



Full wwPDB EM Validation Report ⓘ

Sep 14, 2025 – 12:23 AM JST

PDB ID : 9J6Z / pdb_00009j6z
EMDB ID : EMD-61190
Title : Structure of AAV8 in complex with its receptor
Authors : Xu, H.; Wang, G.P.; Su, X.D.
Deposited on : 2024-08-17
Resolution : 3.02 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

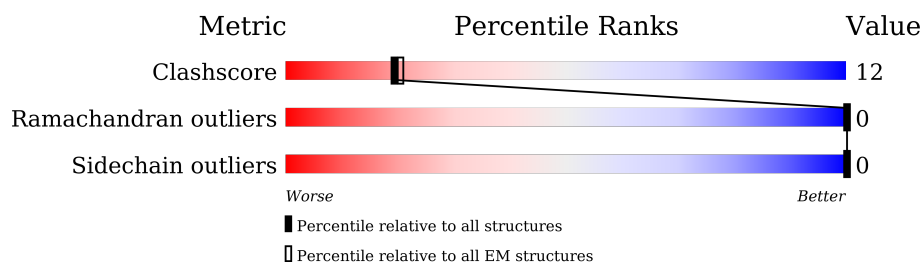
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	5	738	
1	6	738	
1	7	738	
1	c	738	
1	o	738	
1	p	738	
2	A	470	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16127 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	82	Total	C	N	O	S	0	0
			637	397	112	125	3		
1	6	391	Total	C	N	O	S	0	0
			3185	2036	541	596	12		
1	7	335	Total	C	N	O	S	0	0
			2660	1701	453	496	10		
1	c	203	Total	C	N	O	S	0	0
			1643	1034	290	314	5		
1	o	475	Total	C	N	O	S	0	0
			3823	2429	657	724	13		
1	p	166	Total	C	N	O	S	0	0
			1308	835	227	241	5		

- Molecule 2 is a protein called Carboxypeptidase D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	365	Total	C	N	O	S	0	0
			2871	1815	503	544	9		

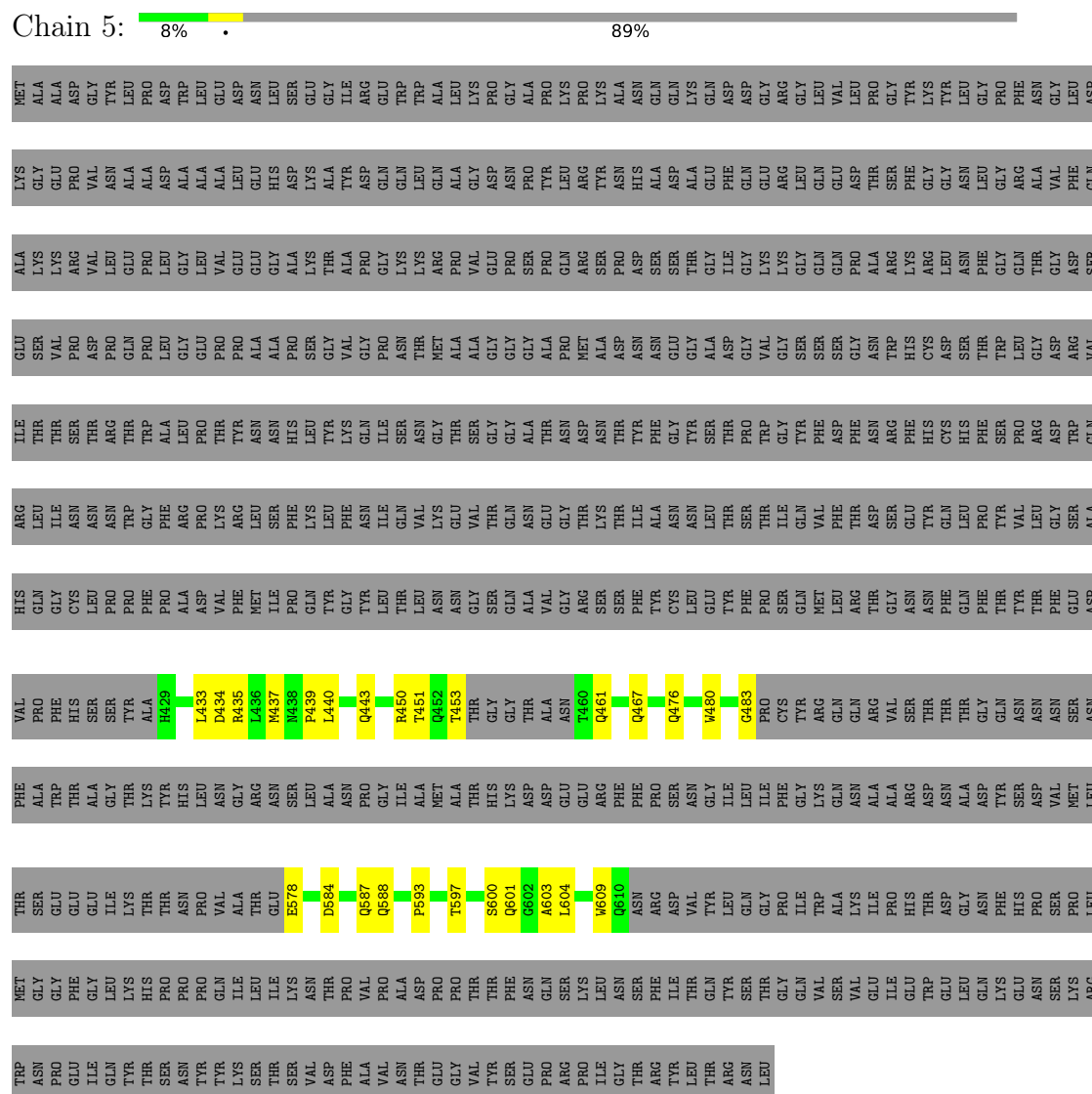
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	expression tag	UNP O75976
A	495	HIS	-	expression tag	UNP O75976
A	496	HIS	-	expression tag	UNP O75976
A	497	HIS	-	expression tag	UNP O75976
A	498	HIS	-	expression tag	UNP O75976
A	499	HIS	-	expression tag	UNP O75976
A	500	HIS	-	expression tag	UNP O75976
A	501	HIS	-	expression tag	UNP O75976

