



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 2GUM / pdb_00002gum
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 : 4-5-2 with Phenix2.0
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

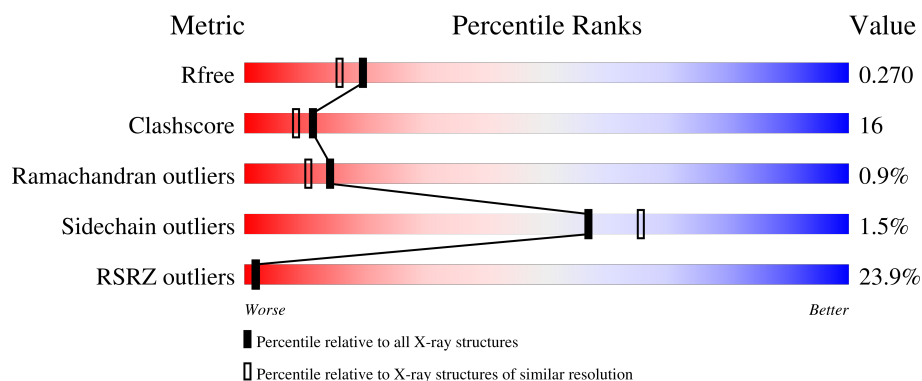
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	30% 58% 32% 8%
1	B	628	16% 65% 27% 7%
1	C	628	20% 65% 25% 8%

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.

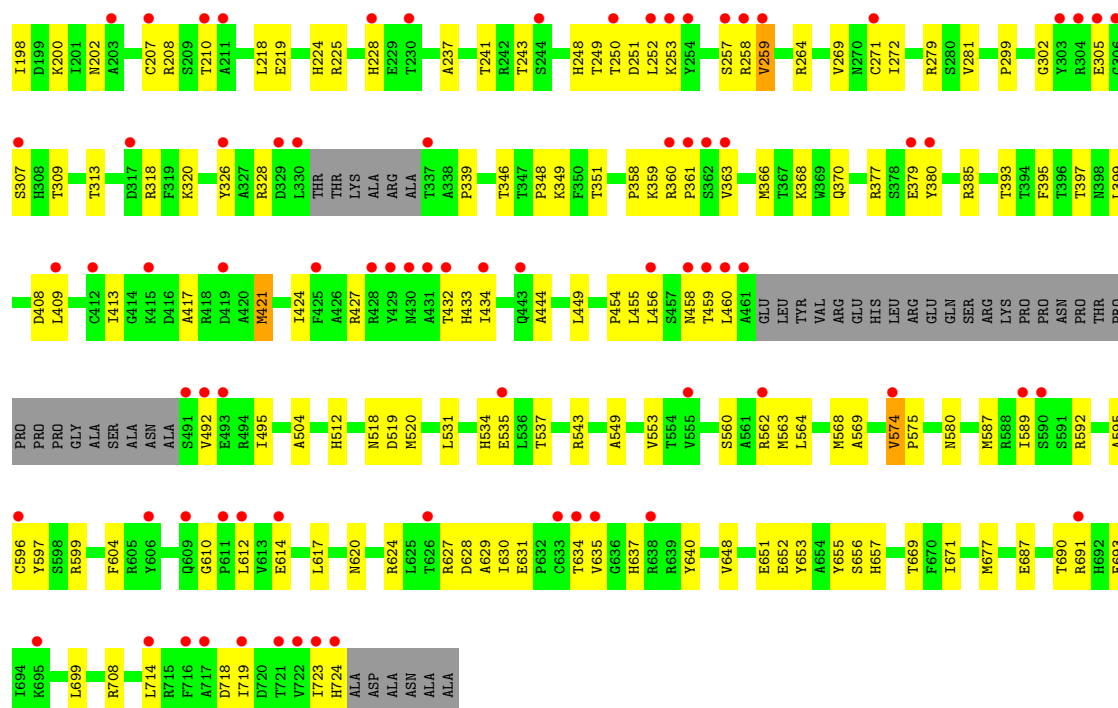
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4658	2941	819	876	22			
1	B	581	Total	C	N	O	S	0	0	0
			4694	2962	824	886	22			
1	C	575	Total	C	N	O	S	0	0	0
			4644	2931	813	878	22			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

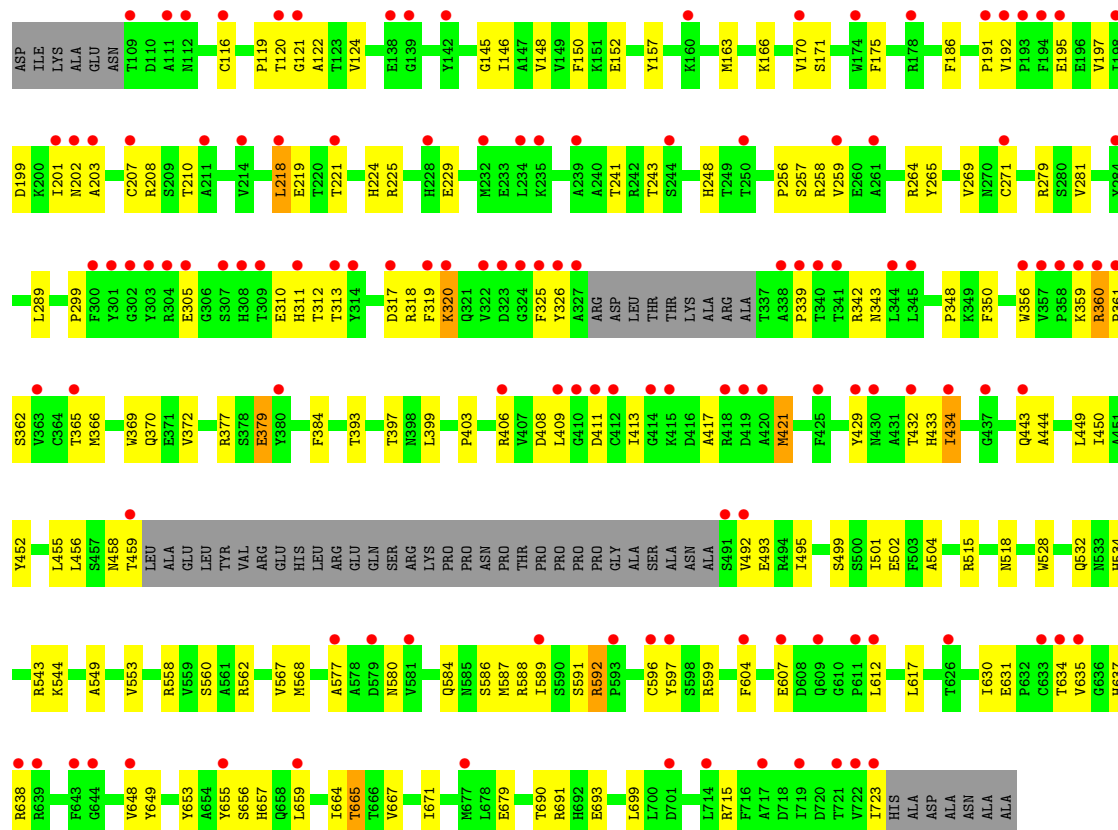
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	2	Total	Na	0	0
			2	2		
2	C	1	Total	Na	0	0
			1	1		

- 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		



• 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	8216 reflections (4.99%)	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 [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/4775	0.93	14/6488 (0.2%)
1	B	0.47	1/4811 (0.0%)	0.95	14/6538 (0.2%)
1	C	0.44	0/4760	0.91	6/6469 (0.1%)
All	All	0.45	1/14346 (0.0%)	0.93	34/19495 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	PRO	N-CD	5.07	1.54	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	B	370	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	B	172	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	B	610	GLY	CA-C-N	7.29	127.25	120.03
1	B	610	GLY	C-N-CA	7.29	127.25	120.03
1	B	370	GLN	CG-CD-NE2	6.78	126.58	116.40
1	A	599	ARG	CA-C-N	6.60	126.64	119.90
1	A	599	ARG	C-N-CA	6.60	126.64	119.90
1	A	584	GLN	CG-CD-NE2	6.46	126.10	116.40
1	B	172	GLN	CG-CD-NE2	6.41	126.02	116.40
1	C	450	ILE	N-CA-C	6.25	116.87	107.80
1	C	362	SER	N-CA-C	6.15	117.66	111.07
1	A	506	LEU	N-CA-C	-6.11	104.63	111.28
1	A	592	ARG	CA-C-N	6.08	126.40	119.83
1	A	592	ARG	C-N-CA	6.08	126.40	119.83
1	A	199	ASP	N-CA-C	6.00	117.89	111.36
1	A	372	VAL	N-CA-C	5.68	116.31	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	PRO	N-CA-C	-5.58	107.17	114.03
1	B	574	VAL	CA-C-N	5.57	125.48	119.85
1	B	574	VAL	C-N-CA	5.57	125.48	119.85
1	B	360	ARG	N-CA-C	5.50	120.98	113.16
1	C	586	SER	N-CA-C	5.37	118.56	109.76
1	C	372	VAL	N-CA-C	5.31	115.23	107.37
1	A	502	GLU	N-CA-C	5.31	117.75	111.33
