



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 AM UTC

PDB ID : 1Q47 / pdb_00001q47
Title : Structure of the Semaphorin 3A Receptor-Binding Module
Authors : Antipenko, A.; Himanen, J.-P.; van Leyen, K.; Nardi-Dei, V.; Lesniak, J.; Barton, W.A.; Rajashankar, K.R.; Lu, M.; Hoemme, C.; Puschel, A.; Nikolov, D.
Deposited on : 2003-08-01
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

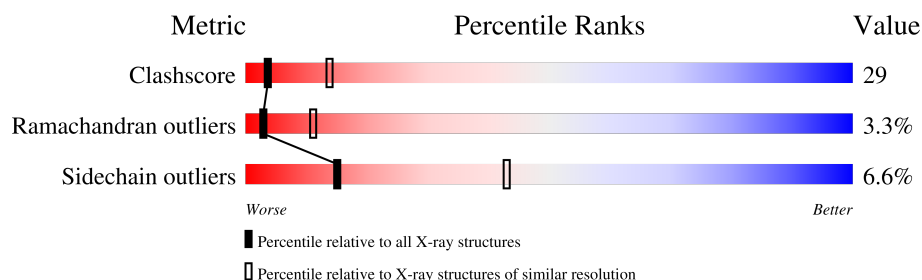
1 Overall quality at a glance

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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	495	
1	B	495	

2 Entry composition [i](#)

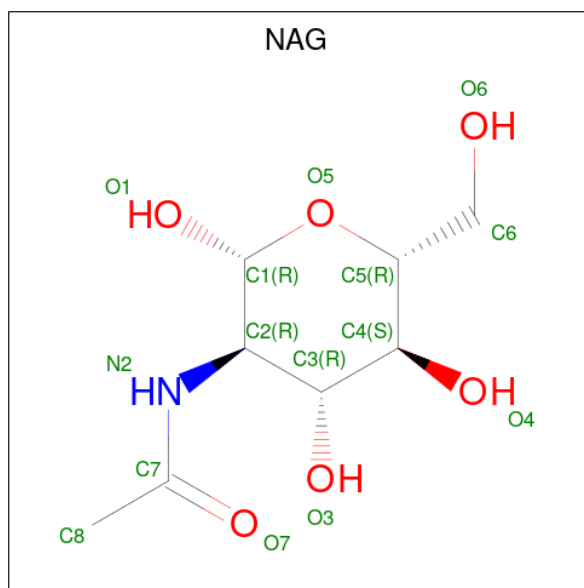
There are 2 unique types of molecules in this entry. The entry contains 7923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Semaphorin 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3883	2474	669	721	19			
1	B	495	Total	C	N	O	S	0	0	0
			3980	2536	684	741	19			

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



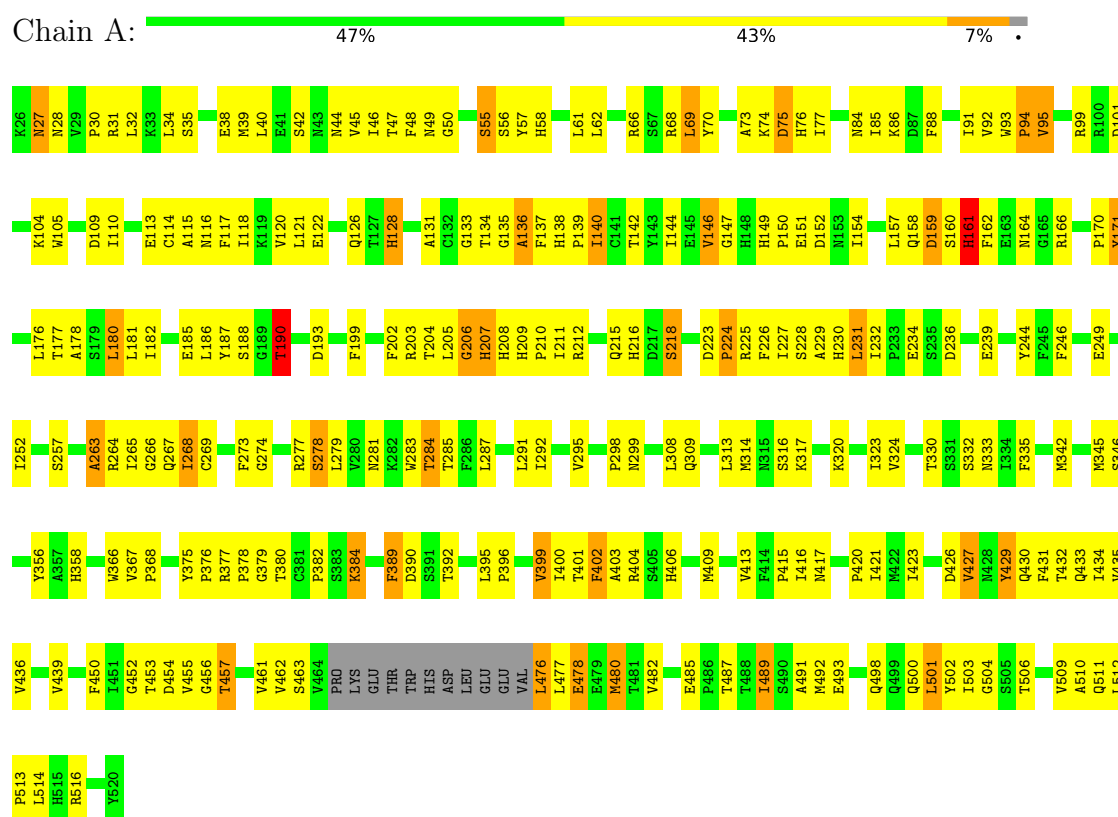
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

3 Residue-property plots

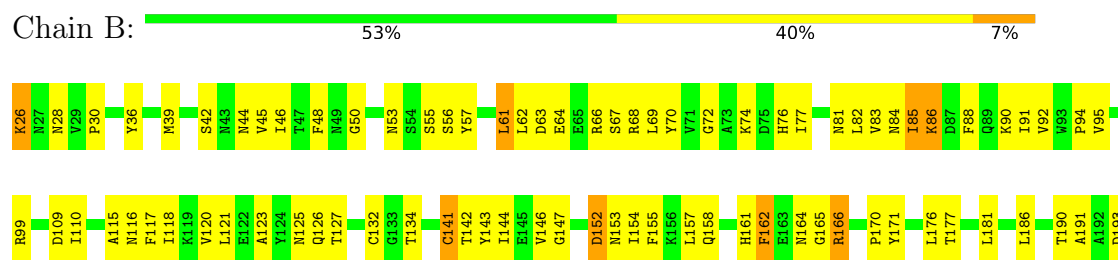
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Semaphorin 3A



