



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:40 PM UTC

PDB ID : 1GWB / pdb_00001gwb
Title : STRUCTURE OF GLYCOPROTEIN 1B
Authors : Emsley, J.; Uff, S.; Clemetson, K.J.M.; Clemetson, J.M.; Harrison, T.
Deposited on : 2002-03-14
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

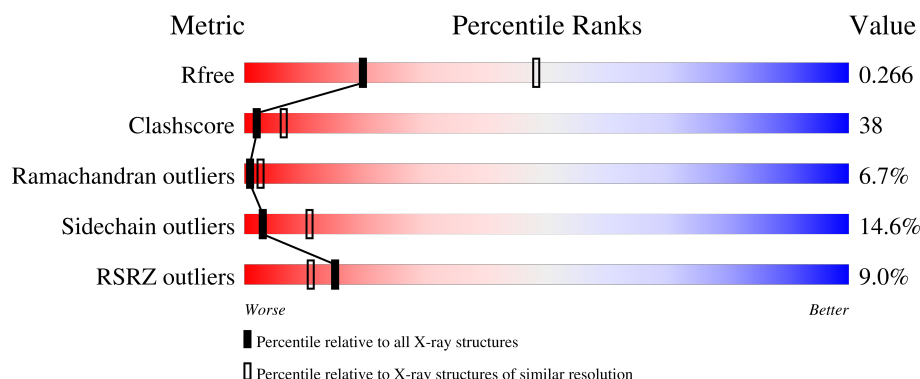
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	281	9% 34% 43% 15% 5%
1	B	281	9% 43% 42% 12% ..

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
4	NAG	A	304	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4451 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.

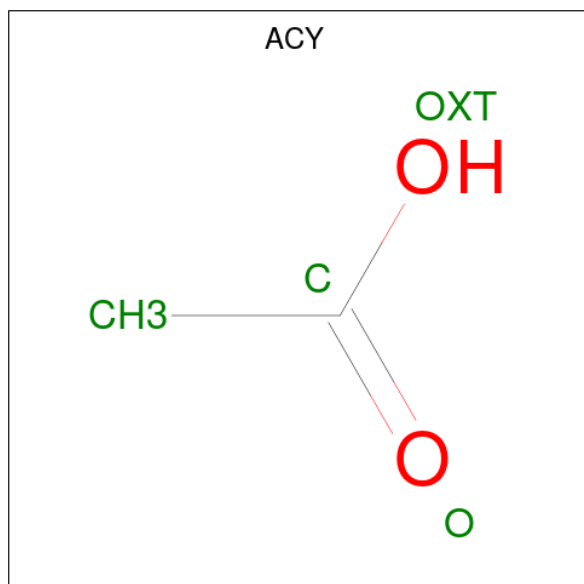
- Molecule 1 is a protein called PLATELET GLYCOPROTEIN IB ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	1
			2063	1326	343	387	7			
1	B	279	Total	C	N	O	S	0	0	0
			2190	1399	356	425	10			

- Molecule 2 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

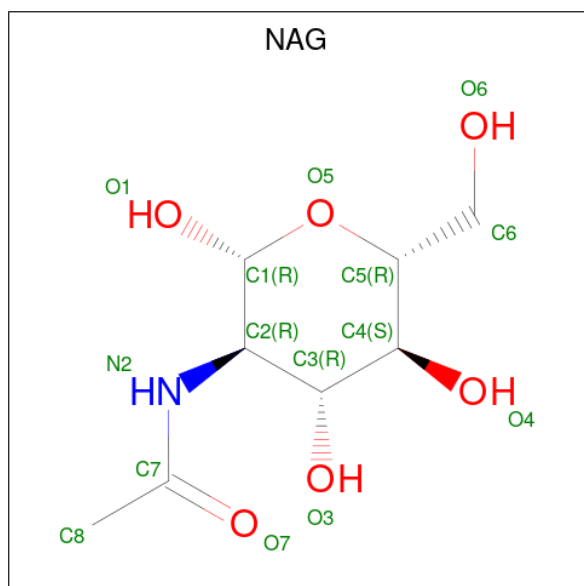
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Pt	0	0
			2	2		
2	B	2	Total	Pt	0	0
			2	2		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



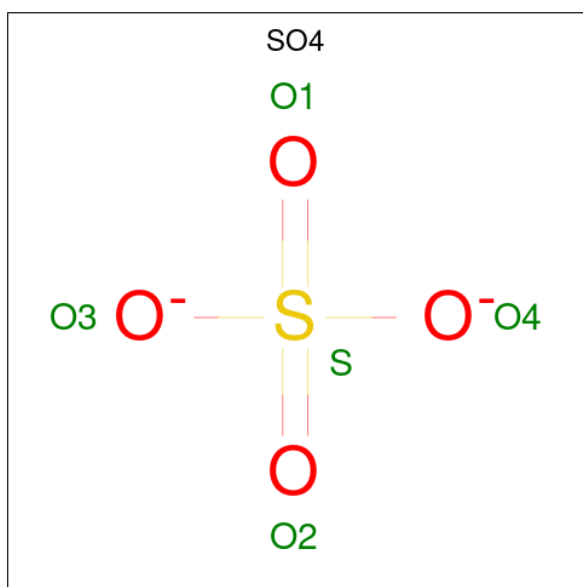
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