1	B	669	THR	N-CA-C	-5.25	106.55	113.17
1	B	183	MET	N-CA-C	-5.24	106.73	113.23
1	C	299	PRO	N-CA-C	-5.15	107.33	113.98
1	A	574	VAL	N-CA-C	5.13	114.11	108.05
1	A	183	MET	N-CA-C	-5.06	107.50	113.97
1	A	322	VAL	N-CA-C	5.04	114.01	106.85
1	B	272	ILE	N-CA-C	5.02	115.14	108.11
1	C	502	GLU	N-CA-C	5.02	117.41	111.33
1	A	328	ARG	N-CA-C	-5.02	104.06	110.53
1	B	198	ILE	N-CA-C	5.01	115.24	110.53

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	186	0
1	B	4694	0	4501	160	0
1	C	4644	0	4450	138	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	444	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 (444) 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:HB	1.08	1.03
1:A:699:LEU:HD13	1:C:281:VAL:HG13	1.51	0.91
1:C:543:ARG:HB2	1:C:568:MET:HE1	1.50	0.91
1:A:677:MET:HE2	1:B:518:ASN:HB3	1.54	0.89
1:B:366:MET:HE1	1:B:495:ILE:CB	2.03	0.86
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:A:202:ASN:OD1	1:A:328:ARG:HD2	1.89	0.72
1:C:591:SER:O	1:C:592:ARG:HB2	1.88	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:B:587:MET:HE3	1:B:599:ARG:C	2.16	0.70
1:B:366:MET:HE3	1:B:495:ILE:HB	1.69	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:C:543:ARG:HB2	1:C:568:MET:CE	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:HG22	1:A:251:ASP:N	2.10	0.66
1:C:256:PRO:HG3	1:C:265:TYR:C	2.20	0.66
1:A:638:ARG:HH11	1:B:121:GLY:HA3	1.61	0.66
1:C:248:HIS:HA	1:C:271:CYS:O	1.94	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:543:ARG:HB2	1:B:568:MET:HE1	1.79	0.65
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:C:148:VAL:HG23	1:C:421:MET:HE3	1.77	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: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:A:543:ARG:HB2	1:A:568:MET:HE1	1.79	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:365:THR:O	1:C:366:MET:HE2	2.00	0.62
1:B:630:ILE:HG22	1:B:631:GLU:N	2.13	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:C:152:GLU:HA	1:C:366:MET:HE2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:259:VAL:HG23	1:A:264:ARG:HH11	1.68	0.59
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:177:HIS:O	1:B:178:ARG:HB2	2.01	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:163:MET:HE3	1:C:289:LEU:HD12	1.85	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:A:120:THR:C	1:A:122:ALA:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:GLN:OE1	1:C:495:ILE:HD12	2.04	0.56