• Molecule 1: Semaphorin 3A



F450		P382		L287		F194
T483		S383		R290		M195
D454				L291		D196
V455		F386		I292		F199
T457		G387		C293		
		G388		S294		F202
V461		F389				R203
		D390		P298		
K466		S391		N299		H207
E467		T392				H208
T468		K393		H304		H209
W469		D394		F305		P210
H470		L395		D306		I211
D471		P396		E307		R212
L472		D397		L308		T213
		D398				E214
L476		P399		L313		Q215
		I400		M314		H216
		T401				D217
H480		P402		K320		S218
T481		A403				
V482		R404		V324		I227
F483		S405		Y325		S228
R484		H406				A229
		P407		T329		
I489		A408		T330		I232
S490		M409		S331		
A491				S332		S235
M492		V413		N333		D236
E493		F414		I334		I237
L494		P415		F335		P238
S495		I416				E239
T496		M417		A339		
K497		M418				Y244
Q498		I421		M342		
Q499		M422		M345		H256
O500		I423				S257
L501		R424		V348		
I502		T425		R349		T261
I503		D426		R350		H262
G504		V427				A263
S505		M428		H358		
T506		Y429		R359		I268
				D360		
Q511		T432		G361		N271
L512		Q433				
P513		I434		W366		G274
		V435		V367		G275
R516		V436		P368		H276
C517		D437		Y369		R277
D518						S278
I519		A441		R372		L279
		E442		V373		V280
Y520		D443		P374		N281
		G444		Y375		K282
		V448		P376		W283
						T284
		M449		G379		T285
						F286

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.79Å 59.73Å 122.72Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.61	0/3989	1.04	21/5411 (0.4%)
1	B	0.52	1/4091 (0.0%)	0.94	10/5553 (0.2%)
All	All	0.57	1/8080 (0.0%)	0.99	31/10964 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	MET	SD-CE	5.03	1.92	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	PHE	N-CA-C	-9.51	98.40	110.19
1	B	263	ALA	N-CA-C	-9.07	97.72	110.50
1	A	126	GLN	N-CA-C	-8.35	103.08	113.18
1	B	402	PHE	N-CA-C	-8.04	100.16	110.53
1	B	498	GLN	N-CA-C	-6.96	105.72	114.56
1	A	399	VAL	N-CA-C	-6.62	104.71	110.74
1	B	379	GLY	N-CA-C	-6.53	106.59	113.58
1	A	171	TYR	N-CA-C	-6.40	105.61	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	N-CA-C	6.29	119.44	109.50
1	A	463	SER	N-CA-C	6.28	118.73	109.69
1	A	47	THR	N-CA-C	6.19	119.56	109.59
1	B	306	ASP	N-CA-C	6.18	118.09	111.36
1	B	88	PHE	N-CA-C	6.08	115.87	107.73
1	A	461	VAL	N-CA-C	6.07	117.51	108.46
1	A	284	THR	N-CA-C	-6.02	105.24	113.30
1	A	346	SER	N-CA-C	-5.88	104.46	111.69
1	A	207	HIS	N-CA-C	5.87	123.30	110.80
1	B	408	ALA	N-CA-C	5.85	119.01	109.59
1	A	480	MET	N-CA-C	5.79	118.24	107.99
1	A	478	GLU	N-CA-C	5.72	117.81	108.55
1	A	263	ALA	N-CA-C	-5.70	102.60	110.35
1	B	435	VAL	N-CA-C	-5.63	100.11	107.88
1	A	136	ALA	N-CA-C	-5.59	103.70	111.52
1	A	489	ILE	N-CA-C	-5.53	101.53	108.84
1	A	236	ASP	N-CA-C	-5.43	106.50	113.02
1	A	128	HIS	N-CA-C	5.43	117.93	109.52
1	A	190	THR	CB-CA-C	-5.41	102.71	113.80
1	A	439	VAL	N-CA-C	5.29	115.72	107.99
1	B	86	LYS	N-CA-C	-5.17	106.82	113.23
1	A	88	PHE	N-CA-C	5.04	116.50	108.79
1	B	126	GLN	N-CA-C	-5.02	107.12	113.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	TYR	Sidechain
1	A	57	TYR	Sidechain
1	B	375	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3883	0	3745	236	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3980	0	3835	221	0
2	A	30	0	27	3	0
2	B	30	0	27	4	0
All	All	7923	0	7634	452	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 29.