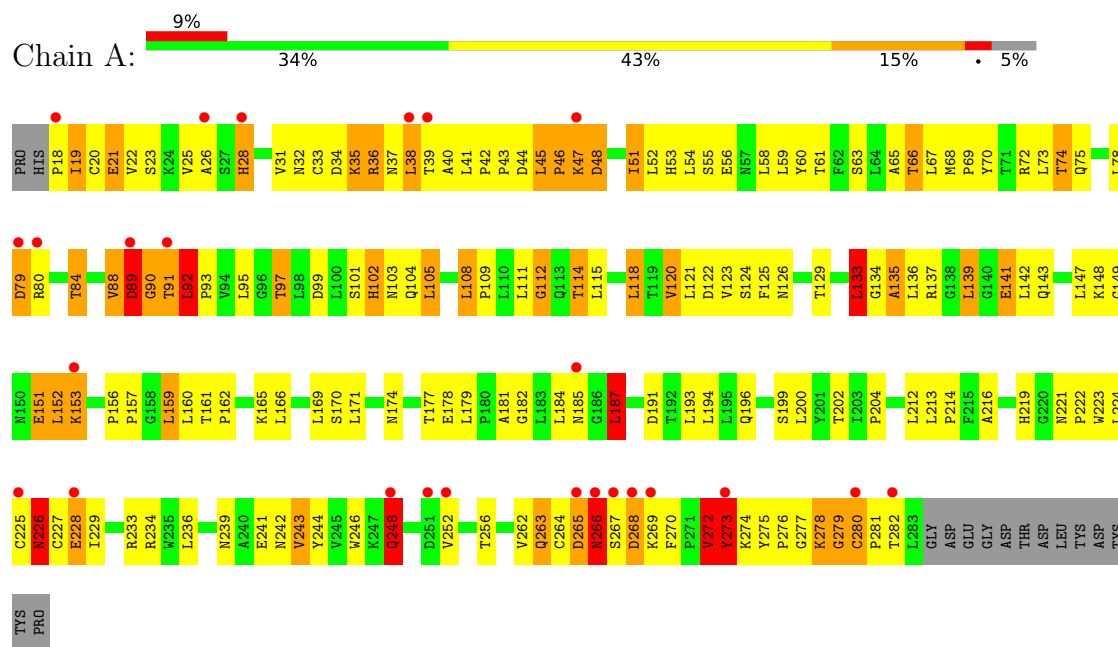
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	B	92	Total	O	0	0
			92	92		

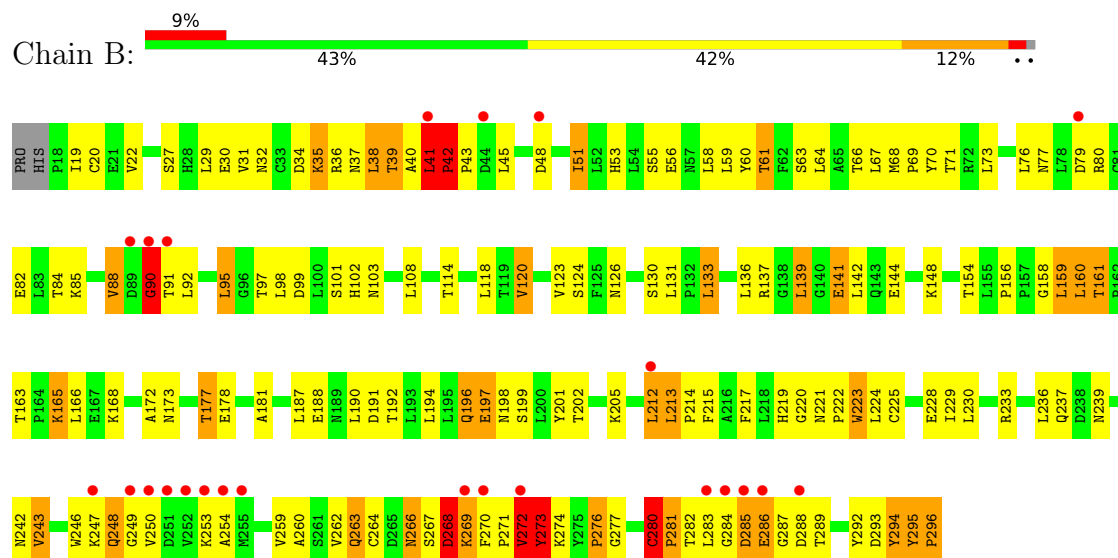
3 Residue-property plots [i](#)

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

• Molecule 1: PLATELET GLYCOPROTEIN IB ALPHA CHAIN



• Molecule 1: PLATELET GLYCOPROTEIN IB ALPHA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	202.00Å 202.00Å 128.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-2.80) 97.7 (15.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.274 0.241 , 0.266	Depositor DCC
R_{free} test set	1929 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4451	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: NAG, SO4, TYS, ACY, PT

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	0.48	1/2109 (0.0%)	1.03	14/2883 (0.5%)
1	B	0.52	0/2187	1.18	23/2984 (0.8%)
All	All	0.50	1/4296 (0.0%)	1.11	37/5867 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	THR	C-N	-5.54	1.25	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	LEU	C-N-CD	-13.85	90.13	120.60
1	B	38	LEU	N-CA-C	10.00	121.88	110.97
1	A	272	VAL	N-CA-C	-9.14	96.47	109.63
1	A	274	LYS	N-CA-C	-8.94	101.70	114.12
1	B	41	LEU	CA-C-N	8.56	147.55	127.00
1	B	41	LEU	C-N-CA	8.56	147.55	127.00
1	B	274	LYS	N-CA-C	-8.55	101.85	113.30
1	B	90	GLY	N-CA-C	7.83	131.75	113.18
1	B	213	LEU	CA-C-N	7.82	127.11	118.97
1	B	213	LEU	C-N-CA	7.82	127.11	118.97
1	A	78	LEU	N-CA-C	-7.58	104.01	112.57
1	B	228	GLU	N-CA-C	-7.13	104.47	113.02
1	B	71	THR	N-CA-C	6.53	119.22	111.71
1	B	88	VAL	N-CA-C	6.00	117.42	108.54
1	A	90	GLY	N-CA-C	6.00	127.40	113.18
1	B	141	GLU	N-CA-C	-5.99	106.02	113.38
1	B	248	GLN	CB-CA-C	-5.85	109.27	117.23
1	B	272	VAL	N-CA-C	-5.84	101.64	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	LEU	N-CA-C	-5.79	105.52	112.59
1	A	84	THR	N-CA-C	-5.74	107.27	114.56
1	A	89	ASP	N-CA-C	5.69	117.39	107.49
1	A	92	LEU	CA-C-N	5.67	125.77	119.87
1	A	92	LEU	C-N-CA	5.67	125.77	119.87
1	A	228	GLU	N-CA-C	-5.63	104.62	112.45
1	A	153	LYS	N-CA-C	-5.60	107.09	114.31
1	A	112	GLY	N-CA-C	5.57	120.68	113.27
1	A	265	ASP	N-CA-C	-5.53	106.60	113.19
1	B	198	ASN	N-CA-C	-5.51	101.12	108.34
1	A	38	LEU	N-CA-C	5.49	119.14	112.23
1	B	215	PHE	N-CA-C	5.42	117.51	108.02
1	B	177	THR	N-CA-C	-5.41	107.69	114.56
1	B	42	PRO	CA-N-CD	-5.41	103.93	111.50
1	B	84	THR	N-CA-C	-5.29	107.38	113.88
1	B	197	GLU	N-CA-C	5.23	117.56	111.02
1	B	263	GLN	N-CA-C	5.23	117.62	109.52
1	B	269	LYS	N-CA-C	-5.20	106.53	112.92
1	B	280	CYS	N-CA-C	5.20	117.99	110.14

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	2063	0	2089	184	1
1	B	2190	0	2181	148	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	0	0
4	A	28	0	26	3	0
4	B	14	0	13	0	0
5	B	5	0	0	0	0
6	A	51	0	0	3	1
6	B	92	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4451	0	4312	328	4

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 38.