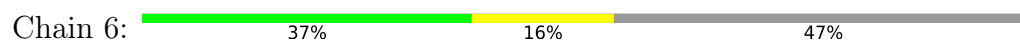
3 Residue-property plots

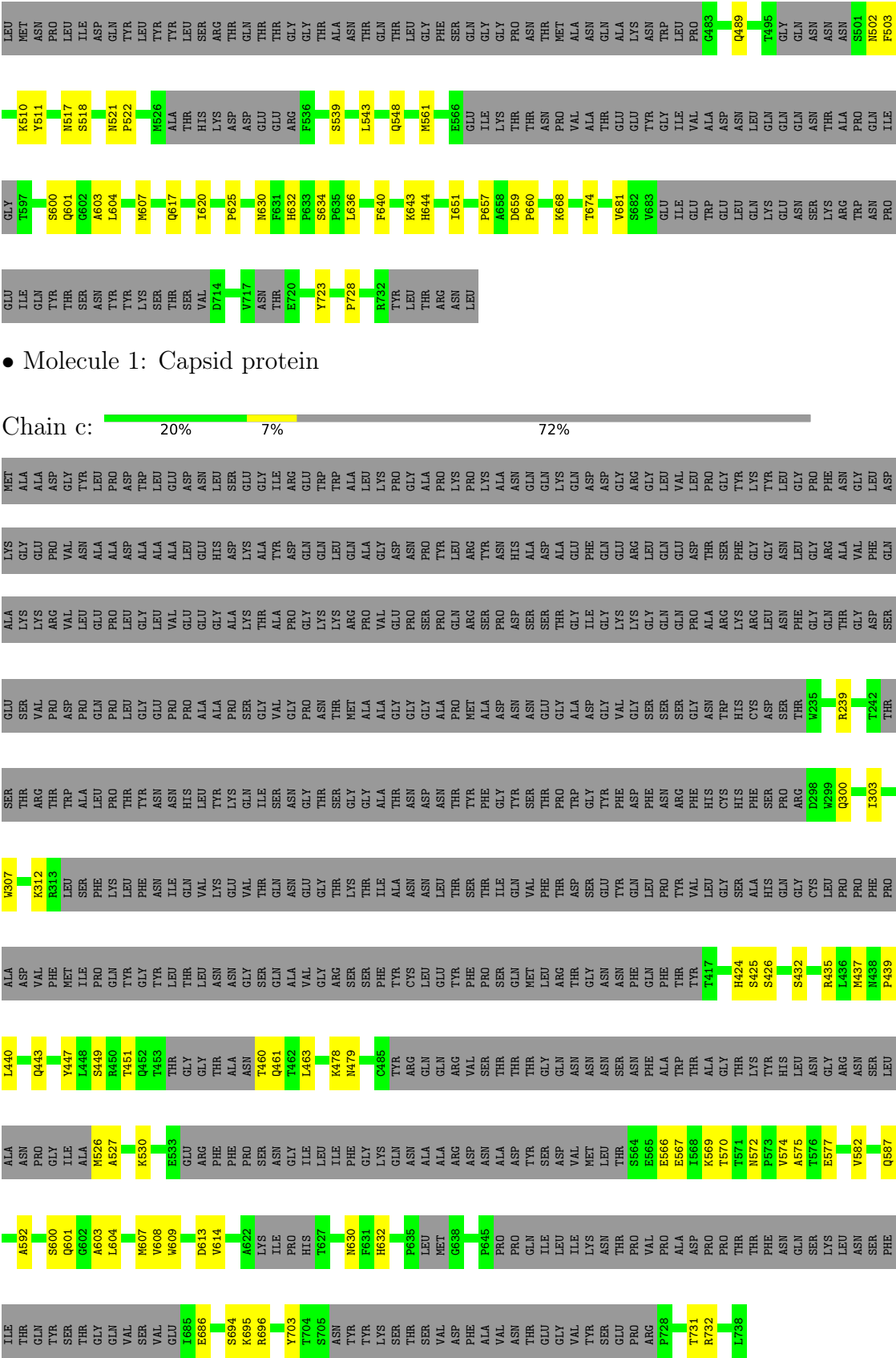
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Capsid protein