All (452) 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:279:LEU:HD21	1:B:404:ARG:HD3	1.41	1.02
1:A:287:LEU:HD22	1:A:409:MET:CE	1.91	0.99
1:A:273:PHE:H	1:A:392:THR:HG21	1.24	0.99
1:B:53:ASN:ND2	2:B:600:NAG:O7	2.01	0.93
1:A:287:LEU:HD22	1:A:409:MET:HE1	1.52	0.89
1:B:190:THR:HG22	1:B:191:ALA:H	1.36	0.88
1:B:116:ASN:HA	1:B:134:THR:O	1.77	0.84
1:A:128:HIS:HB2	2:A:601:NAG:H82	1.59	0.83
1:B:427:VAL:HG13	1:B:429:TYR:H	1.43	0.83
1:A:32:LEU:HD22	1:A:34:LEU:HD21	1.61	0.82
1:A:94:PRO:O	1:A:95:VAL:HB	1.77	0.81
1:B:367:VAL:HG22	1:B:368:PRO:HD2	1.63	0.80
1:A:44:ASN:OD1	1:A:516:ARG:HG3	1.81	0.80
1:A:489:ILE:HG23	1:A:503:ILE:HG23	1.64	0.80
1:B:92:VAL:HG12	1:B:94:PRO:HD3	1.66	0.78
1:A:273:PHE:N	1:A:392:THR:HG21	1.99	0.78
1:B:278:SER:HB3	1:B:400:ILE:HG21	1.66	0.78
1:A:269:CYS:SG	1:A:285:THR:HG21	2.23	0.78
1:A:152:ASP:HB2	1:A:154:ILE:HD11	1.65	0.77
1:B:237:ASN:HD21	1:B:239:GLU:HB3	1.47	0.77
1:B:237:ASN:ND2	1:B:239:GLU:HB3	1.99	0.77
1:B:453:THR:HG22	1:B:455:VAL:H	1.47	0.77
1:A:215:GLN:HE21	1:A:216:HIS:CD2	2.03	0.77
1:B:395:LEU:HD22	1:B:399:VAL:HG21	1.65	0.77
1:A:285:THR:HG22	1:A:285:THR:O	1.84	0.77
1:B:516:ARG:NE	1:B:519:ILE:HG13	1.99	0.76
1:A:453:THR:HG21	1:A:455:VAL:HG12	1.66	0.76
1:A:453:THR:CG2	1:A:455:VAL:HG12	2.17	0.75
1:A:287:LEU:HB3	1:A:409:MET:HE3	1.69	0.74
1:A:402:PHE:O	1:A:403:ALA:HB3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:HE	1:B:211:ILE:HD13	1.53	0.73
1:B:367:VAL:CG2	1:B:368:PRO:HD2	2.19	0.73
1:A:501:LEU:HD22	1:A:503:ILE:CD1	2.19	0.73
1:A:170:PRO:HD3	1:A:190:THR:HG21	1.71	0.72
1:A:273:PHE:H	1:A:392:THR:CG2	2.01	0.72
1:A:453:THR:HG22	1:A:455:VAL:H	1.54	0.72
1:A:186:LEU:HB2	1:A:205:LEU:HD22	1.71	0.72
1:B:90:LYS:HE3	2:B:600:NAG:H5	1.72	0.71
1:B:469:TRP:O	1:B:470:HIS:HB2	1.88	0.71
1:A:498:GLN:O	1:A:500:GLN:HG2	1.90	0.71
1:B:82:LEU:HD13	1:B:498:GLN:HG3	1.71	0.71
1:A:502:TYR:C	1:A:503:ILE:HD12	2.16	0.70
1:B:342:MET:SD	1:B:421:ILE:HD13	2.31	0.70
1:B:345:MET:HA	1:B:348:VAL:HG22	1.73	0.70
1:A:452:GLY:CA	1:A:492:MET:HE1	2.22	0.70
1:A:295:VAL:HG11	1:B:334:ILE:HD11	1.74	0.69
1:A:116:ASN:HA	1:A:134:THR:O	1.91	0.69
1:B:209:HIS:HD2	1:B:210:PRO:HD2	1.56	0.69
1:B:68:ARG:HE	1:B:81:ASN:HA	1.57	0.69
1:A:330:THR:HG22	1:A:332:SER:H	1.57	0.69
1:B:433:GLN:NE2	1:B:491:ALA:HA	2.07	0.69
1:A:226:PHE:O	1:A:227:ILE:HD12	1.93	0.68
1:B:203:ARG:NE	1:B:211:ILE:HD13	2.08	0.68
1:A:30:PRO:HG3	1:A:476:LEU:HD13	1.76	0.68
1:A:420:PRO:HG3	1:A:423:ILE:HD11	1.76	0.68
1:A:274:GLY:O	1:A:392:THR:HG23	1.94	0.67
1:B:235:SER:HA	1:B:320:LYS:HD3	1.76	0.67
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.58	0.67
1:A:516:ARG:HA	1:A:516:ARG:NE	2.10	0.67
1:B:276:HIS:HB2	1:B:393:LYS:O	1.95	0.67
1:B:406:HIS:N	1:B:407:PRO:HD3	2.10	0.66
1:A:95:VAL:HG23	1:A:116:ASN:HB2	1.78	0.66
1:B:432:THR:O	1:B:433:GLN:HG2	1.96	0.66
1:A:180:LEU:HD11	1:A:182:ILE:HD13	1.78	0.65
1:B:164:ASN:HD21	1:B:166:ARG:HB2	1.62	0.65
1:B:190:THR:HG22	1:B:191:ALA:N	2.10	0.65
1:A:56:SER:HA	1:A:506:THR:HG22	1.77	0.64
1:B:330:THR:HG22	1:B:332:SER:H	1.60	0.64
1:A:317:LYS:HA	1:A:317:LYS:HE2	1.79	0.64
1:B:125:ASN:HB3	2:B:601:NAG:HN2	1.61	0.64
1:B:134:THR:HG22	1:B:170:PRO:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:C	1:A:227:ILE:HD12	2.22	0.64
1:A:452:GLY:HA3	1:A:492:MET:HE1	1.79	0.64
1:A:404:ARG:HG2	1:A:404:ARG:HH11	1.62	0.64
1:A:48:PHE:CE2	1:A:50:GLY:HA2	2.33	0.64
1:A:478:GLU:CD	1:A:480:MET:HE2	2.22	0.64
1:B:404:ARG:HG2	1:B:404:ARG:NH1	2.13	0.63
1:A:85:ILE:HG12	1:A:511:GLN:HE21	1.63	0.63
1:B:227:ILE:HG13	1:B:308:LEU:CD1	2.29	0.63
1:A:203:ARG:NH2	1:A:273:PHE:CE2	2.65	0.63
1:A:218:SER:HB2	1:A:252:ILE:HD11	1.80	0.63
1:A:249:GLU:OE2	1:A:264:ARG:CD	2.47	0.62
1:B:152:ASP:O	1:B:154:ILE:HG13	1.99	0.62
1:A:396:PRO:HG2	1:A:399:VAL:HG12	1.81	0.62
1:A:85:ILE:H	1:A:511:GLN:HE22	1.45	0.62
1:A:209:HIS:HD2	1:A:210:PRO:O	1.82	0.62
1:B:492:MET:HE3	1:B:501:LEU:HD21	1.80	0.62
1:A:164:ASN:HD22	1:A:166:ARG:H	1.47	0.62
1:B:39:MET:HE3	1:B:45:VAL:HG13	1.82	0.61
1:A:85:ILE:H	1:A:511:GLN:NE2	1.99	0.61
1:A:164:ASN:ND2	1:A:166:ARG:H	1.98	0.61
1:A:154:ILE:HD12	1:A:154:ILE:H	1.65	0.61
1:A:285:THR:HG23	1:A:379:GLY:HA2	1.82	0.61
1:B:42:SER:HB2	1:B:516:ARG:HH21	1.64	0.61
1:B:227:ILE:HG13	1:B:308:LEU:HD13	1.82	0.61
1:A:268:ILE:HD13	1:A:283:TRP:CD2	2.35	0.61
1:A:427:VAL:HG21	1:A:429:TYR:OH	2.00	0.61
1:B:181:LEU:HD12	1:B:186:LEU:HD23	1.82	0.60
1:B:427:VAL:CG1	1:B:429:TYR:H	2.13	0.60
1:A:105:TRP:HA	1:A:105:TRP:CE3	2.36	0.60
1:A:313:LEU:HD22	1:A:324:VAL:HG22	1.83	0.60
1:A:118:ILE:N	1:A:118:ILE:HD12	2.16	0.60
1:B:292:ILE:O	1:B:415:PRO:HD3	2.00	0.60
1:B:44:ASN:HD21	1:B:516:ARG:NE	1.99	0.60
1:A:128:HIS:HB2	2:A:601:NAG:C8	2.29	0.59
1:A:154:ILE:HD12	1:A:154:ILE:N	2.17	0.59
1:A:501:LEU:HD22	1:A:503:ILE:HD11	1.84	0.59
1:B:95:VAL:HG21	1:B:99:ARG:HG2	1.84	0.59
1:A:66:ARG:HA	1:A:150:PRO:CB	2.32	0.59
1:B:166:ARG:HD2	1:B:171:TYR:OH	2.02	0.59
1:B:170:PRO:HB3	1:B:190:THR:CG2	2.33	0.59