All (328) 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:90:GLY:HA2	1:B:114:THR:HB	1.38	1.04
1:A:105:LEU:HD23	1:A:105:LEU:H	1.19	1.04
1:A:97:THR:HB	1:A:120:VAL:HG13	1.50	0.94
1:B:272:VAL:O	1:B:273:TYR:HB3	1.66	0.92
1:A:151:GLU:HG2	4:A:305:NAG:H82	1.53	0.90
1:A:153:LYS:HE3	1:A:177:THR:HG21	1.53	0.87
1:A:222:PRO:HA	1:A:265:ASP:HB2	1.56	0.87
1:A:272:VAL:O	1:A:273:TYR:HB3	1.76	0.85
1:A:37:ASN:HA	1:A:58:LEU:HD23	1.55	0.85
1:B:90:GLY:HA2	1:B:114:THR:CB	2.07	0.84
1:B:205:LYS:HD3	1:B:294:TYS:HE1	1.57	0.84
1:A:139:LEU:HD23	1:A:139:LEU:H	1.47	0.79
1:A:225:CYS:HB2	1:A:229:ILE:HG21	1.64	0.79
1:B:91:THR:HG22	6:B:469:HOH:O	1.81	0.79
1:B:133:LEU:H	1:B:133:LEU:HD22	1.47	0.78
1:A:47:LYS:O	1:A:48:ASP:HB2	1.84	0.78
1:B:41:LEU:HB3	1:B:42:PRO:O	1.85	0.77
1:B:259:VAL:O	1:B:262:VAL:HG12	1.86	0.76
1:B:212:LEU:HG	1:B:239:ASN:HD21	1.49	0.76
1:B:196:GLN:HG3	1:B:217:PHE:HB3	1.69	0.74
1:A:75:GLN:HG2	1:A:97:THR:HG23	1.68	0.74
1:A:41:LEU:HD12	1:A:42:PRO:HD2	1.69	0.74
1:B:31:VAL:HG11	1:B:45:LEU:HD12	1.70	0.74
1:B:233:ARG:HG2	1:B:273:TYR:HA	1.68	0.74
1:A:224:LEU:HA	1:A:266:ASN:HD21	1.53	0.74
1:B:45:LEU:H	1:B:45:LEU:HD22	1.54	0.73
1:B:295:TYS:CG	1:B:296:PRO:HD2	2.19	0.72
1:A:105:LEU:H	1:A:105:LEU:CD2	2.00	0.72
1:A:56:GLU:HA	1:A:80:ARG:O	1.90	0.71
1:A:151:GLU:CG	4:A:305:NAG:H82	2.20	0.71
1:A:108:LEU:HD22	1:A:109:PRO:HD2	1.72	0.71
1:A:42:PRO:O	1:A:45:LEU:HD23	1.90	0.71
1:B:99:ASP:OD1	1:B:101:SER:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:THR:HG23	1:B:293:ASP:OD1	1.91	0.70
1:A:19:ILE:HG21	1:A:44:ASP:OD2	1.91	0.70
1:B:88:VAL:HG12	1:B:114:THR:HG21	1.74	0.70
1:B:97:THR:HG22	1:B:120:VAL:HG13	1.74	0.70
1:B:20:CYS:HA	1:B:36:ARG:HH12	1.56	0.69
1:A:123:VAL:HG22	1:A:147:LEU:HD23	1.75	0.69
1:A:262:VAL:HG12	1:A:272:VAL:CG1	2.23	0.69
1:B:236:LEU:HD22	1:B:262:VAL:HG11	1.74	0.69
1:A:266:ASN:N	1:A:266:ASN:HD22	1.91	0.68
1:B:90:GLY:CA	1:B:114:THR:HB	2.21	0.68
1:A:105:LEU:HD23	1:A:105:LEU:N	2.03	0.68
1:A:153:LYS:HG3	1:A:177:THR:HG23	1.73	0.68
1:B:233:ARG:HD3	1:B:237:GLN:NE2	2.08	0.68
1:A:19:ILE:HG23	1:A:20:CYS:N	2.08	0.68
1:A:219:HIS:CE1	1:A:246:TRP:H	2.12	0.67
1:B:51:ILE:HD11	1:B:53:HIS:NE2	2.09	0.67
1:A:139:LEU:H	1:A:139:LEU:CD2	2.05	0.67
1:A:241:GLU:HG2	6:A:430:HOH:O	1.94	0.66
1:B:148:LYS:HE3	1:B:173:ASN:HD22	1.59	0.66
1:B:41:LEU:HB3	1:B:42:PRO:C	2.21	0.66
1:A:91:THR:O	1:A:92:LEU:HB2	1.96	0.66
1:B:268:ASP:OD2	1:B:268:ASP:C	2.38	0.66
1:A:88:VAL:HG12	1:A:114:THR:HG21	1.78	0.65
1:A:97:THR:HB	1:A:120:VAL:CG1	2.25	0.65
1:A:99:ASP:OD1	1:A:101:SER:HB2	1.97	0.65
1:A:88:VAL:HG12	1:A:114:THR:CG2	2.27	0.64
1:B:177:THR:O	1:B:178:GLU:HG2	1.98	0.64
1:A:112:GLY:HA3	1:A:137:ARG:O	1.98	0.63
1:B:148:LYS:HE3	1:B:173:ASN:ND2	2.13	0.63
1:A:48:ASP:OD2	1:A:72:ARG:HD2	1.97	0.63
1:A:272:VAL:O	1:A:273:TYR:CB	2.47	0.63
1:B:172:ALA:HB2	1:B:196:GLN:NE2	2.13	0.63
1:A:233:ARG:HG3	1:A:273:TYR:HA	1.79	0.62
1:B:20:CYS:HA	1:B:36:ARG:NH1	2.13	0.62
1:A:268:ASP:OD2	1:A:270:PHE:HB2	2.00	0.62
1:A:280:CYS:SG	1:A:281:PRO:HD2	2.39	0.62
1:B:68:MET:CB	1:B:91:THR:HG21	2.29	0.62
1:A:92:LEU:H	1:A:93:PRO:HD3	1.64	0.62
1:A:222:PRO:HA	1:A:265:ASP:CB	2.30	0.62
1:B:205:LYS:HD3	1:B:294:TYS:CE1	2.27	0.61
1:A:19:ILE:HG23	1:A:20:CYS:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:HB2	1:A:223:TRP:NE1	2.16	0.61
1:B:63:SER:HB3	1:B:66:THR:HG23	1.82	0.61
1:A:263:GLN:OE1	1:A:269:LYS:HG3	2.00	0.61
4:A:305:NAG:H3	4:A:305:NAG:H83	1.81	0.61
1:A:67:LEU:C	1:A:69:PRO:HD2	2.26	0.60
1:A:42:PRO:HB2	1:A:45:LEU:CD2	2.30	0.60
1:A:44:ASP:O	1:A:45:LEU:C	2.45	0.60
1:A:212:LEU:O	1:A:214:PRO:HD3	2.02	0.60
1:B:38:LEU:O	1:B:39:THR:HG22	2.02	0.60
1:B:197:GLU:HG3	1:B:220:GLY:HA3	1.83	0.59
1:A:118:LEU:HD11	1:A:121:LEU:HB2	1.83	0.59
1:A:31:VAL:HG11	1:A:45:LEU:CD1	2.33	0.59
1:B:263:GLN:CD	1:B:268:ASP:HA	2.28	0.59
1:A:228:GLU:HB2	6:A:442:HOH:O	2.03	0.59
1:B:22:VAL:HG13	1:B:29:LEU:HD21	1.85	0.59
1:B:196:GLN:CG	1:B:217:PHE:HB3	2.32	0.59
1:B:282:THR:O	1:B:284:GLY:N	2.36	0.58
1:A:32:ASN:HD22	1:A:33:CYS:N	2.01	0.58
1:A:184:LEU:HA	1:A:187:LEU:HD22	1.85	0.58
1:A:225:CYS:HA	1:A:229:ILE:HB	1.86	0.58
1:B:120:VAL:HB	1:B:144:GLU:HB2	1.85	0.58
1:B:269:LYS:HA	1:B:269:LYS:HE3	1.84	0.58
1:B:34:ASP:O	1:B:36:ARG:HD2	2.03	0.58
1:A:80:ARG:HA	1:A:102:HIS:O	2.03	0.57
1:B:280:CYS:SG	1:B:281:PRO:HD2	2.44	0.57
1:A:234:ARG:HH21	1:A:234:ARG:HG3	1.69	0.57
1:B:225:CYS:HB2	1:B:229:ILE:HG21	1.87	0.57
1:A:125:PHE:CD1	1:A:149:GLY:HA3	2.40	0.57
1:A:68:MET:N	1:A:69:PRO:HD2	2.20	0.57
1:A:265:ASP:O	1:A:267:SER:N	2.38	0.57
1:B:276:PRO:HG2	1:B:277:GLY:H	1.69	0.57
1:B:269:LYS:C	1:B:271:PRO:HD3	2.30	0.57
1:A:32:ASN:HD22	1:A:32:ASN:C	2.12	0.57
1:A:58:LEU:O	1:A:59:LEU:HD23	2.05	0.56
1:A:124:SER:HB2	1:A:148:LYS:O	2.05	0.56
1:A:182:GLY:CA	1:A:185:ASN:ND2	2.69	0.56
1:A:125:PHE:CZ	1:B:288:ASP:HB3	2.41	0.55
1:B:177:THR:C	1:B:178:GLU:HG2	2.31	0.55