1:A:365:THR:O	1:A:366:MET:HE2	2.05	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
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: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:110:ASP:C	1:B:112:ASN:H	2.14	0.54
1:B:366:MET:CE	1:B:495:ILE:CB	2.65	0.54
1:A:212:LYS:HE2	1:A:219:GLU:CD	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:ARG:CZ	1:B:563:MET:HE1	2.39	0.53
1:C:121:GLY:O	1:C:122:ALA:C	2.51	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: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
1:B:281:VAL:HG13	1:C:699:LEU:HD13	1.90	0.52
1:B:519:ASP:CG	1:B:520:MET:HE2	2.34	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:B:200:LYS:HZ1	1:B:208:ARG:NH1	2.08	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: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:B:433:HIS:C	1:B:434:ILE:HD12	2.36	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:408:ASP:O	1:C:409:LEU:HB2	2.11	0.51
1:A:120:THR:C	1:A:122:ALA:N	2.67	0.51
1:C:202:ASN:ND2	1:C:325:PHE:HE1	2.09	0.50
1:B:120:THR:C	1:B:122:ALA:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:458:ASN:O	1:C:459:THR:C	2.55	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:A:224:HIS:C	1:A:226:ASP:H	2.19	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: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
1:B:432:THR:HB	1:B:433:HIS:HD2	1.78	0.49
1:C:634:THR:CG2	1:C:635:VAL:N	2.75	0.49
1:B:120:THR:C	1:B:122:ALA:N	2.70	0.49
1:B:648:VAL:HG13	1:B:648:VAL:O	2.12	0.49
1:B:634:THR:HG22	1:B:635:VAL:H	1.78	0.49
1:B:121:GLY:O	1:B:122:ALA:C	2.56	0.48
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:A:637:HIS:HD2	1:A:653:TYR:H	1.62	0.48
1:B:218:LEU:C	1:B:218:LEU:HD23	2.39	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:C:648:VAL:HG13	1:C:648:VAL:O	2.12	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:B:181:GLN:NE2	1:B:183:MET:HE1	2.28	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:256:PRO:HG3	1:A:265:TYR:C	2.39	0.47
1:A:601:LEU:HD22	1:A:627:ARG:CD	2.43	0.47
1:C:208:ARG:C	1:C:210:THR:H	2.21	0.47
1:A:358:PRO:HG2	1:A:361:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HD22	1:A:627:ARG:HD3	1.96	0.47
1:C:120:THR:C	1:C:122:ALA:N	2.72	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:311:HIS:HE2	1:A:313:THR:HG1	1.61	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
1:B:218:LEU:HD23	1:B:219:GLU:C	2.39	0.47
