



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 12:52 PM EST

PDB ID : 1Q47
Title : Structure of the Semaphorin 3A Receptor-Binding Module
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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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

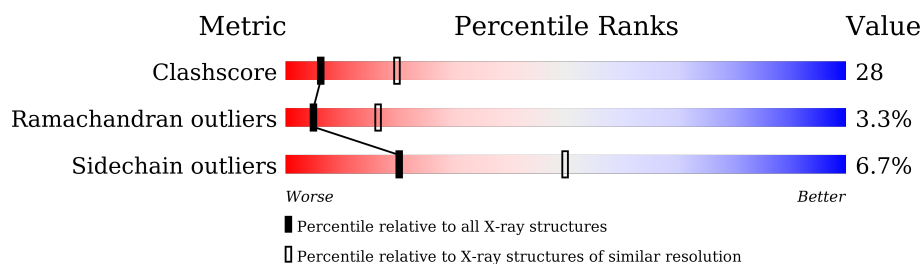
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

2 Entry composition [i](#)

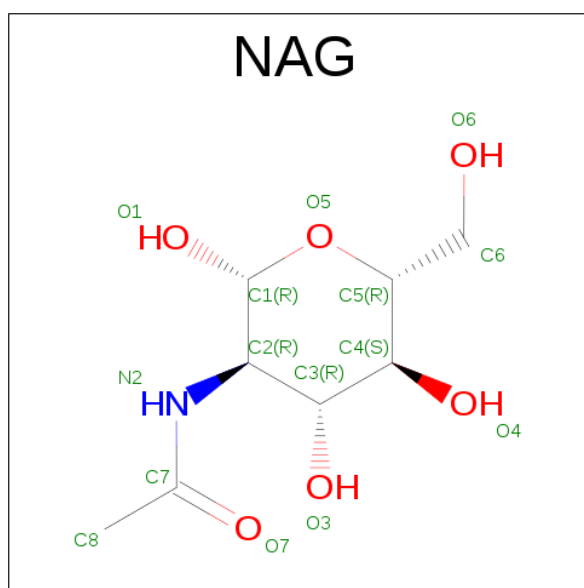
There are 2 unique types of molecules in this entry. The entry contains 7923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



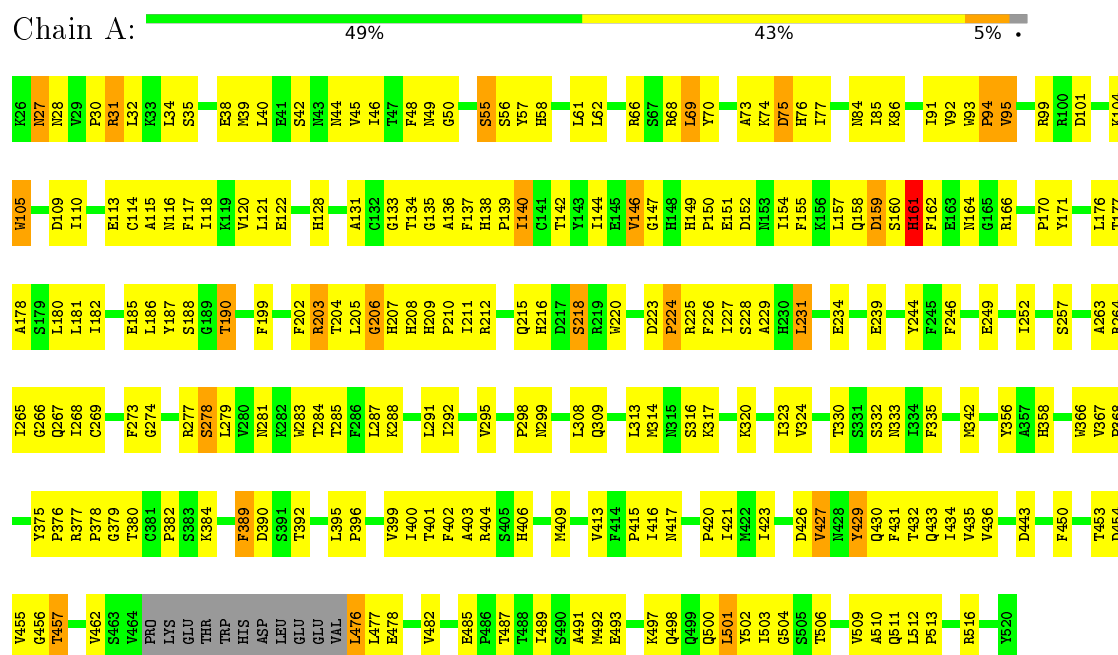
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