1:B:219:HIS:HE1	1:B:246:TRP:H	1.51	0.55
1:A:28:HIS:CD2	1:A:28:HIS:H	2.25	0.55
1:A:63:SER:O	1:A:66:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ALA:HB2	1:B:196:GLN:HE22	1.70	0.55
1:B:263:GLN:HG3	1:B:266:ASN:HA	1.89	0.55
1:B:267:SER:O	1:B:268:ASP:CB	2.55	0.54
1:B:103:ASN:O	1:B:126:ASN:HA	2.08	0.54
1:A:264:CYS:C	1:A:266:ASN:H	2.15	0.54
1:A:277:GLY:O	1:A:279:GLY:N	2.41	0.54
1:A:20:CYS:O	1:A:21:GLU:CB	2.56	0.54
1:A:123:VAL:HG23	1:A:123:VAL:O	2.07	0.54
1:B:262:VAL:HG13	1:B:262:VAL:O	2.08	0.54
1:B:286:GLU:CG	1:B:287:GLY:N	2.68	0.54
1:B:35:LYS:HG3	1:B:56:GLU:HB2	1.89	0.54
1:A:92:LEU:H	1:A:93:PRO:CD	2.21	0.53
1:B:42:PRO:HB3	1:B:45:LEU:HD11	1.89	0.53
1:B:247:LYS:HB3	1:B:250:VAL:HB	1.89	0.53
1:A:170:SER:HB2	1:A:194:LEU:HD13	1.90	0.53
1:A:153:LYS:CE	1:A:177:THR:HG21	2.32	0.53
1:B:124:SER:HB2	1:B:148:LYS:O	2.08	0.53
1:A:59:LEU:C	1:A:61:THR:H	2.15	0.53
1:B:177:THR:C	1:B:178:GLU:CG	2.81	0.53
1:A:266:ASN:N	1:A:266:ASN:ND2	2.57	0.52
1:B:39:THR:HA	1:B:58:LEU:O	2.09	0.52
1:B:191:ASP:HA	1:B:214:PRO:HD2	1.91	0.52
1:A:262:VAL:HG12	1:A:272:VAL:HG11	1.90	0.52
1:B:88:VAL:CG1	1:B:114:THR:HG21	2.39	0.52
1:A:139:LEU:CD2	1:A:139:LEU:N	2.73	0.52
1:B:35:LYS:C	1:B:36:ARG:HD2	2.35	0.52
1:A:136:LEU:HA	1:A:139:LEU:HD21	1.92	0.52
1:B:187:LEU:HD12	1:B:187:LEU:N	2.25	0.52
1:A:151:GLU:O	1:A:174:ASN:HB3	2.10	0.51
1:B:55:SER:OG	1:B:79:ASP:HB3	2.11	0.51
1:A:114:THR:HG23	6:A:410:HOH:O	2.08	0.51
1:A:153:LYS:HE3	1:A:177:THR:CG2	2.35	0.51
1:A:134:GLY:O	1:A:137:ARG:HB3	2.10	0.51
1:B:264:CYS:C	1:B:266:ASN:H	2.19	0.51
1:A:34:ASP:O	1:A:35:LYS:C	2.54	0.51
1:B:19:ILE:HG23	1:B:20:CYS:N	2.26	0.51
1:A:275:TYR:CE2	1:A:277:GLY:HA2	2.46	0.51
1:B:264:CYS:C	1:B:266:ASN:N	2.65	0.51
1:B:267:SER:O	1:B:268:ASP:HB3	2.10	0.50
1:A:41:LEU:HD12	1:A:42:PRO:CD	2.40	0.50
1:B:68:MET:N	1:B:69:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:OG1	1:A:228:GLU:HG3	2.11	0.50
1:B:36:ARG:HB2	1:B:38:LEU:HG	1.93	0.50
1:B:165:LYS:HE2	6:B:403:HOH:O	2.10	0.50
1:B:219:HIS:CE1	1:B:246:TRP:H	2.29	0.50
1:A:278:LYS:HG3	1:A:278:LYS:O	2.12	0.50
1:B:236:LEU:CD2	1:B:262:VAL:HG11	2.40	0.50
1:B:168:LYS:HG3	1:B:192:THR:HB	1.94	0.50
1:A:18:PRO:O	1:A:19:ILE:HG22	2.12	0.49
1:B:233:ARG:HD3	1:B:237:GLN:HE22	1.76	0.49
1:B:263:GLN:NE2	1:B:268:ASP:CB	2.75	0.49
1:A:123:VAL:HG22	1:A:147:LEU:CD2	2.39	0.49
1:B:286:GLU:HG3	1:B:287:GLY:N	2.27	0.49
1:A:226:ASN:O	1:A:227:CYS:HB2	2.13	0.49
1:A:268:ASP:O	1:A:269:LYS:HB3	2.13	0.49
1:A:169:LEU:HD13	1:A:169:LEU:C	2.38	0.49
1:A:219:HIS:HE1	1:A:246:TRP:H	1.58	0.49
1:B:29:LEU:HD23	1:B:29:LEU:C	2.38	0.49
1:B:187:LEU:HD23	1:B:190:LEU:HD13	1.94	0.49
1:A:36:ARG:O	1:A:37:ASN:C	2.55	0.49
1:A:58:LEU:N	1:A:58:LEU:HD22	2.27	0.49
1:A:59:LEU:C	1:A:60:TYR:HD1	2.21	0.49
1:A:161:THR:N	1:A:162:PRO:CD	2.76	0.49
1:B:53:HIS:HD2	1:B:77:ASN:HD22	1.61	0.49
1:A:19:ILE:CG2	1:A:20:CYS:N	2.75	0.49
1:B:213:LEU:HD23	1:B:213:LEU:H	1.78	0.49
1:A:95:LEU:HD12	1:A:118:LEU:HD23	1.95	0.48
1:B:108:LEU:HD22	1:B:131:LEU:HD22	1.94	0.48
1:A:236:LEU:HD11	1:A:262:VAL:HG11	1.95	0.48
1:A:38:LEU:O	1:A:39:THR:HB	2.13	0.48
1:B:38:LEU:O	1:B:39:THR:CB	2.60	0.48
1:A:199:SER:HA	1:A:222:PRO:CD	2.43	0.48
1:B:36:ARG:O	1:B:37:ASN:C	2.55	0.48
1:A:19:ILE:CD1	1:A:42:PRO:HB3	2.44	0.48
1:A:125:PHE:N	1:A:148:LYS:O	2.47	0.48
1:B:35:LYS:HA	1:B:56:GLU:O	2.13	0.48
1:B:59:LEU:O	1:B:61:THR:N	2.42	0.48
1:A:37:ASN:HA	1:A:58:LEU:CD2	2.36	0.47
1:B:137:ARG:HG2	6:B:442:HOH:O	2.14	0.47
1:B:295:TYS:CD1	1:B:296:PRO:HD2	2.43	0.47
1:A:69:PRO:HG2	1:A:70:TYR:CE1	2.49	0.47
1:A:226:ASN:N	1:A:226:ASN:HD22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HD23	1:B:30:GLU:N	2.29	0.47
1:B:133:LEU:H	1:B:133:LEU:CD2	2.24	0.47
1:A:32:ASN:C	1:A:32:ASN:ND2	2.72	0.47
1:A:136:LEU:O	1:A:139:LEU:HD23	2.14	0.47
1:A:22:VAL:HG12	1:A:23:SER:N	2.28	0.47
1:A:103:ASN:HB2	1:A:126:ASN:OD1	2.15	0.47
1:B:60:TYR:HA	1:B:82:GLU:O	2.14	0.47
1:B:67:LEU:C	1:B:69:PRO:HD2	2.40	0.47
1:A:276:PRO:HG2	1:A:277:GLY:H	1.80	0.47
1:B:159:LEU:HD13	1:B:160:LEU:HD13	1.97	0.47
1:A:91:THR:O	1:A:92:LEU:CB	2.62	0.46
1:B:97:THR:HB	1:B:120:VAL:HG22	1.96	0.46
1:B:177:THR:HG22	1:B:199:SER:HB2	1.96	0.46
1:B:194:LEU:HD23	1:B:217:PHE:CG	2.50	0.46
1:A:51:ILE:O	1:A:51:ILE:HG12	2.15	0.46
1:B:271:PRO:O	1:B:272:VAL:C	2.58	0.46
1:B:286:GLU:HG3	1:B:287:GLY:H	1.81	0.46
1:B:253:LYS:HD2	1:B:253:LYS:C	2.40	0.46
1:A:234:ARG:HG3	1:A:234:ARG:NH2	2.31	0.46
1:B:53:HIS:HD2	1:B:77:ASN:ND2	2.14	0.46
1:A:46:PRO:O	1:A:48:ASP:N	2.49	0.46
1:B:136:LEU:O	1:B:139:LEU:HD22	2.16	0.46
1:B:248:GLN:HG2	1:B:249:GLY:N	2.30	0.46
1:A:39:THR:HA	1:A:58:LEU:O	2.16	0.45
1:A:248:GLN:HE22	1:B:286:GLU:HA	1.80	0.45
1:A:266:ASN:O	1:A:267:SER:C	2.59	0.45
1:B:160:LEU:HG	1:B:166:LEU:HD12	1.98	0.45
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.16	0.45
1:A:262:VAL:HG12	1:A:272:VAL:HG13	1.98	0.45