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:A:658:GLN:C	1:A:659:LEU:HD12	2.40	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:152:GLU:HA	1:A:366:MET:CE	2.45	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:124:VAL:O	1:C:665:THR:HG22	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:543:ARG:HB2	1:B:568:MET:CE	2.43	0.46
1:A:244:SER:OG	1:B:708:ARG:NH2	2.46	0.46
1:B:366:MET:HE3	1:B:495:ILE:HD12	1.98	0.46
1:B:655:TYR:C	1:B:655:TYR:CD2	2.93	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:B:543:ARG:HD2	1:B:568:MET:HE3	1.97	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: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: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: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:587:MET:HE3	1:C:599:ARG:C	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ARG:HD2	1:A:568:MET:HE3	1.99	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: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: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:418:ARG:O	1:A:419:ASP:C	2.61	0.44
1:C:120:THR:C	1:C:122:ALA:H	2.26	0.44
1:A:150:PHE:HB2	1:A:449:LEU:HB3	1.99	0.44
1:A:224:HIS:C	1:A:226:ASP:N	2.76	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: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: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:624:ARG:HH22	1:B:628:ASP:CG	2.25	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:543:ARG:NE	1:B:563:MET:HE1	2.33	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:A:543:ARG:HB2	1:A:568:MET:CE	2.48	0.43
1:A:152:GLU:HA	1:A:366:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:PRO:O	1:B:455:LEU:HD23	2.17	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:B:307:SER:C	1:B:309:THR:H	2.28	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: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: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: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: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: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:B:148:VAL:HG23	1:B:421:MET:HE3	2.01	0.41
1:B:458:ASN:C	1:B:460:LEU:N	2.78	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:B:677:MET:HE3	1:C:518:ASN:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ILE:N	1:C:671:ILE:CD1	2.82	0.41