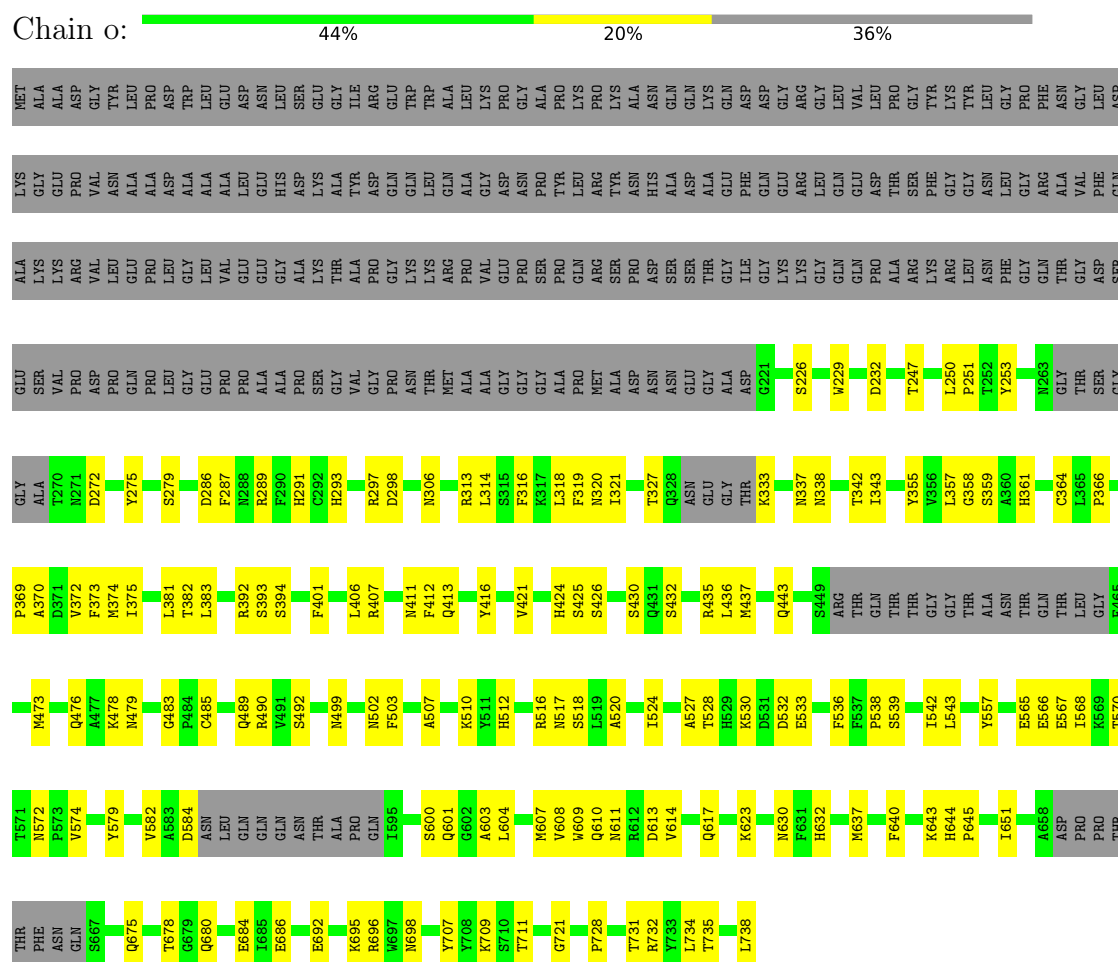


- Molecule 1: Capsid protein



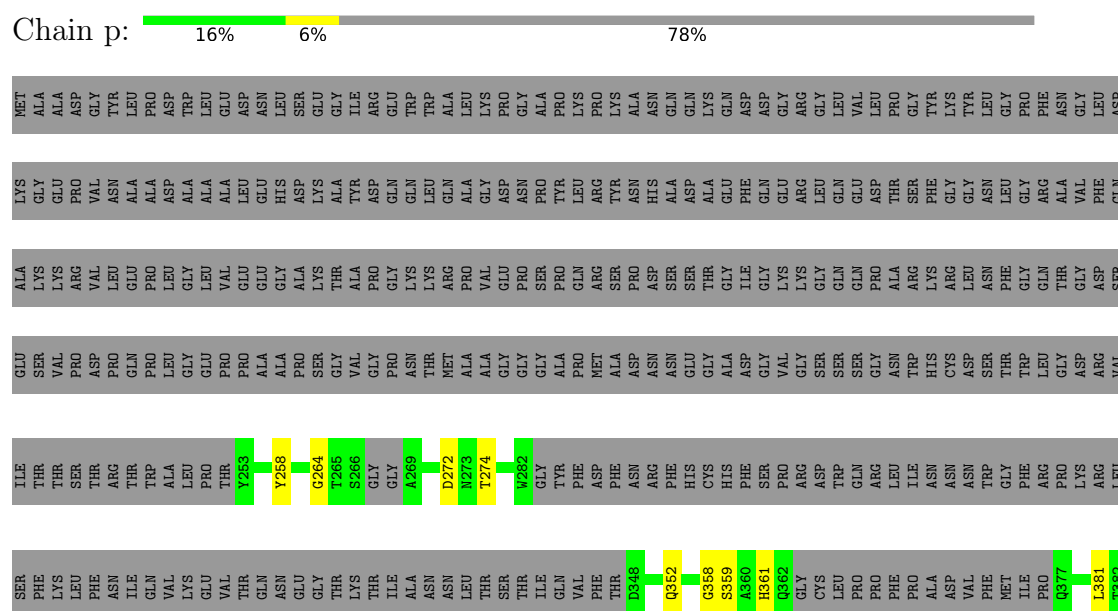


Chain o:



● Molecule 1: Capsid protein

Chain p:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	5	0.13	0/649	0.31	0/882
1	6	0.13	0/3287	0.29	0/4473
1	7	0.15	0/2737	0.32	0/3722
1	c	0.13	0/1683	0.32	0/2280
1	o	0.13	0/3937	0.29	0/5361
1	p	0.13	0/1345	0.28	0/1820
2	A	0.18	0/2935	0.34	0/3979
All	All	0.14	0/16573	0.31	0/22517

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	5	637	0	608	29	0
1	6	3185	0	2968	108	0
1	7	2660	0	2521	71	0
1	c	1643	0	1545	47	0
1	o	3823	0	3605	123	0
1	p	1308	0	1210	38	0
2	A	2871	0	2783	78	0
All	All	16127	0	15240	388	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 12.