1:B:80:ARG:HA	1:B:102:HIS:O	2.16	0.45
1:B:295:TYS:CD2	1:B:296:PRO:HB2	2.47	0.45
1:B:213:LEU:HA	1:B:214:PRO:HD3	1.75	0.45
1:A:177:THR:O	1:A:200:LEU:HA	2.17	0.45
1:A:239:ASN:HD22	1:A:242:ASN:HD22	1.65	0.45
1:B:20:CYS:HB3	1:B:32:ASN:O	2.17	0.45
1:A:51:ILE:HD11	1:A:53:HIS:NE2	2.32	0.44
1:B:196:GLN:HG3	1:B:217:PHE:CB	2.44	0.44
1:A:38:LEU:C	1:A:40:ALA:H	2.25	0.44
1:B:259:VAL:HG13	1:B:260:ALA:N	2.32	0.44
1:A:19:ILE:HD11	1:A:42:PRO:HB3	1.99	0.44
1:A:58:LEU:HB3	1:A:60:TYR:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:HG22	1:A:75:GLN:HG3	1.98	0.44
1:A:216:ALA:O	1:A:243:VAL:HA	2.16	0.44
1:B:69:PRO:HG2	1:B:70:TYR:CE1	2.52	0.44
1:B:194:LEU:HD23	1:B:217:PHE:CD1	2.51	0.44
1:A:124:SER:HB3	1:A:148:LYS:H	1.83	0.44
1:A:269:LYS:O	1:A:269:LYS:HG2	2.17	0.44
1:B:139:LEU:O	1:B:163:THR:HG22	2.17	0.44
1:B:272:VAL:O	1:B:273:TYR:CB	2.50	0.44
1:A:63:SER:C	1:A:65:ALA:N	2.74	0.44
1:B:40:ALA:C	1:B:41:LEU:O	2.60	0.44
1:A:92:LEU:N	1:A:93:PRO:CD	2.78	0.44
1:B:91:THR:OG1	1:B:92:LEU:HG	2.18	0.44
1:A:59:LEU:O	1:A:61:THR:N	2.40	0.44
1:B:92:LEU:HB3	1:B:95:LEU:HB2	2.00	0.44
1:A:133:LEU:C	1:A:135:ALA:H	2.25	0.44
1:A:121:LEU:HD12	1:A:122:ASP:N	2.32	0.43
1:B:38:LEU:O	1:B:39:THR:CG2	2.66	0.43
1:B:156:PRO:O	1:B:159:LEU:HB2	2.18	0.43
1:A:42:PRO:HB2	1:A:45:LEU:HD21	2.00	0.43
1:A:60:TYR:N	1:A:60:TYR:CD1	2.85	0.43
1:A:264:CYS:C	1:A:266:ASN:N	2.73	0.43
1:B:34:ASP:OD1	1:B:55:SER:HB2	2.19	0.43
1:B:177:THR:OG1	1:B:178:GLU:HG3	2.17	0.43
1:A:19:ILE:CG2	1:A:20:CYS:H	2.28	0.43
1:A:181:ALA:HA	1:A:204:PRO:CG	2.48	0.43
1:A:191:ASP:CG	1:B:181:ALA:HB2	2.42	0.43
1:A:35:LYS:HG3	1:A:56:GLU:CD	2.43	0.43
1:B:269:LYS:HA	1:B:269:LYS:CE	2.45	0.43
1:A:32:ASN:ND2	1:A:34:ASP:OD2	2.50	0.43
1:A:277:GLY:O	1:A:278:LYS:C	2.61	0.43
1:A:45:LEU:HA	1:A:46:PRO:HD2	1.83	0.43
1:A:124:SER:O	1:A:125:PHE:HB2	2.19	0.43
1:A:125:PHE:CE2	1:B:288:ASP:HB3	2.54	0.43
1:A:129:THR:O	1:A:152:LEU:HA	2.18	0.43
1:B:270:PHE:N	1:B:271:PRO:HD3	2.33	0.43
1:A:44:ASP:CG	1:A:45:LEU:N	2.77	0.43
1:A:182:GLY:HA3	1:A:185:ASN:ND2	2.33	0.43
1:A:84:THR:HG22	1:A:104:GLN:HB2	2.01	0.42
1:A:74:THR:CG2	1:A:75:GLN:HG3	2.50	0.42
1:A:226:ASN:N	1:A:226:ASN:ND2	2.66	0.42
1:A:244:TYR:CD1	1:A:244:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TRP:NE1	1:B:262:VAL:HG23	2.35	0.42
1:B:286:GLU:CG	1:B:287:GLY:H	2.33	0.42
1:A:32:ASN:HA	1:A:53:HIS:HB2	2.00	0.42
1:A:161:THR:HB	1:A:162:PRO:HD3	2.00	0.42
1:A:65:ALA:HB2	1:A:89:ASP:HB2	2.02	0.42
1:A:79:ASP:HB2	1:A:99:ASP:OD2	2.19	0.42
1:A:278:LYS:O	1:A:278:LYS:CG	2.68	0.42
1:A:39:THR:N	1:A:58:LEU:O	2.52	0.42
1:B:253:LYS:HD2	1:B:254:ALA:N	2.35	0.42
1:A:199:SER:HA	1:A:222:PRO:HD2	2.01	0.41
1:B:223:TRP:O	1:B:264:CYS:HA	2.20	0.41
1:B:248:GLN:HG2	1:B:249:GLY:H	1.85	0.41
1:A:111:LEU:HB3	1:A:115:LEU:HD12	2.02	0.41
1:B:19:ILE:O	1:B:36:ARG:NH1	2.53	0.41
1:B:76:LEU:HD23	1:B:98:LEU:CD1	2.51	0.41
1:B:201:TYR:CE1	1:B:202:THR:HG22	2.56	0.41
1:A:270:PHE:HE2	1:A:275:TYR:HA	1.84	0.41
1:A:278:LYS:O	1:A:279:GLY:C	2.62	0.41
1:B:221:ASN:HB2	1:B:223:TRP:CE2	2.55	0.41
1:B:243:VAL:HG11	1:B:259:VAL:HG23	2.03	0.41
1:A:25:VAL:O	1:A:26:ALA:HB3	2.20	0.41
1:A:143:GLN:HE22	1:B:178:GLU:CD	2.28	0.41
1:B:221:ASN:HA	1:B:222:PRO:HD3	1.81	0.41
1:A:59:LEU:C	1:A:60:TYR:CD1	2.99	0.41
1:B:53:HIS:CD2	1:B:77:ASN:ND2	2.88	0.41
1:A:156:PRO:HA	1:A:157:PRO:HD3	1.75	0.41
1:B:263:GLN:HA	1:B:272:VAL:HG12	2.03	0.41
1:A:102:HIS:HA	1:A:125:PHE:O	2.21	0.41
1:A:159:LEU:HB3	1:A:160:LEU:HD22	2.01	0.41
1:A:225:CYS:HA	1:A:229:ILE:CB	2.49	0.41
1:A:252:VAL:O	1:A:252:VAL:HG12	2.20	0.41
1:B:34:ASP:O	1:B:36:ARG:CD	2.68	0.41
1:B:194:LEU:HB3	1:B:196:GLN:NE2	2.36	0.41
1:B:214:PRO:O	1:B:242:ASN:HB3	2.20	0.41
1:B:268:ASP:OD2	1:B:269:LYS:N	2.53	0.41
1:A:55:SER:C	1:A:56:GLU:HG2	2.46	0.41
1:A:225:CYS:CB	1:A:229:ILE:HG21	2.43	0.41
1:A:136:LEU:HD12	1:A:159:LEU:HD22	2.04	0.40
1:A:222:PRO:O	1:A:223:TRP:C	2.63	0.40
1:B:123:VAL:HG12	1:B:123:VAL:O	2.21	0.40
1:A:34:ASP:OD1	1:A:55:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD11	1:A:123:VAL:CG1	2.51	0.40
1:A:45:LEU:HA	1:A:45:LEU:HD13	1.93	0.40
1:A:52:LEU:HD11	1:A:54:LEU:HG	2.03	0.40
1:A:193:LEU:HB3	1:A:213:LEU:HD21	2.03	0.40
1:B:187:LEU:N	1:B:187:LEU:CD1	2.85	0.40
1:A:31:VAL:HG11	1:A:45:LEU:HD13	2.02	0.40
1:B:158:GLY:O	1:B:161:THR:HB	2.21	0.40
1:A:133:LEU:HD22	1:A:133:LEU:HA	1.95	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:404:HOH:O	6:A:404:HOH:O[12_565]	1.97	0.23
6:B:403:HOH:O	6:B:403:HOH:O[11_556]	2.05	0.15
1:A:39:THR:CG2	1:A:39:THR:CG2[9_555]	2.12	0.08
1:B:188:GLU:OE1	1:B:188:GLU:OE1[11_556]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	264/281 (94%)	200 (76%)	40 (15%)	24 (9%)	0	1
1	B	274/281 (98%)	222 (81%)	40 (15%)	12 (4%)	2	7
All	All	538/562 (96%)	422 (78%)	80 (15%)	36 (7%)	1	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	28	HIS