3 Residue-property plots

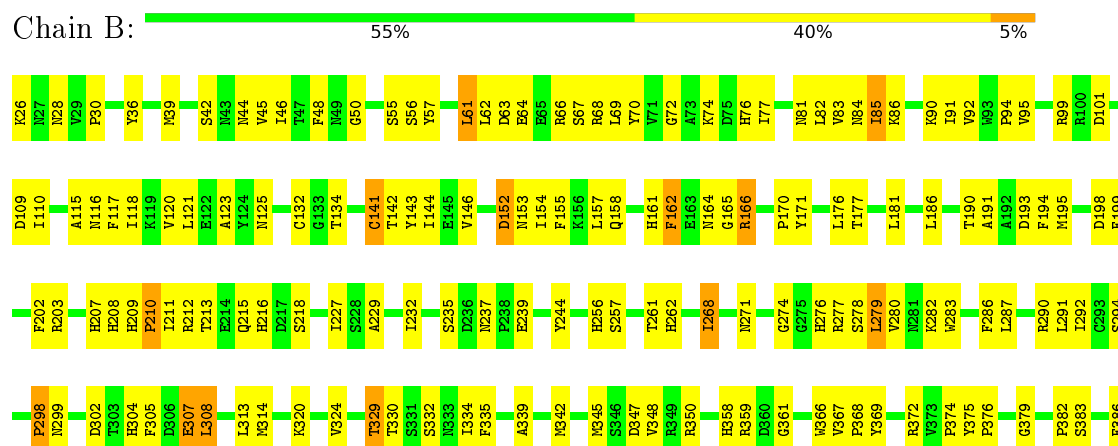
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Semaphorin 3A



• Molecule 1: Semaphorin 3A



T457	G387	G388	G389	S391	T392	K393	T394	T395	T396	T397	T398	T399	T400	T401	F402	F403	F404	S405	H406	P407	A408	M409	V413	F414	P415	F416	M417	N418	I421	M422	T425	D426	V427	M428	Y429	T432	Q433	T434	V435	F436	D437	A441	E442	D443	G444	V448	M449	F450	T453	D454	V455	T456
V461	K466	E467	T468	H470	D471	L472	L476	M480	T481	V482	F483	R484	I489	S490	A491	M492	E493	L494	S495	T496	K497	Q498	Q499	Q500	L501	Y502	I503	G504	S505	T506	Q511	L512	P513	R516	C517	D518	I519	Y520														

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	218.79 Å 59.73 Å 122.72 Å 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 [i](#)

5.1 Standard geometry [i](#)

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	0.53	0/3989	0.72	0/5411
1	B	0.48	0/4091	0.65	0/5553
All	All	0.50	0/8080	0.69	0/10964

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

There are no bond length outliers.

There are no bond angle outliers.

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	226	0
1	B	3980	0	3835	212	0
2	A	30	0	27	3	0
2	B	30	0	27	3	0
All	All	7923	0	7634	433	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 28.