All (388) 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)
2:A:261:VAL:HA	2:A:350:GLU:O	1.74	0.87
1:7:405:MET:SD	1:o:320:ASN:ND2	2.50	0.83
2:A:59:TYR:HB3	2:A:63:GLU:HB3	1.62	0.79
2:A:425:PRO:HA	2:A:447:VAL:O	1.82	0.78
1:o:530:LYS:HG3	1:o:533:GLU:HG3	1.67	0.76
2:A:268:ASP:HA	2:A:324:GLY:HA3	1.70	0.73
1:o:250:LEU:HB2	1:o:375:ILE:HD12	1.68	0.73
1:7:405:MET:HE1	1:o:680:GLN:HG2	1.69	0.72
1:6:530:LYS:NZ	1:6:533:GLU:OE2	2.22	0.72
1:5:443:GLN:NE2	1:6:359:SER:O	2.23	0.71
2:A:137:ASN:HB3	2:A:181:SER:HA	1.73	0.71
1:c:479:ASN:ND2	1:o:358:GLY:O	2.23	0.70
2:A:61:GLU:HG2	2:A:92:ARG:HH11	1.56	0.70
1:6:526:MET:HE3	1:6:575:ALA:HA	1.73	0.69
1:o:601:GLN:NE2	1:p:600:SER:OG	2.25	0.69
1:c:600:SER:OG	1:p:601:GLN:NE2	2.26	0.69
1:6:289:ARG:HH21	1:6:617:GLN:HB3	1.58	0.69
1:6:298:ASP:OD2	1:p:400:TYR:OH	2.11	0.68
1:p:272:ASP:HA	1:p:516:ARG:HG3	1.76	0.67
1:o:382:THR:HG21	1:o:394:SER:H	1.59	0.67
1:7:338:ASN:OD1	1:o:337:ASN:ND2	2.28	0.67
1:7:657:PRO:HG3	1:o:372:VAL:HG11	1.77	0.67
2:A:76:LEU:HD12	2:A:161:ARG:HD2	1.76	0.67
1:5:483:GLY:HA3	1:5:609:TRP:HB3	1.77	0.65
2:A:152:LEU:HD22	2:A:373:LEU:HD23	1.77	0.65
1:o:272:ASP:HA	1:o:516:ARG:HG3	1.79	0.65
1:o:692:GLU:HG3	1:o:734:LEU:HD13	1.78	0.65
2:A:135:VAL:HG13	2:A:179:LEU:HD22	1.77	0.65
2:A:359:ALA:HA	2:A:362:LEU:HD23	1.78	0.65
1:o:251:PRO:HG3	1:o:374:MET:HE3	1.80	0.64
1:5:467:GLN:O	1:6:552:ARG:NH1	2.31	0.63
1:o:503:PHE:HB2	1:o:507:ALA:HB3	1.79	0.63
1:o:608:VAL:HG12	1:p:630:ASN:HB3	1.78	0.63
1:5:584:ASP:OD1	1:6:599:ASN:ND2	2.32	0.62
1:5:593:PRO:HD3	1:6:499:ASN:HD22	1.63	0.62
1:o:327:THR:O	1:o:333:LYS:HA	2.00	0.62
1:5:578:GLU:HG3	1:5:597:THR:HG23	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:291:HIS:HD2	1:6:617:GLN:HA	1.64	0.62
1:7:400:TYR:OH	1:o:298:ASP:OD2	2.17	0.62
2:A:101:ALA:HB3	2:A:129:ARG:HH12	1.63	0.62
1:6:497:GLN:NE2	2:A:188:GLU:OE1	2.31	0.61
1:6:714:ASP:HB2	1:6:726:PRO:HG2	1.81	0.61
2:A:265:TYR:HB2	2:A:288:PHE:HB3	1.82	0.61
1:c:443:GLN:NE2	1:o:359:SER:O	2.33	0.61
1:7:604:LEU:H	1:7:607:MET:HE3	1.64	0.61
1:o:483:GLY:HA3	1:o:609:TRP:HB3	1.82	0.61
2:A:284:ASP:OD1	2:A:421:ARG:NH2	2.33	0.61
1:c:426:SER:HB2	1:c:731:THR:HG22	1.81	0.61
1:o:291:HIS:HD2	1:o:617:GLN:HA	1.65	0.61
2:A:370:ARG:NH1	2:A:371:GLU:OE2	2.34	0.60
1:7:326:VAL:O	1:7:674:THR:OG1	2.20	0.60
2:A:413:THR:HG22	2:A:419:PHE:HB3	1.83	0.60
1:7:405:MET:HE3	1:o:229:TRP:HB2	1.84	0.60
2:A:214:ARG:HD2	2:A:234:GLU:HB3	1.84	0.60
1:6:443:GLN:NE2	1:7:359:SER:O	2.32	0.60
2:A:138:MET:HG3	2:A:182:LEU:HD23	1.84	0.60
2:A:192:GLU:HA	2:A:356:TYR:CD2	2.37	0.60
2:A:433:VAL:HG22	2:A:439:PRO:HB3	1.84	0.60
2:A:137:ASN:HB2	2:A:146:ARG:HB2	1.84	0.60
1:c:239:ARG:NH1	1:c:686:GLU:OE1	2.34	0.60
1:o:584:ASP:OD1	1:p:599:ASN:ND2	2.35	0.59
1:7:263:ASN:O	1:7:274:THR:HA	2.02	0.59
2:A:59:TYR:HD2	2:A:150:ILE:HD13	1.67	0.59
1:o:366:PRO:HG3	1:o:373:PHE:HB3	1.84	0.59
2:A:216:LEU:HD22	2:A:238:VAL:HG23	1.83	0.59
1:o:604:LEU:O	1:o:607:MET:HG2	2.01	0.59
1:6:623:LYS:HB2	1:6:645:PRO:HG3	1.85	0.59
2:A:79:LEU:HD11	2:A:171:LEU:HD13	1.84	0.58
1:p:258:TYR:OH	1:p:399:GLU:OE1	2.17	0.58
1:5:601:GLN:OE1	1:6:600:SER:OG	2.21	0.58
1:c:604:LEU:N	1:c:607:MET:SD	2.73	0.58
1:6:608:VAL:HG12	1:7:630:ASN:HB3	1.85	0.58
1:6:426:SER:HB2	1:6:731:THR:HG22	1.86	0.58
1:7:318:LEU:HD21	1:7:651:ILE:HD12	1.84	0.58
1:o:416:TYR:OH	1:o:644:HIS:O	2.20	0.58
1:6:566:GLU:OE1	1:6:569:LYS:NZ	2.37	0.58
1:p:604:LEU:O	1:p:607:MET:HG2	2.03	0.57
1:o:479:ASN:ND2	1:p:358:GLY:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:479:ASN:ND2	1:7:358:GLY:O	2.38	0.57