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Mol	Chain	Res	Type
1	A	48	ASP
1	A	92	LEU
1	A	248	GLN
1	A	278	LYS
1	B	42	PRO
1	B	90	GLY
1	B	283	LEU
1	B	285	ASP
1	B	286	GLU
1	A	35	LYS
1	A	47	LYS
1	A	91	THR
1	A	133	LEU
1	A	152	LEU
1	A	266	ASN
1	A	273	TYR
1	A	279	GLY
1	B	41	LEU
1	B	268	ASP
1	B	273	TYR
1	A	19	ILE
1	A	43	PRO
1	A	46	PRO
1	A	135	ALA
1	B	223	TRP
1	A	45	LEU
1	A	90	GLY
1	A	102	HIS
1	A	187	LEU
1	A	226	ASN
1	B	35	LYS
1	A	268	ASP
1	B	276	PRO
1	B	281	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	236/249 (95%)	201 (85%)	35 (15%)	3	10
1	B	245/249 (98%)	210 (86%)	35 (14%)	3	11
All	All	481/498 (97%)	411 (85%)	70 (15%)	3	11

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	51	ILE
1	A	66	THR
1	A	73	LEU
1	A	74	THR
1	A	79	ASP
1	A	88	VAL
1	A	89	ASP
1	A	97	THR
1	A	105	LEU
1	A	108	LEU
1	A	114	THR
1	A	118	LEU
1	A	120	VAL
1	A	133	LEU
1	A	139	LEU
1	A	141	GLU
1	A	142	LEU
1	A	151	GLU
1	A	159	LEU
1	A	165	LYS
1	A	166	LEU
1	A	178	GLU
1	A	179	LEU
1	A	187	LEU
1	A	196	GLN
1	A	226	ASN
1	A	243	VAL
1	A	248	GLN
1	A	256	THR
1	A	263	GLN
1	A	266	ASN
1	A	272	VAL
1	A	273	TYR
1	A	280	CYS