All (433) 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:A:287:LEU:HD22	1:A:409:MET:HE1	1.55	0.88
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:B:287:LEU:HD22	1:B:409:MET:HE1	1.68	0.76
1:A:453:THR:HG21	1:A:455:VAL:HG12	1.66	0.76
1:A:287:LEU:HB3	1:A:409:MET:HE3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:THR:CG2	1:A:455:VAL:HG12	2.17	0.75
1:A:402:PHE:O	1:A:403:ALA:HB3	1.86	0.74
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:469:TRP:O	1:B:470:HIS:HB2	1.88	0.71
1:B:90:LYS:HE3	2:B:600:NAG:H5	1.72	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: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: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:A:433:GLN:HB2	1:A:492:MET:HE3	1.76	0.67
1:B:235:SER:HA	1:B:320:LYS:HD3	1.76	0.67
1:B:404:ARG:HG2	1:B:404:ARG:HH11	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:502:TYR:C	1:A:503:ILE:HD12	2.16	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:HE2	1:A:317:LYS:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.62	0.64
1:A:48:PHE:CE2	1:A:50:GLY:HA2	2.33	0.64
1:B:404:ARG:HG2	1:B:404:ARG:NH1	2.13	0.63
1:A:287:LEU:HD22	1:A:409:MET:HE2	1.79	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:218:SER:HB2	1:A:252:ILE:HD11	1.80	0.63
1:A:203:ARG:NH2	1:A:273:PHE:CE2	2.65	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:A:164:ASN:HD22	1:A:166:ARG:H	1.47	0.62
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:H	1:A:154:ILE:HD12	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:HD12	1:A:118:ILE:N	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:226:PHE:C	1:A:227:ILE:HD12	2.22	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
1:A:176:LEU:O	1:A:190:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:VAL:HG13	1:A:368:PRO:HD2	1.85	0.59
1:A:453:THR:HG22	1:A:455:VAL:N	2.15	0.59
1:A:48:PHE:CZ	1:A:50:GLY:HA2	2.37	0.59
1:A:209:HIS:CD2	1:A:210:PRO:O	2.56	0.59
1:A:46:ILE:O	1:A:85:ILE:HD11	2.03	0.59
1:B:198:ASP:OD1	1:B:212:ARG:NH2	2.36	0.59
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:A:66:ARG:HA	1:A:150:PRO:HB3	1.84	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: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:NH1	1:A:404:ARG:HG2	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:A:140:ILE:H	1:A:140:ILE:HD13	1.68	0.57
1:B:472:LEU:H	1:B:472:LEU:HD23	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:309:GLN:HA	1:A:309:GLN:OE1	2.04	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: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:376:PRO:HG2	1:B:389:PHE:CZ	2.41	0.55
1:A:389:PHE:H	1:A:389:PHE:HD2	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:396:PRO:HD2	1:B:399:VAL:HG21	1.88	0.55
1:B:66:ARG:O	1:B:68:ARG:HG2	2.07	0.55
1:B:395:LEU:HB3	1:B:399:VAL:CG2	2.36	0.55
1:B:76:HIS:CE1	1:B:92:VAL:HG22	2.42	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:31:ARG:N	1:A:31:ARG:HD2	2.23	0.54
1:A:401:THR:O	1:A:404:ARG:HB3	2.07	0.54
1:A:30:PRO:HG3	1:A:476:LEU:CD1	2.37	0.54
1:A:56:SER:CA	1:A:506:THR:HG22	2.38	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:366:TRP:HB2	1:B:256:HIS:CE1	2.44	0.52
1:A:333:ASN:HB2	1:B:298:PRO:HD2	1.91	0.52
1:B:395:LEU:HB3	1:B:399:VAL:HG21	1.92	0.52
1:B:279:LEU:CD2	1:B:404:ARG:HD3	2.27	0.52
1:A:402:PHE:O	1:A:403:ALA:CB	2.52	0.52
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:N	1:A:503:ILE:HD12	2.25	0.52
1:B:503:ILE:N	1:B:503:ILE:HD12	2.25	0.52