2:A:409:HIS:O	2:A:421:ARG:NH1	2.36	0.57
1:6:300:GLN:NE2	1:6:703:TYR:O	2.31	0.57
1:6:436:LEU:HD21	1:6:738:LEU:HD12	1.85	0.57
1:p:521:ASN:HB2	1:p:540:ASN:HB2	1.87	0.57
1:5:600:SER:OG	1:7:601:GLN:OE1	2.23	0.57
2:A:156:LEU:HD23	2:A:167:LEU:HD22	1.87	0.57
1:c:574:VAL:HB	1:c:577:GLU:HG2	1.85	0.57
1:o:528:THR:HG23	1:o:538:PRO:HD2	1.87	0.57
1:c:582:VAL:HG11	1:o:600:SER:HB2	1.86	0.57
2:A:165:PRO:O	2:A:169:ARG:HG2	2.05	0.57
1:c:696:ARG:NH2	1:o:393:SER:O	2.38	0.56
1:o:421:VAL:HG21	1:o:640:PHE:HB3	1.86	0.56
1:7:416:TYR:OH	1:7:644:HIS:O	2.18	0.56
1:c:601:GLN:OE1	1:o:600:SER:OG	2.23	0.56
1:p:510:LYS:HD3	1:p:517:ASN:HB3	1.87	0.56
1:6:601:GLN:OE1	1:7:600:SER:OG	2.23	0.56
1:7:657:PRO:HD2	1:o:678:THR:HG21	1.88	0.56
1:c:300:GLN:NE2	1:c:703:TYR:O	2.35	0.56
1:o:247:THR:HB	1:o:372:VAL:HG22	1.88	0.56
1:5:433:LEU:HD11	1:5:480:TRP:HB2	1.87	0.56
2:A:249:LYS:NZ	2:A:412:THR:OG1	2.38	0.56
1:c:478:LYS:NZ	1:o:518:SER:OG	2.30	0.55
1:6:700:GLU:OE1	1:o:297:ARG:NE	2.31	0.55
1:o:435:ARG:NH2	1:p:272:ASP:O	2.40	0.55
1:6:280:THR:HG21	1:6:398:LEU:HD13	1.89	0.55
1:6:303:ILE:HG22	1:6:731:THR:HG23	1.87	0.55
2:A:166:ARG:NH1	2:A:371:GLU:OE1	2.40	0.55
2:A:149:LEU:HD21	2:A:256:LEU:HD13	1.88	0.54
1:7:617:GLN:HE22	1:7:728:PRO:HA	1.73	0.54
2:A:265:TYR:HB2	2:A:266:PRO:HD2	1.90	0.54
1:c:587:GLN:NE2	1:o:490:ARG:O	2.40	0.54
1:o:623:LYS:HB2	1:o:645:PRO:HG3	1.90	0.54
1:o:250:LEU:HD22	1:o:651:ILE:HG12	1.89	0.53
1:6:481:LEU:HG	1:7:636:LEU:HD11	1.90	0.53
1:c:312:LYS:HB2	1:c:686:GLU:HG2	1.89	0.53
1:7:421:VAL:HG21	1:7:640:PHE:HB3	1.89	0.53
1:6:530:LYS:HB3	1:6:574:VAL:HG21	1.90	0.53
2:A:267:PHE:CD2	2:A:282:THR:HG22	2.44	0.53
1:o:226:SER:HB2	1:o:319:PHE:HB2	1.91	0.53
1:o:253:TYR:OH	1:o:375:ILE:O	2.17	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:473:MET:HA	1:o:476:GLN:HG3	1.89	0.53
1:7:366:PRO:HG3	1:7:373:PHE:HB3	1.89	0.53
1:p:524:ILE:HA	1:p:636:LEU:HD22	1.90	0.53
2:A:142:GLU:OE1	2:A:257:HIS:ND1	2.42	0.53
1:o:582:VAL:HA	1:p:509:THR:HG23	1.91	0.53
2:A:434:LEU:HB3	2:A:437:TYR:HB2	1.89	0.52
1:c:566:GLU:OE2	1:o:392:ARG:NH2	2.34	0.52
1:o:406:LEU:HD21	1:o:412:PHE:HB2	1.92	0.52
1:6:481:LEU:HB2	1:6:607:MET:HG2	1.91	0.52
1:p:538:PRO:HG2	1:p:542:ILE:HG23	1.92	0.52
2:A:409:HIS:HB3	2:A:421:ARG:HH22	1.74	0.52
1:o:306:ASN:O	1:o:426:SER:OG	2.28	0.52
1:c:451:THR:HB	1:o:502:ASN:HA	1.91	0.52
1:6:566:GLU:OE2	1:o:707:TYR:OH	2.27	0.52
1:5:588:GLN:OE1	1:6:490:ARG:NH2	2.42	0.52
1:7:342:THR:HG22	1:7:407:ARG:HG2	1.90	0.52
1:o:286:ASP:HB3	1:o:364:CYS:HA	1.91	0.52
1:o:382:THR:HG22	1:o:383:LEU:H	1.75	0.52
1:o:572:ASN:HD21	1:o:609:TRP:HB2	1.75	0.52
1:7:253:TYR:OH	1:7:375:ILE:O	2.22	0.52
2:A:217:ASN:HB3	2:A:218:ARG:HH11	1.75	0.52
1:c:435:ARG:HD2	1:o:381:LEU:HD13	1.91	0.52
1:c:566:GLU:O	1:c:569:LYS:HG2	2.09	0.52
1:o:696:ARG:NE	1:o:698:ASN:OD1	2.39	0.52
1:c:460:THR:OG1	1:c:461:GLN:N	2.42	0.52
1:o:617:GLN:HE22	1:o:728:PRO:HA	1.75	0.52
1:7:250:LEU:HB2	1:7:375:ILE:HD12	1.91	0.51
2:A:71:ALA:HB2	2:A:154:ARG:HG3	1.91	0.51
1:6:298:ASP:OD1	1:6:301:ARG:NH1	2.43	0.51
1:7:291:HIS:HD2	1:7:617:GLN:HA	1.73	0.51
1:7:346:PHE:HB3	1:7:403:SER:HA	1.91	0.51
1:7:659:ASP:OD1	1:7:659:ASP:N	2.43	0.51
1:7:510:LYS:HD3	1:7:517:ASN:HB3	1.92	0.51
1:c:608:VAL:HG12	1:o:630:ASN:HB3	1.92	0.51
2:A:135:VAL:HA	2:A:179:LEU:HB3	1.93	0.51
1:o:432:SER:HA	1:o:570:THR:HB	1.93	0.50
1:c:463:LEU:HD23	1:o:557:TYR:HB2	1.92	0.50
2:A:306:GLU:OE1	2:A:316:THR:OG1	2.25	0.50
1:o:425:SER:HG	1:o:732:ARG:HH21	1.58	0.50
1:p:483:GLY:HA2	1:p:609:TRP:HB3	1.93	0.50