1:C:679:GLU:H	1:C:679:GLU:CD	2.28	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: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: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
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:259:VAL:O	1:A:260:GLU:C	2.63	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:C:655:TYR:CD2	1:C:655:TYR:C	2.99	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:256:PRO:HG2	1:A:264:ARG:C	2.46	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

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%)	11	8
1	B	575/628 (92%)	538 (94%)	32 (6%)	5 (1%)	14	10
1	C	569/628 (91%)	533 (94%)	32 (6%)	4 (1%)	18	15
All	All	1714/1884 (91%)	1602 (94%)	97 (6%)	15 (1%)	14	10

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	502/543 (92%)	495 (99%)	7 (1%)	59	67
1	B	507/543 (93%)	501 (99%)	6 (1%)	63	72
1	C	502/543 (92%)	493 (98%)	9 (2%)	51	60
All	All	1511/1629 (93%)	1489 (98%)	22 (2%)	57	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	265	TYR
1	A	320	LYS
1	A	328	ARG
1	A	368	LYS
1	A	567	VAL
1	A	620	ASN
1	B	195	GLU
1	B	320	LYS
1	B	368	LYS
1	B	377	ARG
1	B	421	MET
1	B	620	ASN
1	C	195	GLU
1	C	218	LEU
1	C	317	ASP
1	C	320	LYS
1	C	377	ARG
1	C	379	GLU
1	C	421	MET
1	C	434	ILE
1	C	665	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	172	GLN
1	A	181	GLN
1	A	217	ASN
1	A	238	ASN
1	A	248	HIS
1	A	263	HIS

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	430	ASN
1	A	443	GLN
1	A	445	ASN
1	A	534	HIS
1	A	580	ASN
1	A	585	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	534	HIS
1	B	580	ASN
1	B	584	GLN
1	B	585	ASN
1	B	620	ASN
1	B	637	HIS
1	B	724	HIS
1	C	126	GLN
1	C	140	GLN
1	C	181	GLN
1	C	370	GLN
1	C	433	HIS
1	C	580	ASN
1	C	584	GLN
1	C	585	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 [i](#)

There are no oligosaccharides 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, 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%)	1.54	191 (33%) 1 1	24, 62, 87, 113	0
1	B	581/628 (92%)	0.98	98 (16%) 4 4	22, 50, 82, 109	0
1	C	575/628 (91%)	1.22	125 (21%) 2 2	21, 56, 82, 95	0
All	All	1732/1884 (91%)	1.24	414 (23%) 2 2	21, 56, 85, 113	0

All (414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	CYS	8.9
1	B	330	LEU	6.9
1	A	330	LEU	6.7
1	B	460	LEU	5.9
1	A	234	LEU	5.6
1	A	725	ALA	5.3
1	B	174	TRP	5.3
1	C	194	PHE	5.1
1	A	322	VAL	5.0
1	B	111	ALA	4.9
1	C	327	ALA	4.9
1	A	303	TYR	4.9
1	B	361	PRO	4.8