1:A:35:SER:OG	1:A:38:GLU:HG3	2.09	0.52
1:A:204:THR:O	1:A:205:LEU:HB2	2.09	0.52
1:A:455:VAL:HG13	1:A:455:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:HD23	1:B:413:VAL:CG1	2.40	0.52
1:A:335:PHE:HB3	1:B:335:PHE:CD2	2.45	0.51
1:B:402:PHE:O	1:B:403:ALA:HB3	2.09	0.51
1:B:46:ILE:N	1:B:46:ILE:HD12	2.26	0.51
1:B:48:PHE:CZ	1:B:50:GLY:HA2	2.45	0.51
1:A:39:MET:HE3	1:A:44:ASN:HB3	1.90	0.51
1:A:46:ILE:HB	1:A:511:GLN:HB3	1.91	0.51
1:B:198:ASP:CG	1:B:212:ARG:HH22	2.14	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:462:VAL:CG2	1:A:477:LEU:HD11	2.41	0.51
1:A:453:THR:H	1:A:489:ILE:HD12	1.75	0.51
1:A:66:ARG:O	1:A:68:ARG:HG3	2.11	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:149:HIS:C	1:A:151:GLU:H	2.13	0.51
1:B:402:PHE:C	1:B:404:ARG:H	2.14	0.51
1:A:234:GLU:O	1:A:320:LYS:HD3	2.12	0.50
1:B:90:LYS:HG3	1:B:90:LYS:O	2.11	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:46:ILE:HB	1:B:511:GLN:HB3	1.94	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: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
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:491:ALA:HB3	1:A:504:GLY:HA3	1.94	0.49
1:A:69:LEU:O	1:A:69:LEU:HD13	2.12	0.49
1:A:313:LEU:CD2	1:A:324:VAL:HG22	2.42	0.49
1:B:110:ILE:N	1:B:110:ILE:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HB2	1:B:26:LYS:NZ	2.27	0.49
1:A:335:PHE:CE2	1:B:425:THR:HG23	2.47	0.49
1:B:67:SER:O	1:B:68:ARG:HD2	2.13	0.49
1:B:313:LEU:CD2	1:B:324:VAL:HG22	2.42	0.49
1:B:91:ILE:HG13	1:B:155:PHE:CD1	2.48	0.49
1:A:140:ILE:HD13	1:A:140:ILE:N	2.27	0.49
1:A:157:LEU:O	1:A:157:LEU:HD13	2.13	0.48
1:B:287:LEU:HD22	1:B:409:MET:CE	2.41	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: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:HH11	1:B:350:ARG:HG3	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: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:A:134:THR:O	1:A:136:ALA:N	2.42	0.47
1:B:142:THR:OG1	1:B:143:TYR:N	2.48	0.47
1:B:85:ILE:H	1:B:511:GLN:NE2	2.11	0.47
1:A:263:ALA:O	1:A:264:ARG:HG2	2.15	0.47
1:A:509:VAL:HG12	1:A:510:ALA:N	2.30	0.47
1:B:110:ILE:H	1:B:110:ILE:HD12	1.80	0.47
1:B:77:ILE:HG12	1:B:118:ILE:HG12	1.95	0.47
1:B:170:PRO:HB3	1:B:190:THR:HG21	1.97	0.47
1:A:427:VAL:CG1	1:A:429:TYR:H	2.27	0.47
1:A:160:SER:HB3	1:A:161:HIS:CE1	2.49	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:B:62:LEU:HD23	1:B:69:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:323:ILE:N	1:A:323:ILE:HD12	2.31	0.46
1:A:92:VAL:HG12	1:A:94:PRO:HD3	1.98	0.46
1:A:287:LEU:HD11	1:A:379:GLY:HA3	1.96	0.46
1:B:208:HIS:CG	1:B:209:HIS:N	2.83	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:342:MET:HG3	1:A:421:ILE:CG1	2.46	0.46
1:A:128:HIS:ND1	2:A:601:NAG:H83	2.31	0.46
1:A:482:VAL:HG12	1:A:510:ALA:HB1	1.97	0.46
1:B:170:PRO:HD3	1:B:190:THR:HG21	1.98	0.46
1:B:85:ILE:H	1:B:511:GLN:HE22	1.64	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:432:THR:C	1:B:433:GLN:HG2	2.37	0.45
1:A:180:LEU:HD11	1:A:182:ILE:CD1	2.46	0.45
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:220:TRP:O	1:A:288:LYS:NZ	2.45	0.45
1:B:141:CYS:O	1:B:162:PHE:HA	2.17	0.45
1:B:389:PHE:CD2	1:B:389:PHE:N	2.84	0.45
1:B:422:MET:HE1	1:B:461:VAL:HG21	1.99	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:453:THR:HG22	1:A:455:VAL:HG12	1.93	0.45
1:A:66:ARG:HA	1:A:150:PRO:HB2	1.99	0.45
1:A:149:HIS:HB2	1:A:152:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PRO:O	1:B:399:VAL:HG22	2.17	0.44