2:A:418:ASP:OD1	2:A:418:ASP:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:355:TYR:CE2	1:o:357:LEU:HB2	2.47	0.50
1:o:435:ARG:HD2	1:p:381:LEU:HD13	1.94	0.50
1:c:527:ALA:O	1:c:575:ALA:N	2.36	0.50
2:A:253:SER:HB3	2:A:344:CYS:SG	2.52	0.50
1:c:424:HIS:NE2	1:c:614:VAL:HG22	2.27	0.50
1:o:313:ARG:HG3	1:o:686:GLU:HB3	1.93	0.50
1:7:399:GLU:HG3	1:o:370:ALA:HB2	1.94	0.49
1:6:503:PHE:HB2	1:6:507:ALA:HB3	1.95	0.49
1:c:604:LEU:HD22	1:o:524:ILE:HD13	1.94	0.49
1:5:437:MET:HB2	1:6:361:HIS:NE2	2.28	0.49
1:6:451:THR:HB	1:7:502:ASN:HA	1.95	0.49
1:6:492:SER:HB2	1:6:536:PHE:CE1	2.47	0.49
1:c:695:LYS:HE2	1:o:401:PHE:HA	1.95	0.49
1:6:572:ASN:HD21	1:6:609:TRP:HB2	1.78	0.49
1:o:492:SER:HB2	1:o:536:PHE:CE1	2.48	0.49
1:6:372:VAL:HG12	1:p:669:LEU:HD12	1.94	0.49
1:7:382:THR:HG21	1:7:394:SER:H	1.77	0.49
1:6:512:HIS:ND1	1:6:517:ASN:OD1	2.45	0.49
1:7:561:MET:HB3	1:7:728:PRO:HD3	1.95	0.49
1:c:432:SER:HA	1:c:570:THR:HB	1.94	0.49
2:A:137:ASN:N	2:A:145:SER:OG	2.37	0.49
1:6:416:TYR:OH	1:6:644:HIS:O	2.24	0.48
1:6:424:HIS:NE2	1:6:614:VAL:HG22	2.28	0.48
1:7:399:GLU:HB2	1:o:369:PRO:HB2	1.95	0.48
2:A:256:LEU:HG	2:A:349:LEU:HD12	1.95	0.48
1:p:623:LYS:HB2	1:p:645:PRO:HG3	1.95	0.48
1:6:291:HIS:CD2	1:6:617:GLN:HA	2.47	0.48
1:6:435:ARG:NH2	1:7:272:ASP:O	2.46	0.48
1:6:440:LEU:HD11	1:7:279:SER:HB2	1.94	0.48
1:c:572:ASN:HD21	1:c:609:TRP:HB2	1.78	0.48
1:p:264:GLY:HA2	1:p:274:THR:HG22	1.94	0.48
1:5:587:GLN:NE2	1:6:490:ARG:O	2.43	0.48
1:o:443:GLN:NE2	1:p:359:SER:O	2.46	0.48
1:5:604:LEU:HB3	1:6:524:ILE:HG21	1.95	0.48
1:7:382:THR:HG22	1:7:383:LEU:H	1.78	0.48
1:c:609:TRP:HE1	1:c:632:HIS:CD2	2.32	0.48
1:6:483:GLY:HA3	1:6:609:TRP:HB3	1.96	0.48
1:7:548:GLN:NE2	1:7:723:TYR:O	2.43	0.48
1:5:439:PRO:HB3	1:6:381:LEU:HD21	1.95	0.48
2:A:253:SER:O	2:A:346:GLU:HA	2.14	0.48
1:c:307:TRP:HZ2	1:c:694:SER:HB2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:528:THR:HG23	1:6:538:PRO:HD2	1.96	0.48
1:7:288:ASN:O	1:7:620:ILE:N	2.45	0.48
1:p:383:LEU:HD12	1:p:392:ARG:HB3	1.95	0.48
1:6:604:LEU:O	1:6:607:MET:HG3	2.14	0.48
1:6:355:TYR:CE2	1:6:357:LEU:HB2	2.49	0.47
1:6:707:TYR:OH	1:o:566:GLU:OE1	2.32	0.47
1:o:695:LYS:NZ	1:p:400:TYR:O	2.34	0.47
1:6:243:THR:HB	1:6:684:GLU:HG3	1.94	0.47
1:7:264:GLY:N	1:7:387:SER:HB3	2.28	0.47
2:A:217:ASN:HB3	2:A:218:ARG:NH1	2.29	0.47
1:o:291:HIS:CD2	1:o:617:GLN:HA	2.47	0.47
1:6:565:GLU:OE2	1:6:615:TYR:OH	2.22	0.47
1:7:489:GLN:HB3	1:7:539:SER:HB2	1.96	0.47
1:o:430:SER:HB3	1:o:735:THR:HB	1.96	0.47
1:6:435:ARG:HD2	1:7:381:LEU:HD13	1.96	0.47
1:o:527:ALA:HB3	1:o:574:VAL:HA	1.95	0.47
2:A:59:TYR:O	2:A:146:ARG:NH2	2.48	0.47
1:5:450:ARG:HH21	1:6:554:ASN:ND2	2.13	0.47
1:6:434:ASP:O	1:6:435:ARG:NH1	2.42	0.47
1:7:399:GLU:O	1:o:229:TRP:NE1	2.42	0.47
1:c:239:ARG:HD3	1:c:239:ARG:HA	1.77	0.47
1:6:286:ASP:OD1	1:6:357:LEU:HD22	2.14	0.47
2:A:220:PHE:HZ	2:A:241:LEU:HD23	1.79	0.47
1:6:470:PRO:HA	1:6:473:MET:HE3	1.96	0.47
2:A:60:HIS:H	2:A:63:GLU:CD	2.22	0.47
2:A:74:ALA:O	2:A:161:ARG:HG3	2.14	0.47
1:6:244:SER:HB2	1:6:246:ARG:HH12	1.80	0.47
1:7:604:LEU:HB2	1:7:607:MET:HE3	1.97	0.47
1:c:603:ALA:HB3	1:o:603:ALA:HB3	1.97	0.47
1:o:275:TYR:HB2	1:o:381:LEU:HD22	1.97	0.46
1:6:738:LEU:HB3	1:7:625:PRO:HB3	1.96	0.46
2:A:133:LYS:NZ	2:A:338:ASN:OD1	2.43	0.46
1:o:738:LEU:HD22	1:p:625:PRO:HB3	1.97	0.46
1:5:450:ARG:HH21	1:6:554:ASN:HD21	1.63	0.46
1:6:532:ASP:OD2	1:o:709:LYS:NZ	2.49	0.46
1:7:660:PRO:HG2	1:o:251:PRO:HB3	1.97	0.46
1:o:437:MET:HB2	1:p:361:HIS:NE2	2.31	0.46
1:6:288:ASN:O	1:6:620:ILE:N	2.46	0.46
2:A:306:GLU:HG3	2:A:308:HIS:HB2	1.96	0.46