1:A:135:GLY:H	1:A:139:PRO:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:O	1:A:190:THR:HG23	2.03	0.59
1:A:367:VAL:HG13	1:A:368:PRO:HD2	1.85	0.59
1:A:48:PHE:CZ	1:A:50:GLY:HA2	2.37	0.59
1:A:453:THR:HG22	1:A:455:VAL:N	2.15	0.59
1:A:46:ILE:O	1:A:85:ILE:HD11	2.03	0.59
1:A:209:HIS:CD2	1:A:210:PRO:O	2.56	0.59
1:B:198:ASP:OD1	1:B:212:ARG:NH2	2.36	0.59
1:A:66:ARG:HA	1:A:150:PRO:HB3	1.84	0.58
1:A:186:LEU:O	1:A:203:ARG:HA	2.04	0.58
1:A:493:GLU:O	1:A:501:LEU:HD23	2.04	0.58
1:B:382:PRO:HA	1:B:389:PHE:CZ	2.39	0.58
1:A:178:ALA:O	1:A:188:SER:HA	2.03	0.58
1:A:287:LEU:HD22	1:A:409:MET:HE2	1.83	0.58
1:B:211:ILE:N	1:B:211:ILE:HD12	2.19	0.58
1:A:70:TYR:OH	1:A:146:VAL:HG21	2.04	0.58
1:B:66:ARG:HD3	1:B:146:VAL:HG11	1.85	0.58
1:B:232:ILE:HD12	1:B:244:TYR:CD1	2.39	0.58
1:A:249:GLU:OE2	1:A:264:ARG:HD2	2.02	0.57
1:A:404:ARG:HG2	1:A:404:ARG:NH1	2.18	0.57
1:A:227:ILE:O	1:A:228:SER:HB3	2.04	0.57
1:A:120:VAL:O	1:A:131:ALA:HA	2.04	0.57
1:A:435:VAL:HG23	1:A:450:PHE:HB2	1.87	0.57
1:B:325:TYR:CZ	1:B:342:MET:HE3	2.40	0.57
1:A:140:ILE:H	1:A:140:ILE:HD13	1.68	0.57
1:B:472:LEU:HD23	1:B:472:LEU:H	1.69	0.57
1:B:433:GLN:HE21	1:B:491:ALA:HA	1.68	0.57
1:A:501:LEU:HD22	1:A:503:ILE:HD12	1.86	0.57
1:B:472:LEU:H	1:B:472:LEU:CD2	2.17	0.57
1:B:291:LEU:HD23	1:B:413:VAL:HG13	1.86	0.56
1:A:170:PRO:HD3	1:A:177:THR:OG1	2.05	0.56
1:A:187:TYR:CE2	1:A:203:ARG:HD3	2.40	0.56
1:A:309:GLN:HA	1:A:309:GLN:OE1	2.04	0.56
1:A:104:LYS:HD2	1:A:110:ILE:HD11	1.87	0.56
1:A:378:PRO:HG3	1:A:399:VAL:HG23	1.88	0.56
1:B:469:TRP:O	1:B:470:HIS:CB	2.54	0.56
1:A:457:THR:H	1:A:489:ILE:HD11	1.70	0.56
1:B:84:ASN:OD1	1:B:86:LYS:HB2	2.06	0.56
1:A:265:ILE:HB	1:A:291:LEU:HD11	1.87	0.56
1:B:141:CYS:SG	1:B:165:GLY:HA2	2.45	0.56
1:B:198:ASP:CG	1:B:212:ARG:HH22	2.14	0.56
1:B:376:PRO:HG2	1:B:389:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:PHE:H	1:A:389:PHE:HD2	1.53	0.55
1:B:402:PHE:C	1:B:404:ARG:H	2.14	0.55
1:A:149:HIS:C	1:A:151:GLU:H	2.13	0.55
1:A:285:THR:O	1:A:285:THR:CG2	2.52	0.55
1:B:307:GLU:HB2	1:B:329:THR:HG22	1.88	0.55
1:B:239:GLU:OE2	1:B:383:SER:HA	2.06	0.55
1:B:374:PRO:HB3	1:B:399:VAL:HG12	1.88	0.55
1:B:30:PRO:HA	1:B:476:LEU:HG	1.89	0.55
1:B:66:ARG:O	1:B:68:ARG:HG2	2.07	0.55
1:B:396:PRO:HD2	1:B:399:VAL:HG21	1.88	0.55
1:B:76:HIS:CE1	1:B:92:VAL:HG22	2.42	0.55
1:B:359:ARG:HH21	1:B:366:TRP:NE1	2.05	0.55
1:B:395:LEU:HB3	1:B:399:VAL:CG2	2.36	0.55
1:A:420:PRO:CG	1:A:423:ILE:HD11	2.37	0.54
1:A:426:ASP:N	1:A:426:ASP:OD2	2.40	0.54
1:A:249:GLU:OE2	1:A:264:ARG:HD3	2.07	0.54
1:A:32:LEU:HB2	1:A:478:GLU:HB3	1.89	0.54
1:A:93:TRP:CH2	1:A:142:THR:HG22	2.43	0.54
1:A:384:LYS:NZ	1:A:384:LYS:HB3	2.23	0.54
1:B:176:LEU:O	1:B:190:THR:HG23	2.07	0.54
1:B:427:VAL:HG13	1:B:428:ASN:N	2.23	0.54
1:A:30:PRO:HG3	1:A:476:LEU:CD1	2.37	0.54
1:A:31:ARG:HD2	1:A:31:ARG:N	2.23	0.54
1:A:56:SER:CA	1:A:506:THR:HG22	2.38	0.54
1:A:401:THR:O	1:A:404:ARG:HB3	2.07	0.54
1:A:45:VAL:HG11	1:A:482:VAL:HG13	1.88	0.53
1:B:186:LEU:O	1:B:203:ARG:HA	2.08	0.53
1:A:161:HIS:O	1:A:162:PHE:HB2	2.08	0.53
1:B:278:SER:O	1:B:280:VAL:N	2.38	0.53
1:A:279:LEU:HD12	1:A:400:ILE:HG23	1.90	0.53
1:B:359:ARG:NH2	1:B:366:TRP:NE1	2.56	0.53
1:A:218:SER:HB2	1:A:252:ILE:CD1	2.39	0.53
1:B:45:VAL:HG12	1:B:482:VAL:HG13	1.90	0.53
1:A:199:PHE:CZ	1:A:225:ARG:NH1	2.76	0.53
1:A:267:GLN:O	1:A:268:ILE:HG13	2.09	0.53
1:A:427:VAL:HG13	1:A:429:TYR:CD2	2.44	0.53
1:A:333:ASN:HB2	1:B:298:PRO:HD2	1.91	0.52
1:A:366:TRP:HB2	1:B:256:HIS:CE1	2.44	0.52
1:B:279:LEU:CD2	1:B:404:ARG:HD3	2.27	0.52
1:B:395:LEU:HB3	1:B:399:VAL:HG21	1.92	0.52
1:A:402:PHE:O	1:A:403:ALA:CB	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD11	1:B:64:GLU:OE2	2.08	0.52
1:A:134:THR:HG23	1:A:171:TYR:O	2.08	0.52
1:A:503:ILE:HD12	1:A:503:ILE:N	2.25	0.52
1:B:503:ILE:HD12	1:B:503:ILE:N	2.25	0.52
1:A:35:SER:OG	1:A:38:GLU:HG3	2.09	0.52
1:B:422:MET:HE1	1:B:461:VAL:HG21	1.91	0.52
1:A:204:THR:O	1:A:205:LEU:HB2	2.09	0.52
1:A:455:VAL:O	1:A:455:VAL:HG13	2.10	0.52
1:B:291:LEU:HD23	1:B:413:VAL:CG1	2.40	0.52
1:A:39:MET:HE3	1:A:45:VAL:HG13	1.91	0.51
1:A:335:PHE:HB3	1:B:335:PHE:CD2	2.45	0.51
1:B:46:ILE:N	1:B:46:ILE:HD12	2.26	0.51
1:B:402:PHE:O	1:B:403:ALA:HB3	2.09	0.51
1:B:48:PHE:CZ	1:B:50:GLY:HA2	2.45	0.51
1:A:46:ILE:HB	1:A:511:GLN:HB3	1.91	0.51
1:B:212:ARG:HG2	1:B:213:THR:N	2.24	0.51
1:B:489:ILE:HG23	1:B:503:ILE:HG23	1.92	0.51
1:A:274:GLY:HA2	1:A:284:THR:HG23	1.92	0.51
1:A:66:ARG:O	1:A:68:ARG:HG3	2.11	0.51
1:A:453:THR:H	1:A:489:ILE:HD12	1.75	0.51
1:A:462:VAL:CG2	1:A:477:LEU:HD11	2.41	0.51
1:B:42:SER:HB2	1:B:516:ARG:NH2	2.26	0.51
1:B:466:LYS:O	1:B:467:GLU:HG2	2.11	0.51
1:A:234:GLU:O	1:A:320:LYS:HD3	2.12	0.50
1:B:90:LYS:O	1:B:90:LYS:HG3	2.11	0.50
1:B:46:ILE:HB	1:B:511:GLN:HB3	1.94	0.50
1:B:235:SER:CA	1:B:320:LYS:HD3	2.42	0.50
1:B:427:VAL:HG11	1:B:429:TYR:CE1	2.47	0.50
1:B:203:ARG:HB2	1:B:283:TRP:CZ2	2.46	0.50
1:A:152:ASP:HB2	1:A:154:ILE:CD1	2.40	0.50
1:A:46:ILE:HD12	1:A:511:GLN:NE2	2.26	0.50