1:A:512:LEU:HD23	1:A:512:LEU:C	2.38	0.44
1:B:72:GLY:HA3	1:B:118:ILE:HG21	1.98	0.44
1:B:386:PHE:C	1:B:388:GLY:H	2.20	0.44
1:B:39:MET:SD	1:B:480:MET:HB3	2.57	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: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:A:95:VAL:HG13	1:A:99:ARG:HB3	1.99	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:A:287:LEU:CD2	1:A:409:MET:HE1	2.39	0.44
1:B:330:THR:HG22	1:B:332:SER:N	2.32	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: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:417:ASN:O	1:B:418:ASN:HB2	2.18	0.43
1:B:76:HIS:CE1	1:B:92:VAL:HG13	2.52	0.43
1:B:171:TYR:CG	1:B:194:PHE:HA	2.53	0.43
1:B:422:MET:HE3	1:B:461:VAL:HG11	1.99	0.43
1:A:39:MET:HE3	1:A:45:VAL:HG13	2.00	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:B:81:ASN:HD21	1:B:83:VAL:HB	1.83	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: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:HE3	1:A:105:TRP:HA	1.80	0.43
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.76	0.43
1:B:492:MET:HE3	1:B:501:LEU:HD21	2.00	0.43
1:B:453:THR:CG2	1:B:454:ASP:N	2.81	0.43
1:A:118:ILE:HA	1:A:133:GLY:CA	2.49	0.43
1:B:441:ALA:C	1:B:443:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HA	1:A:389:PHE:CZ	2.53	0.43
1:A:292:ILE:O	1:A:415:PRO:HD3	2.18	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:435:VAL:HG22	1:B:492:MET:HE2	1.99	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: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:B:132:CYS:HG	1:B:141:CYS:HB3	1.84	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:503:ILE:HG22	1:B:504:GLY:N	2.34	0.42
1:B:77:ILE:HD13	1:B:144:ILE:HD11	2.02	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: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:389:PHE:HD2	1:B:389:PHE:N	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
1:B:229:ALA:HA	1:B:244:TYR:O	2.19	0.42
1:A:121:LEU:C	1:A:122:GLU:HG2	2.40	0.42
1:A:427:VAL:HG21	1:A:429:TYR:CZ	2.55	0.42
1:A:55:SER:O	1:A:73:ALA:HB1	2.19	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:B:66:ARG:CD	1:B:146:VAL:HG11	2.47	0.42
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:A:56:SER:HB3	1:A:58:HIS:CD2	2.54	0.41
1:A:84:ASN:C	1:A:86:LYS:H	2.23	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:B:56:SER:N	1:B:506:THR:HG22	2.35	0.41
1:A:416:ILE:O	1:A:417:ASN:HB2	2.20	0.41
1:B:193:ASP:OD1	1:B:195:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:401:THR:C	1:A:402:PHE:O	2.58	0.41
1:A:427:VAL:HG12	1:A:429:TYR:H	1.85	0.41
1:A:77:ILE:HD13	1:A:144:ILE:HD11	2.02	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:B:191:ALA:HA	1:B:199:PHE:HA	2.02	0.41
1:B:57:TYR:HE1	1:B:506:THR:O	2.04	0.41
1:A:62:LEU:C	1:A:62:LEU:HD13	2.41	0.41
1:B:209:HIS:CD2	1:B:210:PRO:HD2	2.46	0.41
1:B:26:LYS:HZ2	1:B:466:LYS:HZ2	1.69	0.41
1:A:342:MET:HG3	1:A:421:ILE:HG12	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:B:56:SER:HA	1:B:506:THR:HG22	2.02	0.41
1:A:244:TYR:HA	1:A:266:GLY:O	2.21	0.41
1:A:180:LEU:HD13	1:A:180:LEU:C	2.42	0.41
1:A:392:THR:O	1:A:395:LEU:HD12	2.21	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
1:B:77:ILE:HG22	1:B:155:PHE:HZ	1.86	0.41
1:A:268:ILE:HD13	1:A:283:TRP:CE2	2.56	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: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%)	4	15
1	B	493/495 (100%)	410 (83%)	68 (14%)	15 (3%)	5	18
All	All	973/990 (98%)	818 (84%)	123 (13%)	32 (3%)	5	16