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Mol	Chain	Res	Type
1	B	27	SER
1	B	39	THR
1	B	42	PRO
1	B	43	PRO
1	B	48	ASP
1	B	51	ILE
1	B	61	THR
1	B	64	LEU
1	B	73	LEU
1	B	85	LYS
1	B	95	LEU
1	B	118	LEU
1	B	120	VAL
1	B	130	SER
1	B	133	LEU
1	B	139	LEU
1	B	141	GLU
1	B	142	LEU
1	B	154	THR
1	B	159	LEU
1	B	160	LEU
1	B	161	THR
1	B	165	LYS
1	B	196	GLN
1	B	212	LEU
1	B	224	LEU
1	B	230	LEU
1	B	243	VAL
1	B	266	ASN
1	B	268	ASP
1	B	272	VAL
1	B	273	TYR
1	B	280	CYS
1	B	285	ASP
1	B	296	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	32	ASN
1	A	75	GLN

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Mol	Chain	Res	Type
1	A	87	GLN
1	A	113	GLN
1	A	143	GLN
1	A	185	ASN
1	A	196	GLN
1	A	211	HIS
1	A	219	HIS
1	A	226	ASN
1	A	239	ASN
1	A	266	ASN
1	B	28	HIS
1	B	53	HIS
1	B	75	GLN
1	B	77	ASN
1	B	87	GLN
1	B	102	HIS
1	B	106	GLN
1	B	173	ASN
1	B	189	ASN
1	B	196	GLN
1	B	219	HIS
1	B	237	GLN
1	B	239	ASN
1	B	242	ASN
1	B	248	GLN
1	B	263	GLN
1	B	266	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TYS	B	292	1	15,16,17	1.59	2 (13%)	15,22,24	0.45	0
1	TYS	B	294	1	15,16,17	1.68	2 (13%)	15,22,24	0.52	0
1	TYS	B	295	1	15,16,17	1.41	2 (13%)	15,22,24	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYS	B	292	1	-	1/10/11/13	0/1/1/1
1	TYS	B	294	1	-	2/10/11/13	0/1/1/1
1	TYS	B	295	1	-	2/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	TYS	OH-S	-5.53	1.47	1.58
1	B	292	TYS	OH-S	-5.20	1.48	1.58
1	B	295	TYS	OH-S	-3.65	1.51	1.58
1	B	294	TYS	OH-CZ	-2.82	1.38	1.42
1	B	292	TYS	OH-CZ	-2.57	1.38	1.42
1	B	295	TYS	CE2-CD2	2.37	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	294	TYS	C-CA-CB-CG
1	B	295	TYS	O-C-CA-CB
1	B	294	TYS	N-CA-CB-CG
1	B	292	TYS	C-CA-CB-CG
1	B	295	TYS	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	294	TYS	2	0
1	B	295	TYS	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACY	A	303	-	3,3,3	1.38	1 (33%)	3,3,3	1.60	1 (33%)
4	NAG	A	305	1	14,14,15	0.61	0	17,19,21	0.58	0
4	NAG	B	303	1	14,14,15	0.61	0	17,19,21	0.61	0
5	SO4	B	304	-	4,4,4	0.39	0	6,6,6	0.07	0
4	NAG	A	304	1	14,14,15	0.74	0	17,19,21	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	305	1	-	4/6/23/26	0/1/1/1
4	NAG	B	303	1	-	3/6/23/26	0/1/1/1
4	NAG	A	304	1	1/1/5/7	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	ACY	O-C	2.12	1.31	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	303	ACY	O-C-CH3	-2.18	113.59	122.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	304	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	NAG	C8-C7-N2-C2
4	A	304	NAG	O7-C7-N2-C2
4	A	305	NAG	C3-C2-N2-C7
4	A	305	NAG	C8-C7-N2-C2
4	A	305	NAG	O7-C7-N2-C2
4	B	303	NAG	C3-C2-N2-C7
4	B	303	NAG	C8-C7-N2-C2
4	B	303	NAG	O7-C7-N2-C2
4	A	305	NAG	O5-C5-C6-O6
4	A	304	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	NAG	3	0

