PRO	2.8
1	A	177	HIS	2.8
1	C	659	LEU	2.8
1	A	208	ARG	2.8
1	A	638	ARG	2.8
1	B	691	ARG	2.8
1	B	303	TYR	2.8
1	A	612	LEU	2.8
1	C	714	LEU	2.8
1	B	555	VAL	2.8
1	C	338	ALA	2.7
1	A	313	THR	2.7
1	C	358	PRO	2.7
1	A	195	GLU	2.7
1	C	112	ASN	2.7
1	A	278	ALA	2.7
1	C	211	ALA	2.7
1	B	178	ARG	2.7
1	C	593	PRO	2.7
1	A	555	VAL	2.7
1	B	194	PHE	2.7
1	A	340	THR	2.7
1	A	307	SER	2.7
1	C	111	ALA	2.7
1	C	420	ALA	2.7
1	A	418	ARG	2.7
1	B	412	CYS	2.6
1	B	380	TYR	2.6
1	C	326	TYR	2.6
1	A	111	ALA	2.6
1	A	210	THR	2.6
1	B	175	PHE	2.6
1	C	634	THR	2.6
1	C	719	ILE	2.6
1	C	430	ASN	2.6
1	A	412	CYS	2.6
1	B	716	PHE	2.6
1	A	201	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	2.6
1	A	180	SER	2.6
1	C	139	GLY	2.6
1	A	269	VAL	2.6
1	C	284	TYR	2.6
1	B	415	LYS	2.6
1	C	415	LYS	2.6
1	A	351	THR	2.6
1	A	297	MET	2.6
1	A	140	GLN	2.6
1	C	609	GLN	2.6
1	C	307	SER	2.6
1	B	305	GLU	2.6
1	A	122	ALA	2.5
1	A	315	ALA	2.5
1	B	253	LYS	2.5
1	A	355	ASP	2.5
1	A	635	VAL	2.5
1	C	357	VAL	2.5
1	B	432	THR	2.5
1	B	425	PHE	2.5
1	B	612	LEU	2.5
1	C	121	GLY	2.5
1	B	635	VAL	2.5
1	C	655	TYR	2.5
1	C	195	GLU	2.5
1	C	308	HIS	2.5
1	A	345	LEU	2.5
1	A	414	GLY	2.5
1	B	456	LEU	2.5
1	A	222	ALA	2.5
1	B	120	THR	2.5
1	B	112	ASN	2.5
1	A	257	SER	2.5
1	B	228	HIS	2.5
1	A	253	LYS	2.5
1	C	160	LYS	2.5
1	A	443	GLN	2.5
1	A	197	VAL	2.5
1	C	221	THR	2.5
1	A	202	ASN	2.5
1	A	305	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	606	TYR	2.4
1	C	142	TYR	2.4
1	C	311	HIS	2.4
1	B	252	LEU	2.4
1	B	609	GLN	2.4
1	B	717	ALA	2.4
1	A	400	THR	2.4
1	C	313	THR	2.4
1	C	235	LYS	2.4
1	A	198	ILE	2.4
1	A	324	GLY	2.4
1	C	178	ARG	2.4
1	C	304	ARG	2.4
1	C	203	ALA	2.4
1	A	312	THR	2.4
1	C	340	THR	2.4
1	A	115	VAL	2.4
1	A	259	VAL	2.4
1	C	170	VAL	2.4
1	A	191	PRO	2.4
1	C	339	PRO	2.4
1	A	175	PHE	2.4
1	A	719	ILE	2.4
1	B	329	ASP	2.4
1	A	233	GLU	2.4
1	A	143	THR	2.4
1	B	574	VAL	2.4
1	C	648	VAL	2.4
1	A	193	PRO	2.4
1	B	257	SER	2.4
1	B	306	GLY	2.4
1	B	719	ILE	2.4
1	C	201	ILE	2.4
1	C	305	GLU	2.3
1	B	714	LEU	2.3
1	A	349	LYS	2.3
1	C	250	THR	2.3
1	C	214	VAL	2.3
1	B	443	GLN	2.3
1	A	302	GLY	2.3
1	C	411	ASP	2.3
1	A	424	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	202	ASN	2.3
1	C	120	THR	2.3
1	C	259	VAL	2.3
1	C	581	VAL	2.3
1	B	203	ALA	2.3
1	B	211	ALA	2.3
1	B	250	THR	2.3
1	C	232	MET	2.3
1	A	656	SER	2.3
1	A	648	VAL	2.3
1	A	579	ASP	2.3
1	B	317	ASP	2.3
1	B	695	LYS	2.3
1	B	258	ARG	2.3
1	C	638	ARG	2.3
1	A	237	ALA	2.3
1	A	417	ALA	2.3
1	C	239	ALA	2.3
1	C	261	ALA	2.3
1	C	309	THR	2.3
1	C	432	THR	2.3
1	A	171	SER	2.3
1	B	170	VAL	2.2
1	A	184	GLY	2.2
1	A	223	PHE	2.2
1	A	456	LEU	2.2
1	B	254	TYR	2.2
1	A	243	THR	2.2
1	C	721	THR	2.2
1	C	324	GLY	2.2
1	B	363	VAL	2.2
1	A	264	ARG	2.2
1	A	270	ASN	2.2
1	A	409	LEU	2.2
1	B	122	ALA	2.2
1	B	271	CYS	2.2
1	C	596	CYS	2.2
1	A	592	ARG	2.2
1	C	325	PHE	2.2
1	C	425	PHE	2.2
1	A	554	THR	2.2
1	C	459	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	307	SER	2.2
1	A	359	LYS	2.2
1	C	579	ASP	2.2
1	C	701	ASP	2.2
1	B	136	ARG	2.2
1	A	433	HIS	2.2
1	C	138	GLU	2.1
1	C	612	LEU	2.1
1	B	459	THR	2.1
1	A	354	TRP	2.1
1	A	240	ALA	2.1
1	C	577	ALA	2.1
1	A	321	GLN	2.1
1	B	116	CYS	2.1
1	C	271	CYS	2.1
1	B	614	GLU	2.1
1	A	422	ASP	2.1
1	A	432	THR	2.1
1	A	591	SER	2.1
1	B	244	SER	2.1
1	B	626	THR	2.1
1	C	639	ARG	2.1
1	C	356	TRP	2.1
1	A	594	GLY	2.1
1	A	583	VAL	2.1
1	A	434	ILE	2.1
1	B	419	ASP	2.1
1	C	345	LEU	2.1
1	C	434	ILE	2.1
1	C	643	PHE	2.1
1	A	306	GLY	2.1
1	A	382	GLY	2.1
1	A	610	GLY	2.1
1	A	636	GLY	2.1
1	C	193	PRO	2.1
1	B	326	TYR	2.1
1	A	570	VAL	2.1
1	B	259	VAL	2.1
1	B	638	ARG	2.1
1	C	418	ARG	2.1
1	A	665	THR	2.1
1	A	117	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	535	GLU	2.0
1	A	606	TYR	2.0
1	A	435	LYS	2.0
1	A	244	SER	2.0
1	C	626	THR	2.0
1	A	630	ILE	2.0
1	C	198	ILE	2.0
1	A	437	GLY	2.0
1	C	607	GLU	2.0
1	C	406	ARG	2.0
1	A	407	VAL	2.0
1	B	124	VAL	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
2	NA	B	732	1/1	0.78	0.23	52,52,52,52	0
2	NA	B	731	1/1	0.95	0.08	50,50,50,50	0
2	NA	C	731	1/1	0.95	0.10	44,44,44,44	0
2	NA	A	731	1/1	0.97	0.08	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.