1:B:287:LEU:HD22	1:B:409:MET:CE	2.41	0.50
1:B:432:THR:C	1:B:433:GLN:HG2	2.37	0.50
1:B:345:MET:O	1:B:348:VAL:HG22	2.11	0.50
1:A:178:ALA:HB1	1:A:228:SER:HA	1.94	0.50
1:B:453:THR:HG22	1:B:455:VAL:N	2.21	0.50
1:A:109:ASP:HB3	1:A:113:GLU:HG3	1.93	0.49
1:A:206:GLY:O	1:A:208:HIS:N	2.41	0.49
1:A:399:VAL:HG13	1:A:400:ILE:H	1.77	0.49
1:A:333:ASN:HB2	1:B:298:PRO:CD	2.42	0.49
1:B:85:ILE:HG23	1:B:511:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:HB	1:B:132:CYS:HB2	1.93	0.49
1:B:212:ARG:NH2	1:B:215:GLN:HB3	2.27	0.49
1:B:367:VAL:HG22	1:B:368:PRO:CD	2.40	0.49
1:A:69:LEU:HD13	1:A:69:LEU:O	2.12	0.49
1:A:491:ALA:HB3	1:A:504:GLY:HA3	1.94	0.49
1:A:512:LEU:C	1:A:512:LEU:HD23	2.38	0.49
1:B:386:PHE:C	1:B:388:GLY:H	2.20	0.49
1:A:313:LEU:CD2	1:A:324:VAL:HG22	2.42	0.49
1:A:335:PHE:CE2	1:B:425:THR:HG23	2.47	0.49
1:B:26:LYS:NZ	1:B:26:LYS:HB2	2.27	0.49
1:B:110:ILE:N	1:B:110:ILE:HD12	2.27	0.49
1:B:67:SER:O	1:B:68:ARG:HD2	2.13	0.49
1:B:91:ILE:HG13	1:B:155:PHE:CD1	2.48	0.49
1:B:313:LEU:CD2	1:B:324:VAL:HG22	2.42	0.49
1:A:140:ILE:HD13	1:A:140:ILE:N	2.27	0.49
1:A:157:LEU:HD13	1:A:157:LEU:O	2.13	0.48
1:B:441:ALA:HB3	1:B:444:GLY:O	2.13	0.48
1:A:427:VAL:HG11	1:A:429:TYR:CE1	2.48	0.48
1:B:207:HIS:CG	1:B:208:HIS:N	2.82	0.48
1:A:118:ILE:N	1:A:118:ILE:CD1	2.76	0.48
1:A:202:PHE:CZ	1:A:212:ARG:HD2	2.48	0.48
1:A:246:PHE:CZ	1:A:265:ILE:HD12	2.49	0.48
1:A:433:GLN:HB2	1:A:492:MET:HE3	1.95	0.48
1:B:305:PHE:CD2	1:B:339:ALA:HB2	2.49	0.48
1:B:453:THR:HG22	1:B:454:ASP:N	2.27	0.48
1:B:358:HIS:HD2	1:B:406:HIS:HE1	1.61	0.48
1:B:350:ARG:HG3	1:B:350:ARG:HH11	1.78	0.48
1:A:377:ARG:O	1:A:380:THR:HB	2.14	0.48
1:B:158:GLN:HB3	1:B:161:HIS:CD2	2.49	0.48
1:B:278:SER:O	1:B:280:VAL:HG23	2.14	0.48
1:B:427:VAL:HG21	1:B:429:TYR:CZ	2.49	0.48
1:A:211:ILE:CD1	1:A:281:ASN:HA	2.44	0.47
1:B:441:ALA:C	1:B:443:ASP:H	2.22	0.47
1:A:429:TYR:O	1:A:430:GLN:HG3	2.14	0.47
1:B:146:VAL:HA	1:B:154:ILE:O	2.14	0.47
1:A:170:PRO:CD	1:A:190:THR:HG21	2.42	0.47
1:B:287:LEU:HD22	1:B:409:MET:HE1	1.95	0.47
1:A:134:THR:O	1:A:136:ALA:N	2.42	0.47
1:B:85:ILE:H	1:B:511:GLN:NE2	2.11	0.47
1:B:142:THR:OG1	1:B:143:TYR:N	2.48	0.47
1:A:263:ALA:O	1:A:264:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:VAL:HG12	1:A:510:ALA:N	2.30	0.47
1:B:77:ILE:HG12	1:B:118:ILE:HG12	1.95	0.47
1:B:110:ILE:HD12	1:B:110:ILE:H	1.80	0.47
1:A:121:LEU:C	1:A:122:GLU:HG2	2.40	0.47
1:A:427:VAL:CG1	1:A:429:TYR:H	2.27	0.47
1:B:170:PRO:HB3	1:B:190:THR:HG21	1.97	0.47
1:A:160:SER:HB3	1:A:161:HIS:CE1	2.49	0.47
1:B:62:LEU:HD23	1:B:69:LEU:HD23	1.96	0.47
1:B:209:HIS:HD2	1:B:210:PRO:CD	2.23	0.47
1:B:268:ILE:HD11	1:B:286:PHE:HB2	1.96	0.47
1:B:358:HIS:HB2	1:B:369:TYR:HB2	1.96	0.47
1:B:427:VAL:HG13	1:B:429:TYR:N	2.22	0.47
1:A:115:ALA:HB3	1:A:117:PHE:CE1	2.50	0.47
1:A:358:HIS:CD2	1:A:406:HIS:HE1	2.33	0.47
1:B:212:ARG:HG2	1:B:213:THR:H	1.79	0.47
1:B:437:ASP:HB2	1:B:494:LEU:HD21	1.96	0.47
1:A:453:THR:CG2	1:A:454:ASP:N	2.77	0.46
1:B:287:LEU:HB3	1:B:409:MET:HE3	1.98	0.46
1:A:92:VAL:HG12	1:A:94:PRO:HD3	1.98	0.46
1:A:323:ILE:N	1:A:323:ILE:HD12	2.31	0.46
1:A:84:ASN:C	1:A:86:LYS:H	2.23	0.46
1:A:287:LEU:HD11	1:A:379:GLY:HA3	1.96	0.46
1:B:215:GLN:HG3	1:B:216:HIS:ND1	2.30	0.46
1:A:27:ASN:ND2	1:A:28:ASN:H	2.14	0.46
1:A:164:ASN:ND2	1:A:166:ARG:HG3	2.31	0.46
1:A:285:THR:HG23	1:A:379:GLY:CA	2.44	0.46
1:B:62:LEU:HD13	1:B:63:ASP:N	2.30	0.46
1:A:128:HIS:ND1	2:A:601:NAG:H83	2.31	0.46
1:A:342:MET:HG3	1:A:421:ILE:CG1	2.46	0.46
1:A:482:VAL:HG12	1:A:510:ALA:HB1	1.97	0.46
1:B:85:ILE:H	1:B:511:GLN:HE22	1.64	0.46
1:B:170:PRO:HD3	1:B:190:THR:HG21	1.98	0.46
1:A:62:LEU:HD13	1:A:62:LEU:C	2.41	0.46
1:A:77:ILE:CD1	1:A:144:ILE:HD11	2.47	0.46
1:B:190:THR:CG2	1:B:191:ALA:H	2.19	0.46
1:B:298:PRO:HG2	1:B:299:ASN:H	1.81	0.46
1:A:432:THR:CG2	1:A:454:ASP:HB3	2.46	0.45
1:B:170:PRO:HB3	1:B:190:THR:HG22	1.96	0.45
1:B:208:HIS:CG	1:B:209:HIS:N	2.83	0.45
1:A:180:LEU:C	1:A:180:LEU:HD13	2.42	0.45
1:A:180:LEU:HD11	1:A:182:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HA	1:A:114:CYS:HB2	1.98	0.45
1:A:399:VAL:HG13	1:A:400:ILE:N	2.32	0.45
1:B:268:ILE:HG13	1:B:286:PHE:HA	1.99	0.45
1:B:359:ARG:HD3	1:B:361:GLY:O	2.16	0.45
1:B:450:PHE:CD2	1:B:501:LEU:HD22	2.51	0.45
1:A:427:VAL:HG13	1:A:429:TYR:CE2	2.52	0.45
1:A:181:LEU:C	1:A:181:LEU:HD23	2.42	0.45
1:B:141:CYS:O	1:B:162:PHE:HA	2.17	0.45
1:B:389:PHE:N	1:B:389:PHE:CD2	2.84	0.45
1:A:91:ILE:HD13	1:A:157:LEU:HB2	1.98	0.45
1:B:56:SER:H	1:B:506:THR:HG22	1.81	0.45
1:A:66:ARG:HA	1:A:150:PRO:HB2	1.99	0.45
1:A:453:THR:HG22	1:A:455:VAL:HG12	1.93	0.45
1:A:149:HIS:HB2	1:A:152:ASP:OD2	2.17	0.44
1:B:396:PRO:O	1:B:399:VAL:HG22	2.17	0.44
1:B:39:MET:SD	1:B:480:MET:HB3	2.57	0.44
1:B:72:GLY:HA3	1:B:118:ILE:HG21	1.98	0.44
1:A:181:LEU:HA	1:A:185:GLU:O	2.17	0.44
1:A:512:LEU:HD23	1:A:513:PRO:O	2.17	0.44
1:B:69:LEU:HD13	1:B:69:LEU:O	2.17	0.44
1:A:239:GLU:OE1	1:A:384:LYS:HG3	2.17	0.44
1:A:431:PHE:N	1:A:431:PHE:CD2	2.83	0.44