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
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

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Mol	Chain	Res	Type
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%)	397 (93%)	31 (7%)	18	45
1	B	439/439 (100%)	412 (94%)	27 (6%)	23	54
All	All	867/878 (99%)	809 (93%)	58 (7%)	20	50

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	31	ARG
1	A	40	LEU
1	A	61	LEU
1	A	69	LEU
1	A	94	PRO
1	A	101	ASP
1	A	105	TRP
1	A	140	ILE
1	A	155	PHE
1	A	159	ASP
1	A	161	HIS
1	A	190	THR
1	A	203	ARG
1	A	218	SER
1	A	224	PRO

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Mol	Chain	Res	Type
1	A	231	LEU
1	A	308	LEU
1	A	314	MET
1	A	389	PHE
1	A	390	ASP
1	A	413	VAL
1	A	427	VAL
1	A	436	VAL
1	A	443	ASP
1	A	457	THR
1	A	476	LEU
1	A	485	GLU
1	A	487	THR
1	A	497	LYS
1	A	501	LEU
1	B	28	ASN
1	B	61	LEU
1	B	101	ASP
1	B	109	ASP
1	B	121	LEU
1	B	141	CYS
1	B	152	ASP
1	B	166	ARG
1	B	210	PRO
1	B	218	SER
1	B	268	ILE
1	B	271	ASN
1	B	290	ARG
1	B	302	ASP
1	B	308	LEU
1	B	314	MET
1	B	329	THR
1	B	347	ASP
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	496	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	76	HIS
1	A	164	ASN
1	A	209	HIS
1	A	215	GLN
1	A	216	HIS
1	A	370	GLN
1	A	406	HIS
1	A	411	ASN
1	A	417	ASN
1	A	433	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
1	B	164	ASN
1	B	209	HIS
1	B	215	GLN
1	B	267	GLN
1	B	281	ASN
1	B	315	ASN
1	B	358	HIS
1	B	365	GLN
1	B	406	HIS
1	B	411	ASN
1	B	417	ASN
1	B	433	GLN
1	B	445	GLN
1	B	499	GLN
1	B	500	GLN
1	B	511	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	600	1	15,15,15	0.71	0	17,21,21	0.77	0
2	NAG	A	601	1	15,15,15	0.64	0	17,21,21	1.18	1 (5%)
2	NAG	B	600	1	15,15,15	0.48	0	17,21,21	0.61	0
2	NAG	B	601	1	15,15,15	0.55	0	17,21,21	0.65	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	A	600	1	-	0/6/26/26	0/1/1/1
2	NAG	A	601	1	-	2/6/26/26	0/1/1/1
2	NAG	B	600	1	-	0/6/26/26	0/1/1/1
2	NAG	B	601	1	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAG	C4-C3-C2	-3.66	104.82	110.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	3	0
2	B	600	NAG	1	0
2	B	601	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.