1	B	173	VAL	4.7
1	A	232	MET	4.7
1	A	192	VAL	4.7
1	A	230	THR	4.6
1	A	116	CYS	4.6
1	C	303	TYR	4.6
1	B	724	HIS	4.6
1	B	461	ALA	4.5
1	A	328	ARG	4.5
1	A	344	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	247	TRP	4.5
1	C	322	VAL	4.5
1	B	491	SER	4.4
1	A	326	TYR	4.4
1	A	160	LYS	4.4
1	A	249	THR	4.4
1	C	244	SER	4.4
1	A	206	VAL	4.4
1	B	429	TYR	4.3
1	C	300	PHE	4.3
1	C	722	VAL	4.3
1	A	724	HIS	4.3
1	B	138	GLU	4.3
1	A	194	PHE	4.2
1	C	360	ARG	4.2
1	A	319	PHE	4.2
1	B	633	CYS	4.2
1	B	177	HIS	4.2
1	A	164	TYR	4.1
1	C	443	GLN	4.1
1	A	316	ALA	4.1
1	B	431	ALA	4.1
1	B	207	CYS	4.0
1	B	723	ILE	4.0
1	B	360	ARG	4.0
1	C	717	ALA	3.9
1	B	337	THR	3.9
1	A	415	LYS	3.9
1	C	723	ILE	3.9
1	A	170	VAL	3.9
1	A	265	TYR	3.8
1	A	139	GLY	3.8
1	A	343	ASN	3.8
1	A	250	THR	3.8
1	A	218	LEU	3.8
1	A	254	TYR	3.8
1	C	109	THR	3.8
1	A	203	ALA	3.7
1	A	578	ALA	3.7
1	A	162	THR	3.7
1	C	633	CYS	3.7
1	A	380	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	410	GLY	3.7
1	A	611	PRO	3.6
1	C	359	LYS	3.6
1	C	174	TRP	3.6
1	A	329	ASP	3.6
1	A	169	THR	3.6
1	A	459	THR	3.6
1	B	634	THR	3.6
1	C	341	THR	3.6
1	A	723	ILE	3.5
1	A	353	ALA	3.5
1	B	139	GLY	3.5
1	C	492	VAL	3.5
1	A	431	ALA	3.5
1	C	380	TYR	3.5
1	C	635	VAL	3.5
1	C	412	CYS	3.4
1	B	430	ASN	3.4
1	A	590	SER	3.4
1	A	262	PHE	3.4
1	C	419	ASP	3.4
1	A	228	HIS	3.4
1	C	314	TYR	3.4
1	A	357	VAL	3.4
1	B	611	PRO	3.4
1	C	302	GLY	3.4
1	A	235	LYS	3.3
1	A	613	VAL	3.3
1	A	420	ALA	3.3
1	A	426	ALA	3.3
1	C	409	LEU	3.3
1	A	271	CYS	3.3
1	C	361	PRO	3.3
1	B	492	VAL	3.3
1	A	248	HIS	3.3
1	C	319	PHE	3.3
1	A	341	THR	3.3
1	A	173	VAL	3.3
1	B	179	TYR	3.3
1	C	363	VAL	3.3
1	B	434	ILE	3.3
1	A	178	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	174	TRP	3.2
1	C	207	CYS	3.2
1	A	342	ARG	3.2
1	A	659	LEU	3.2
1	A	425	PHE	3.2
1	A	205	GLY	3.2
1	A	142	TYR	3.2
1	A	429	TYR	3.2
1	C	234	LEU	3.2
1	B	109	THR	3.2
1	A	273	VAL	3.2
1	A	338	ALA	3.2
1	C	301	TYR	3.2
1	C	228	HIS	3.2
1	A	634	THR	3.2
1	A	327	ALA	3.1
1	C	192	VAL	3.1
1	B	589	ILE	3.1
1	A	251	ASP	3.1
1	A	436	VAL	3.1
1	C	317	ASP	3.1
1	C	589	ILE	3.1
1	A	209	SER	3.1
1	A	633	CYS	3.1
1	A	492	VAL	3.1
1	A	320	LYS	3.1
1	A	339	PRO	3.1
1	B	428	ARG	3.1
1	A	272	ILE	3.1
1	C	597	TYR	3.0
1	A	141	ASN	3.0
1	A	325	PHE	3.0
1	B	180	SER	3.0
1	A	410	GLY	3.0
1	A	214	VAL	3.0
1	A	255	ASN	3.0
1	C	491	SER	3.0
1	A	352	VAL	3.0
1	A	301	TYR	3.0
1	A	360	ARG	2.9
1	B	304	ARG	2.9
1	A	430	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	659	LEU	2.9