1:B:359:ARG:NH2	1:B:366:TRP:HE1	2.15	0.44
1:A:95:VAL:HG13	1:A:99:ARG:HB3	1.99	0.44
1:A:160:SER:O	1:A:161:HIS:C	2.60	0.44
1:A:263:ALA:C	1:A:264:ARG:HG2	2.42	0.44
1:A:277:ARG:O	1:A:278:SER:O	2.35	0.44
1:A:287:LEU:HD11	1:A:378:PRO:O	2.17	0.44
1:B:157:LEU:HD13	1:B:157:LEU:C	2.42	0.44
1:B:500:GLN:NE2	1:B:513:PRO:HA	2.33	0.44
1:A:502:TYR:CD1	1:A:502:TYR:N	2.85	0.44
1:B:36:TYR:CD1	1:B:484:ARG:HA	2.53	0.44
1:B:55:SER:H	1:B:74:LYS:HB3	1.83	0.44
1:B:330:THR:HG22	1:B:332:SER:N	2.32	0.44
1:A:182:ILE:CD1	1:A:231:LEU:HG	2.48	0.44
1:B:453:THR:HB	1:B:457:THR:HG22	2.00	0.44
1:A:492:MET:HG3	1:A:501:LEU:HD21	2.01	0.43
1:B:76:HIS:CE1	1:B:92:VAL:HG13	2.52	0.43
1:B:417:ASN:O	1:B:418:ASN:HB2	2.18	0.43
1:B:171:TYR:CG	1:B:194:PHE:HA	2.53	0.43
1:A:375:TYR:HA	1:A:376:PRO:C	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:HD21	1:B:83:VAL:HB	1.83	0.43
1:B:127:THR:HG22	1:B:147:GLY:C	2.43	0.43
1:B:202:PHE:CZ	1:B:212:ARG:HG3	2.54	0.43
1:B:277:ARG:HD3	1:B:397:ASP:OD1	2.18	0.43
1:A:137:PHE:CD2	1:A:171:TYR:HB3	2.53	0.43
1:B:83:VAL:HG22	1:B:498:GLN:OE1	2.18	0.43
1:B:422:MET:C	1:B:423:ILE:HG13	2.43	0.43
1:A:375:TYR:CD1	1:A:376:PRO:HA	2.53	0.43
1:B:294:SER:HB3	1:B:304:HIS:ND1	2.34	0.43
1:A:105:TRP:HA	1:A:105:TRP:HE3	1.80	0.43
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.76	0.43
1:A:285:THR:HG23	1:A:379:GLY:C	2.43	0.43
1:A:118:ILE:HA	1:A:133:GLY:CA	2.49	0.43
1:A:478:GLU:CG	1:A:480:MET:HE2	2.48	0.43
1:A:292:ILE:O	1:A:415:PRO:HD3	2.18	0.43
1:A:382:PRO:HA	1:A:389:PHE:CZ	2.53	0.43
1:B:115:ALA:HB3	1:B:117:PHE:CE1	2.53	0.43
1:B:212:ARG:HH21	1:B:215:GLN:HB3	1.83	0.43
1:B:287:LEU:HA	1:B:407:PRO:O	2.19	0.43
1:B:436:VAL:HG23	1:B:448:VAL:O	2.18	0.43
1:A:229:ALA:HA	1:A:244:TYR:O	2.19	0.43
1:B:453:THR:CG2	1:B:454:ASP:N	2.81	0.43
1:A:203:ARG:NH2	1:A:273:PHE:CZ	2.87	0.42
1:A:356:TYR:OH	1:A:377:ARG:NH1	2.52	0.42
1:A:287:LEU:CD1	1:A:379:GLY:HA3	2.49	0.42
1:B:123:ALA:O	1:B:181:LEU:HD22	2.20	0.42
1:B:77:ILE:HD13	1:B:144:ILE:HD11	2.02	0.42
1:B:299:ASN:O	1:B:299:ASN:CG	2.62	0.42
1:B:503:ILE:HG22	1:B:504:GLY:N	2.34	0.42
1:A:503:ILE:CD1	1:A:503:ILE:N	2.82	0.42
1:B:170:PRO:HD3	1:B:177:THR:OG1	2.19	0.42
1:B:237:ASN:CG	1:B:239:GLU:HB3	2.44	0.42
1:B:402:PHE:C	1:B:404:ARG:N	2.78	0.42
1:A:208:HIS:ND1	1:A:209:HIS:N	2.68	0.42
1:B:287:LEU:HD11	1:B:379:GLY:HA3	2.00	0.42
1:A:75:ASP:HB3	1:A:94:PRO:HB3	2.00	0.42
1:B:375:TYR:HA	1:B:376:PRO:C	2.45	0.42
1:B:389:PHE:N	1:B:389:PHE:HD2	2.18	0.42
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.82	0.42
1:A:434:ILE:CG1	1:A:435:VAL:N	2.83	0.42
1:B:77:ILE:CG1	1:B:118:ILE:HG12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ALA:HA	1:B:244:TYR:O	2.19	0.42
1:A:55:SER:O	1:A:73:ALA:HB1	2.19	0.42
1:A:427:VAL:HG21	1:A:429:TYR:CZ	2.55	0.42
1:B:66:ARG:CD	1:B:146:VAL:HG11	2.47	0.42
1:B:202:PHE:CE1	1:B:212:ARG:HG3	2.54	0.42
1:B:345:MET:CA	1:B:348:VAL:HG22	2.47	0.42
1:A:56:SER:HB3	1:A:58:HIS:CD2	2.54	0.41
1:A:232:ILE:HD12	1:A:345:MET:HE2	2.02	0.41
1:A:400:ILE:O	1:A:402:PHE:O	2.38	0.41
1:A:453:THR:HG22	1:A:454:ASP:N	2.34	0.41
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.83	0.41
1:B:56:SER:N	1:B:506:THR:HG22	2.35	0.41
1:B:110:ILE:H	1:B:110:ILE:CD1	2.34	0.41
1:B:472:LEU:CD2	1:B:472:LEU:N	2.83	0.41
1:A:416:ILE:O	1:A:417:ASN:HB2	2.20	0.41
1:A:500:GLN:C	1:A:514:LEU:HD21	2.45	0.41
1:B:26:LYS:NZ	1:B:466:LYS:NZ	2.68	0.41
1:B:61:LEU:HB3	1:B:70:TYR:HB2	2.01	0.41
1:B:193:ASP:OD1	1:B:195:MET:HB2	2.20	0.41
1:B:203:ARG:HB2	1:B:283:TRP:HZ2	1.85	0.41
1:B:261:THR:HG22	1:B:262:HIS:N	2.35	0.41
1:A:223:ASP:N	1:A:224:PRO:CD	2.83	0.41
1:B:518:ASP:O	1:B:519:ILE:HG12	2.21	0.41
1:A:77:ILE:HD13	1:A:144:ILE:HD11	2.02	0.41
1:A:427:VAL:HG12	1:A:429:TYR:H	1.85	0.41
1:B:395:LEU:CD2	1:B:399:VAL:HG21	2.43	0.41
1:A:74:LYS:O	1:A:76:HIS:N	2.54	0.41
1:A:229:ALA:C	1:A:230:HIS:CD2	2.99	0.41
1:B:57:TYR:HE1	1:B:506:THR:O	2.04	0.41
1:B:191:ALA:HA	1:B:199:PHE:HA	2.02	0.41
1:B:209:HIS:CD2	1:B:210:PRO:HD2	2.46	0.41
1:A:244:TYR:HA	1:A:266:GLY:O	2.21	0.41
1:A:342:MET:HG3	1:A:421:ILE:HG12	2.02	0.41
1:B:56:SER:HA	1:B:506:THR:HG22	2.02	0.41
1:B:207:HIS:CG	1:B:208:HIS:H	2.38	0.41
1:B:212:ARG:HH21	1:B:215:GLN:CB	2.34	0.41
1:B:396:PRO:HD2	1:B:399:VAL:CG2	2.50	0.41
1:A:392:THR:O	1:A:395:LEU:HD12	2.21	0.41
1:B:77:ILE:HG22	1:B:155:PHE:HZ	1.86	0.41
1:B:450:PHE:HD2	1:B:501:LEU:HD22	1.86	0.41
2:B:601:NAG:O3	2:B:601:NAG:C7	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:C	1:A:50:GLY:H	2.29	0.40
1:A:268:ILE:HD13	1:A:283:TRP:CE2	2.56	0.40
1:A:399:VAL:O	1:A:400:ILE:C	2.64	0.40
1:B:157:LEU:HD13	1:B:158:GLN:N	2.35	0.40
1:A:402:PHE:O	1:A:404:ARG:N	2.50	0.40
1:A:316:SER:HB2	1:A:323:ILE:CD1	2.50	0.40
1:A:482:VAL:HG12	1:A:482:VAL:O	2.21	0.40
1:B:274:GLY:HA2	1:B:282:LYS:O	2.20	0.40
1:B:26:LYS:HZ2	1:B:466:LYS:HZ2	1.69	0.40
1:A:135:GLY:HA3	1:A:138:HIS:O	2.21	0.40
1:B:208:HIS:CG	1:B:209:HIS:H	2.39	0.40
1:B:212:ARG:O	1:B:282:LYS:HA	2.21	0.40