1:c:695:LYS:HD3	1:o:401:PHE:CE2	2.51	0.46
1:5:450:ARG:NH1	1:5:453:THR:HA	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:490:ARG:HG3	1:6:576:THR:HG21	1.96	0.46
1:c:437:MET:HB2	1:o:361:HIS:NE2	2.31	0.46
1:7:258:TYR:O	1:o:721:GLY:HA2	2.15	0.46
1:7:264:GLY:HA2	1:7:274:THR:HG22	1.97	0.46
1:p:264:GLY:HA3	1:p:387:SER:HB3	1.98	0.46
1:5:450:ARG:HH21	1:6:554:ASN:CG	2.23	0.46
1:6:366:PRO:HG3	1:6:373:PHE:HB3	1.97	0.46
1:6:490:ARG:HB2	1:6:576:THR:HB	1.98	0.46
1:o:289:ARG:HH21	1:o:617:GLN:HB3	1.80	0.46
1:o:695:LYS:HG2	1:p:352:GLN:NE2	2.30	0.46
1:7:291:HIS:CD2	1:7:617:GLN:HA	2.50	0.46
1:7:388:GLN:HG3	1:o:711:THR:HA	1.98	0.45
2:A:68:LEU:HD11	2:A:180:PRO:HG2	1.99	0.45
2:A:192:GLU:HA	2:A:356:TYR:CE2	2.52	0.45
2:A:274:LYS:O	2:A:329:ASP:HB2	2.15	0.45
1:c:439:PRO:HB3	1:o:381:LEU:HD21	1.98	0.45
1:6:432:SER:HA	1:6:570:THR:HB	1.97	0.45
1:p:613:ASP:OD1	1:p:614:VAL:N	2.50	0.45
1:5:434:ASP:O	1:5:437:MET:HE1	2.16	0.45
1:6:374:MET:HE3	1:p:665:ASN:H	1.81	0.45
1:c:567:GLU:HG2	1:c:732:ARG:HB2	1.98	0.45
2:A:269:ASP:HB3	2:A:330:VAL:O	2.17	0.45
1:o:425:SER:OG	1:o:732:ARG:NH2	2.41	0.45
1:5:450:ARG:HH11	1:5:453:THR:HA	1.82	0.45
1:c:303:ILE:HG22	1:c:731:THR:HG23	1.97	0.45
1:c:425:SER:O	1:c:732:ARG:NE	2.50	0.45
1:c:447:TYR:CE2	1:c:449:SER:HB3	2.51	0.45
1:6:603:ALA:HB3	1:7:603:ALA:HB3	1.98	0.45
1:o:613:ASP:OD1	1:o:731:THR:HB	2.17	0.45
1:6:289:ARG:NH2	1:6:617:GLN:HB3	2.29	0.45
1:c:526:MET:HA	1:c:572:ASN:HB3	1.98	0.45
2:A:58:TYR:CZ	2:A:362:LEU:HD21	2.52	0.45
2:A:264:SER:HA	2:A:322:THR:O	2.17	0.45
1:c:592:ALA:HA	1:o:499:ASN:ND2	2.32	0.45
1:o:565:GLU:O	1:o:568:ILE:HG12	2.17	0.45
1:6:430:SER:HB3	1:6:735:THR:HB	1.99	0.44
1:6:585:ASN:OD1	1:6:594:GLN:N	2.50	0.44
1:5:435:ARG:HD2	1:6:381:LEU:HD13	2.00	0.44
1:o:512:HIS:ND1	1:o:517:ASN:OD1	2.50	0.44
1:6:346:PHE:HB3	1:6:403:SER:HA	1.98	0.44
1:6:437:MET:HB2	1:7:361:HIS:NE2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:451:THR:HG21	1:6:503:PHE:CE2	2.53	0.44
1:5:461:GLN:HE21	1:6:500:ASN:HB2	1.83	0.44
1:6:556:ASP:OD2	1:6:558:SER:OG	2.30	0.44
2:A:98:ARG:NH1	2:A:122:ALA:O	2.46	0.44
1:o:567:GLU:HG3	1:o:732:ARG:HB2	2.00	0.44
1:6:695:LYS:NZ	1:o:232:ASP:OD1	2.30	0.44
1:5:440:LEU:HD21	1:6:279:SER:HB3	2.00	0.44
2:A:60:HIS:HA	2:A:187:PHE:HE2	1.83	0.44
1:6:285:PHE:HB2	1:6:649:ILE:HB	1.99	0.43
1:5:604:LEU:HD22	1:6:524:ILE:HD13	2.00	0.43
1:6:445:LEU:HD13	1:7:543:LEU:HD22	2.00	0.43
1:o:611:ASN:HD21	1:o:632:HIS:CD2	2.36	0.43
1:7:382:THR:HG22	1:7:383:LEU:N	2.32	0.43
2:A:98:ARG:NH2	2:A:124:PRO:O	2.50	0.43
2:A:400:ALA:N	2:A:413:THR:OG1	2.51	0.43
1:o:342:THR:HG22	1:o:407:ARG:HG2	2.00	0.43
1:6:524:ILE:HA	1:6:636:LEU:HD22	2.01	0.43
2:A:280:SER:C	2:A:323:ASN:HD21	2.25	0.43
1:6:306:ASN:O	1:6:426:SER:OG	2.36	0.43
1:6:490:ARG:HD2	1:6:536:PHE:CG	2.53	0.43
1:o:338:ASN:ND2	1:o:675:GLN:OE1	2.50	0.43
1:o:572:ASN:ND2	1:o:609:TRP:HB2	2.34	0.43
1:6:696:ARG:HD2	1:7:394:SER:OG	2.18	0.43
1:7:643:LYS:HB2	1:7:643:LYS:HE2	1.76	0.43
2:A:259:GLY:C	2:A:353:CYS:HA	2.44	0.43
1:5:437:MET:HG3	1:5:476:GLN:OE1	2.19	0.43
1:6:695:LYS:NZ	1:7:400:TYR:O	2.46	0.43
2:A:214:ARG:HH12	2:A:231:ALA:HB3	1.84	0.43
2:A:274:LYS:HD3	2:A:278:ILE:HD11	2.01	0.43
1:o:424:HIS:CE1	1:o:614:VAL:HG13	2.54	0.43
1:o:510:LYS:HA	1:o:520:ALA:H	1.84	0.43
1:o:318:LEU:HD21	1:o:651:ILE:HD12	2.00	0.42
1:o:538:PRO:HG2	1:o:542:ILE:HG23	2.00	0.42
1:o:610:GLN:HG2	1:p:627:THR:HG23	2.01	0.42
1:o:604:LEU:HB3	1:p:524:ILE:HG21	2.01	0.42
1:6:523:GLY:C	1:6:636:LEU:HD13	2.44	0.42
1:7:318:LEU:HB3	1:7:412:PHE:HB3	2.01	0.42