1	A	120	THR	2.9
1	B	210	THR	2.9
1	A	358	PRO	2.9
1	B	303	TYR	2.9
1	C	338	ALA	2.9
1	A	612	LEU	2.9
1	C	320	LYS	2.9
1	C	714	LEU	2.9
1	B	555	VAL	2.9
1	A	177	HIS	2.9
1	A	304	ARG	2.9
1	A	278	ALA	2.9
1	C	211	ALA	2.9
1	A	313	THR	2.9
1	C	358	PRO	2.9
1	B	194	PHE	2.9
1	A	208	ARG	2.8
1	A	638	ARG	2.8
1	B	691	ARG	2.8
1	A	555	VAL	2.8
1	C	593	PRO	2.8
1	C	112	ASN	2.8
1	C	111	ALA	2.8
1	C	420	ALA	2.8
1	A	340	THR	2.8
1	B	175	PHE	2.8
1	B	380	TYR	2.8
1	C	326	TYR	2.8
1	A	111	ALA	2.8
1	A	195	GLU	2.8
1	B	412	CYS	2.8
1	A	307	SER	2.8
1	B	178	ARG	2.8
1	B	716	PHE	2.8
1	A	210	THR	2.8
1	C	634	THR	2.8
1	A	412	CYS	2.8
1	C	719	ILE	2.8
1	C	139	GLY	2.7
1	C	284	TYR	2.7
1	A	418	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	2.7
1	A	201	ILE	2.7
1	C	430	ASN	2.7
1	A	122	ALA	2.7
1	A	315	ALA	2.7
1	B	425	PHE	2.7
1	A	351	THR	2.7
1	A	112	ASN	2.7
1	A	635	VAL	2.7
1	C	357	VAL	2.7
1	A	180	SER	2.7
1	C	121	GLY	2.7
1	B	432	THR	2.7
1	B	612	LEU	2.7
1	A	297	MET	2.7
1	C	655	TYR	2.7
1	B	635	VAL	2.7
1	C	307	SER	2.7
1	A	414	GLY	2.7
1	A	140	GLN	2.6
1	C	609	GLN	2.6
1	A	222	ALA	2.6
1	A	345	LEU	2.6
1	B	456	LEU	2.6
1	A	355	ASP	2.6
1	B	415	LYS	2.6
1	C	415	LYS	2.6
1	B	305	GLU	2.6
1	C	308	HIS	2.6
1	B	120	THR	2.6
1	B	253	LYS	2.6
1	B	606	TYR	2.6
1	C	142	TYR	2.6
1	A	197	VAL	2.6
1	B	228	HIS	2.6
1	B	112	ASN	2.6
1	B	717	ALA	2.6
1	C	221	THR	2.6
1	B	252	LEU	2.6
1	A	257	SER	2.6
1	C	195	GLU	2.6
1	A	324	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	311	HIS	2.6
1	A	202	ASN	2.6
1	A	400	THR	2.6
1	C	203	ALA	2.6
1	C	313	THR	2.6
1	A	175	PHE	2.5
1	A	443	GLN	2.5
1	A	115	VAL	2.5
1	A	198	ILE	2.5
1	A	259	VAL	2.5
1	C	170	VAL	2.5
1	A	253	LYS	2.5
1	C	160	LYS	2.5
1	A	312	THR	2.5
1	C	340	THR	2.5
1	A	191	PRO	2.5
1	C	339	PRO	2.5
1	B	609	GLN	2.5
1	A	305	GLU	2.5
1	A	719	ILE	2.5
1	B	306	GLY	2.5
1	B	574	VAL	2.5
1	C	648	VAL	2.5
1	A	143	THR	2.5
1	A	193	PRO	2.5
1	B	714	LEU	2.5
1	A	302	GLY	2.5
1	C	235	LYS	2.5
1	B	719	ILE	2.5
1	C	178	ARG	2.5
1	C	201	ILE	2.5
1	C	214	VAL	2.5
1	C	304	ARG	2.5
1	B	329	ASP	2.5
1	B	257	SER	2.5
1	C	250	THR	2.5
1	A	424	ILE	2.5
1	C	259	VAL	2.4
1	C	581	VAL	2.4
1	A	233	GLU	2.4
1	C	120	THR	2.4
1	B	203	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	211	ALA	2.4
1	C	202	ASN	2.4
1	B	443	GLN	2.4
1	C	305	GLU	2.4
1	A	648	VAL	2.4
1	C	411	ASP	2.4
1	B	250	THR	2.4
1	A	237	ALA	2.4
1	A	349	LYS	2.4
1	A	417	ALA	2.4
1	C	239	ALA	2.4
1	C	261	ALA	2.4
1	A	184	GLY	2.4