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	266/281 (94%)	0.42	25 (9%) 14 10	33, 58, 90, 105	0
1	B	276/281 (98%)	0.11	24 (8%) 16 11	24, 44, 91, 115	0
All	All	542/562 (96%)	0.26	49 (9%) 15 11	24, 51, 90, 115	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	ASP	10.0
1	A	91	THR	7.2
1	B	252	VAL	7.2
1	B	254	ALA	4.9
1	B	249	GLY	4.4
1	B	90	GLY	4.2
1	B	283	LEU	4.1
1	B	250	VAL	4.1
1	A	248	GLN	3.9
1	A	18	PRO	3.9
1	A	252	VAL	3.8
1	B	212	LEU	3.5
1	A	267	SER	3.5
1	A	280	CYS	3.4
1	B	288	ASP	3.2
1	A	79	ASP	3.1
1	A	268	ASP	3.1
1	B	285	ASP	3.0
1	A	28	HIS	3.0
1	B	48	ASP	3.0
1	A	266	ASN	2.9
1	B	284	GLY	2.9
1	A	228	GLU	2.9
1	A	225	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	269	LYS	2.8
1	B	89	ASP	2.8
1	A	251	ASP	2.7
1	A	273	TYR	2.6
1	B	255	MET	2.6
1	A	80	ARG	2.6
1	B	253	LYS	2.5
1	A	265	ASP	2.4
1	A	38	LEU	2.3
1	B	91	THR	2.3
1	B	247	LYS	2.3
1	A	269	LYS	2.2
1	B	270	PHE	2.2
1	A	153	LYS	2.2
1	A	89	ASP	2.2
1	B	44	ASP	2.1
1	A	39	THR	2.1
1	B	41	LEU	2.1
1	B	79	ASP	2.1
1	B	286	GLU	2.1
1	A	185	ASN	2.0
1	A	282	THR	2.0
1	A	47	LYS	2.0
1	B	272	VAL	2.0
1	A	26	ALA	2.0

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

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(Å ²)	Q<0.9
1	TYS	B	295	16/17	0.69	0.28	84,103,114,115	0
1	TYS	B	292	16/17	0.92	0.11	61,63,72,72	0
1	TYS	B	294	16/17	0.93	0.11	74,77,79,79	0

6.3 Carbohydrates ⓘ

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
3	ACY	A	303	4/4	0.52	0.40	91,92,92,92	0
4	NAG	A	304	14/15	0.60	0.17	102,103,104,104	0
4	NAG	A	305	14/15	0.75	0.13	83,87,88,89	0
4	NAG	B	303	14/15	0.79	0.12	51,63,74,75	0
2	PT	B	302	1/1	0.95	0.09	143,143,143,143	0
2	PT	A	302	1/1	0.97	0.10	98,98,98,98	0
2	PT	A	301	1/1	0.97	0.14	117,117,117,117	0
5	SO4	B	304	5/5	0.97	0.10	70,70,70,71	0
2	PT	B	301	1/1	0.99	0.09	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.