There are no symmetry-related clashes.

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	480/495 (97%)	408 (85%)	55 (12%)	17 (4%)	3	10
1	B	493/495 (100%)	410 (83%)	68 (14%)	15 (3%)	3	12
All	All	973/990 (98%)	818 (84%)	123 (13%)	32 (3%)	3	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	207	HIS
1	A	257	SER
1	B	153	ASN
1	B	372	ARG
1	B	443	ASP

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Mol	Chain	Res	Type
1	B	516	ARG
1	A	42	SER
1	A	75	ASP
1	A	95	VAL
1	A	147	GLY
1	A	158	GLN
1	A	159	ASP
1	A	206	GLY
1	A	278	SER
1	A	456	GLY
1	B	85	ILE
1	B	162	PHE
1	B	307	GLU
1	B	391	SER
1	B	470	HIS
1	B	497	LYS
1	A	55	SER
1	B	279	LEU
1	A	49	ASN
1	B	257	SER
1	A	299	ASN
1	B	466	LYS
1	B	519	ILE
1	A	298	PRO
1	B	298	PRO
1	A	146	VAL

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	428/439 (98%)	400 (94%)	28 (6%)	15	43
1	B	439/439 (100%)	410 (93%)	29 (7%)	15	43
All	All	867/878 (99%)	810 (93%)	57 (7%)	15	43