1	A	223	PHE	2.4
1	B	170	VAL	2.4
1	A	656	SER	2.4
1	C	232	MET	2.4
1	B	254	TYR	2.4
1	C	309	THR	2.4
1	C	432	THR	2.4
1	A	456	LEU	2.4
1	C	324	GLY	2.4
1	A	579	ASP	2.4
1	B	317	ASP	2.4
1	B	363	VAL	2.4
1	A	171	SER	2.4
1	A	243	THR	2.4
1	C	721	THR	2.4
1	B	122	ALA	2.3
1	A	409	LEU	2.3
1	B	258	ARG	2.3
1	B	695	LYS	2.3
1	C	325	PHE	2.3
1	C	425	PHE	2.3
1	C	638	ARG	2.3
1	B	271	CYS	2.3
1	C	596	CYS	2.3
1	A	354	TRP	2.3
1	A	270	ASN	2.3
1	A	554	THR	2.3
1	C	459	THR	2.3
1	A	240	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	577	ALA	2.3
1	C	356	TRP	2.3
1	A	264	ARG	2.3
1	C	612	LEU	2.3
1	A	433	HIS	2.3
1	B	307	SER	2.3
1	B	459	THR	2.3
1	A	592	ARG	2.3
1	B	116	CYS	2.3
1	C	271	CYS	2.3
1	C	579	ASP	2.3
1	C	701	ASP	2.3
1	A	594	GLY	2.3
1	C	643	PHE	2.2
1	A	432	THR	2.2
1	A	583	VAL	2.2
1	B	626	THR	2.2
1	B	136	ARG	2.2
1	A	359	LYS	2.2
1	A	306	GLY	2.2
1	A	382	GLY	2.2
1	A	610	GLY	2.2
1	A	636	GLY	2.2
1	C	345	LEU	2.2
1	B	326	TYR	2.2
1	C	138	GLU	2.2
1	A	321	GLN	2.2
1	A	591	SER	2.2
1	B	244	SER	2.2
1	A	434	ILE	2.2
1	B	259	VAL	2.2
1	C	193	PRO	2.2
1	C	434	ILE	2.2
1	A	570	VAL	2.2
1	A	422	ASP	2.2
1	B	614	GLU	2.2
1	A	606	TYR	2.2
1	C	639	ARG	2.2
1	A	117	PRO	2.2
1	A	665	THR	2.2
1	B	419	ASP	2.2
1	A	437	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	626	THR	2.2
1	A	630	ILE	2.1
1	C	198	ILE	2.1
1	A	407	VAL	2.1
1	B	124	VAL	2.1
1	A	404	LEU	2.1
1	B	638	ARG	2.1
1	C	418	ARG	2.1
1	A	244	SER	2.1
1	A	655	TYR	2.1
1	B	535	GLU	2.1
1	A	356	TRP	2.1
1	C	604	PHE	2.1
1	C	437	GLY	2.1
1	A	435	LYS	2.1
1	A	660	SER	2.1
1	B	596	CYS	2.1
1	C	607	GLU	2.1
1	A	221	THR	2.1
1	A	309	THR	2.1
1	B	230	THR	2.1
1	C	191	PRO	2.1
1	C	406	ARG	2.1
1	A	363	VAL	2.1
1	A	623	LEU	2.1
1	A	625	LEU	2.1
1	B	409	LEU	2.1
1	B	590	SER	2.1
1	C	344	LEU	2.1
1	A	585	ASN	2.1
1	A	118	PRO	2.1
1	A	308	HIS	2.1
1	A	314	TYR	2.1
1	C	365	THR	2.1
1	C	414	GLY	2.1
1	A	350	PHE	2.1
1	B	362	SER	2.1
1	C	677	MET	2.0
1	C	323	ASP	2.0
1	A	593	PRO	2.0
1	B	721	THR	2.0
1	A	213	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	644	GLY	2.0
1	A	287	PHE	2.0
1	B	379	GLU	2.0
1	B	493	GLU	2.0
1	B	722	VAL	2.0
1	B	458	ASN	2.0
1	A	601	LEU	2.0
1	B	140	GLN	2.0
1	C	218	LEU	2.0
1	B	562	ARG	2.0
1	C	116	CYS	2.0
1	C	611	PRO	2.0
1	C	429	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NA	B	732	1/1	0.78	0.23	52,52,52,52	0
2	NA	C	731	1/1	0.94	0.10	44,44,44,44	0
2	NA	B	731	1/1	0.95	0.08	50,50,50,50	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.