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	40	LEU
1	A	61	LEU
1	A	69	LEU
1	A	94	PRO
1	A	101	ASP
1	A	140	ILE
1	A	159	ASP
1	A	161	HIS
1	A	180	LEU
1	A	190	THR
1	A	218	SER
1	A	224	PRO
1	A	231	LEU
1	A	268	ILE
1	A	308	LEU
1	A	314	MET
1	A	384	LYS
1	A	389	PHE
1	A	390	ASP
1	A	413	VAL
1	A	427	VAL
1	A	436	VAL
1	A	457	THR
1	A	476	LEU
1	A	485	GLU
1	A	487	THR
1	A	501	LEU
1	B	26	LYS
1	B	28	ASN
1	B	61	LEU
1	B	109	ASP
1	B	121	LEU
1	B	141	CYS
1	B	152	ASP
1	B	166	ARG
1	B	195	MET
1	B	210	PRO
1	B	211	ILE
1	B	218	SER
1	B	268	ILE
1	B	271	ASN
1	B	284	THR

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Mol	Chain	Res	Type
1	B	290	ARG
1	B	308	LEU
1	B	314	MET
1	B	329	THR
1	B	389	PHE
1	B	413	VAL
1	B	417	ASN
1	B	426	ASP
1	B	427	VAL
1	B	436	VAL
1	B	469	TRP
1	B	472	LEU
1	B	482	VAL
1	B	496	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	27	ASN
1	A	28	ASN
1	A	76	HIS
1	A	89	GLN
1	A	158	GLN
1	A	164	ASN
1	A	209	HIS
1	A	215	GLN
1	A	216	HIS
1	A	256	HIS
1	A	262	HIS
1	A	358	HIS
1	A	365	GLN
1	A	370	GLN
1	A	406	HIS
1	A	411	ASN
1	A	417	ASN
1	A	430	GLN
1	A	511	GLN
1	B	27	ASN
1	B	76	HIS
1	B	81	ASN
1	B	138	HIS
1	B	161	HIS

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Mol	Chain	Res	Type
1	B	164	ASN
1	B	209	HIS
1	B	267	GLN
1	B	281	ASN
1	B	315	ASN
1	B	358	HIS
1	B	363	ASN
1	B	365	GLN
1	B	406	HIS
1	B	411	ASN
1	B	417	ASN
1	B	430	GLN
1	B	433	GLN
1	B	500	GLN
1	B	511	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
2	NAG	B	601	-	15,15,15	0.56	0	21,21,21	0.65	0
2	NAG	A	600	-	15,15,15	0.74	0	21,21,21	1.04	1 (4%)
2	NAG	A	601	-	15,15,15	0.65	0	21,21,21	1.31	2 (9%)
2	NAG	B	600	-	15,15,15	0.51	0	21,21,21	0.64	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
2	NAG	B	601	-	-	6/6/26/26	0/1/1/1
2	NAG	A	600	-	-	4/6/26/26	0/1/1/1
2	NAG	A	601	-	-	3/6/26/26	0/1/1/1
2	NAG	B	600	-	-	3/6/26/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAG	C4-C3-C2	-3.83	104.82	110.40
2	A	601	NAG	O5-C1-C2	2.80	112.33	109.52
2	A	600	NAG	C1-C2-N2	-2.03	108.37	110.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAG	C8-C7-N2-C2
2	A	600	NAG	O7-C7-N2-C2
2	A	601	NAG	C3-C2-N2-C7
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	B	600	NAG	C8-C7-N2-C2
2	B	600	NAG	O7-C7-N2-C2
2	B	601	NAG	C1-C2-N2-C7
2	B	601	NAG	C8-C7-N2-C2
2	B	601	NAG	O7-C7-N2-C2
2	A	600	NAG	O5-C5-C6-O6
2	B	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	600	NAG	C4-C5-C6-O6
2	B	601	NAG	C3-C2-N2-C7
2	B	600	NAG	O5-C5-C6-O6
2	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAG	2	0
2	A	601	NAG	3	0
2	B	600	NAG	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.