1:7:521:ASN:HA	1:7:522:PRO:HA	1.88	0.42
1:c:530:LYS:HB3	1:c:574:VAL:HG21	2.01	0.42
1:o:485:CYS:HB3	1:o:579:TYR:HB2	2.00	0.42
2:A:261:VAL:HG12	2:A:302:MET:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:668:LYS:NZ	1:o:721:GLY:O	2.53	0.42
1:c:451:THR:HG21	1:o:503:PHE:CE2	2.55	0.42
1:6:437:MET:HE1	1:6:478:LYS:HE3	2.01	0.42
1:6:567:GLU:HG3	1:7:392:ARG:NH2	2.35	0.42
1:7:314:LEU:HD23	1:7:418:PHE:CE1	2.54	0.42
2:A:161:ARG:HG3	2:A:161:ARG:HH11	1.84	0.42
1:o:314:LEU:HA	1:o:684:GLU:O	2.20	0.42
1:o:321:ILE:HD13	1:o:343:ILE:HD11	2.02	0.42
1:o:437:MET:HE1	1:o:478:LYS:HE3	2.01	0.42
1:7:312:LYS:HD3	1:7:312:LYS:HA	1.89	0.42
1:c:312:LYS:HD2	1:c:312:LYS:HA	1.70	0.42
2:A:56:ASP:OD1	2:A:56:ASP:N	2.53	0.41
1:c:613:ASP:OD1	1:c:731:THR:HB	2.20	0.41
1:6:451:THR:HG21	1:7:503:PHE:CE2	2.55	0.41
2:A:133:LYS:HA	2:A:177:TYR:O	2.20	0.41
1:o:287:PHE:HB2	1:o:293:HIS:CE1	2.56	0.41
1:o:436:LEU:HD21	1:o:738:LEU:HB2	2.02	0.41
1:o:643:LYS:HD2	1:o:643:LYS:HA	1.90	0.41
1:5:603:ALA:N	1:7:603:ALA:O	2.51	0.41
1:o:382:THR:CG2	1:o:394:SER:H	2.29	0.41
1:o:489:GLN:O	1:o:539:SER:N	2.52	0.41
1:5:450:ARG:NH2	1:6:554:ASN:HD21	2.18	0.41
1:6:709:LYS:HD2	1:p:388:GLN:HE21	1.85	0.41
1:6:721:GLY:HA2	1:p:258:TYR:O	2.20	0.41
1:7:406:LEU:HD21	1:7:412:PHE:HB2	2.02	0.41
2:A:283:SER:HB3	2:A:407:ILE:HG23	2.00	0.41
1:o:543:LEU:HD11	1:o:637:MET:O	2.21	0.41
1:6:565:GLU:O	1:6:568:ILE:HG12	2.20	0.41
1:7:604:LEU:N	1:7:607:MET:HE3	2.33	0.41
2:A:389:LYS:HD2	2:A:389:LYS:HA	1.83	0.41
1:6:434:ASP:OD1	1:6:434:ASP:N	2.48	0.41
2:A:219:SER:OG	2:A:238:VAL:HG21	2.19	0.41
2:A:252:LEU:HD12	2:A:253:SER:H	1.85	0.41
1:5:461:GLN:HG2	1:6:500:ASN:HA	2.01	0.41
1:6:510:LYS:HB3	1:6:519:LEU:HD12	2.02	0.41
1:6:604:LEU:H	1:6:607:MET:HE2	1.86	0.41
1:c:307:TRP:CZ2	1:c:694:SER:HB2	2.55	0.41
1:6:297:ARG:NH2	1:o:692:GLU:OE1	2.53	0.41
1:6:428:ALA:O	1:6:735:THR:HA	2.20	0.41
1:6:489:GLN:O	1:6:539:SER:N	2.48	0.41
1:6:538:PRO:HG2	1:6:542:ILE:HG23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:75:GLY:HA2	2:A:161:ARG:HG2	2.03	0.41
2:A:98:ARG:HH22	2:A:125:LEU:HA	1.85	0.41
2:A:138:MET:HA	2:A:182:LEU:HB3	2.02	0.41
1:c:440:LEU:HD11	1:o:279:SER:HB2	2.03	0.41
1:c:630:ASN:HB3	1:p:608:VAL:HG12	2.02	0.41
1:6:452:GLN:HA	1:6:461:GLN:HA	2.03	0.40
1:6:617:GLN:HE22	1:6:728:PRO:HA	1.86	0.40
2:A:403:SER:HG	2:A:431:THR:HB	1.86	0.40
1:o:316:PHE:O	1:o:413:GLN:HA	2.21	0.40
1:o:382:THR:HG21	1:o:394:SER:N	2.32	0.40
1:o:435:ARG:NH2	1:p:516:ARG:HD2	2.36	0.40
1:o:532:ASP:OD2	1:p:385:ASN:ND2	2.54	0.40
1:7:245:THR:HA	1:7:681:VAL:O	2.21	0.40
1:o:226:SER:HB3	1:o:411:ASN:HB3	2.03	0.40
1:o:382:THR:HG22	1:o:383:LEU:N	2.36	0.40
1:7:247:THR:HB	1:7:372:VAL:HG22	2.02	0.40
1:7:632:HIS:O	1:7:634:SER:N	2.48	0.40
2:A:87:ARG:NH1	2:A:91:GLY:O	2.42	0.40
1:o:425:SER:HB3	1:p:628:ASP:OD1	2.21	0.40
1:7:511:TYR:CE1	1:7:518:SER:HB3	2.57	0.40
1:6:603:ALA:O	1:7:603:ALA:N	2.53	0.40
1:6:609:TRP:HE1	1:6:632:HIS:CD2	2.39	0.40
1:p:486:TYR:H	1:p:526:MET:CE	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	5	76/738 (10%)	74 (97%)	2 (3%)	0	100	100
1	6	373/738 (50%)	364 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	315/738 (43%)	304 (96%)	11 (4%)	0	100	100
1	c	183/738 (25%)	177 (97%)	6 (3%)	0	100	100
1	o	463/738 (63%)	452 (98%)	11 (2%)	0	100	100
1	p	144/738 (20%)	138 (96%)	6 (4%)	0	100	100
2	A	353/470 (75%)	340 (96%)	13 (4%)	0	100	100
All	All	1907/4898 (39%)	1849 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	5	69/618 (11%)	69 (100%)	0	100	100
1	6	345/618 (56%)	345 (100%)	0	100	100
1	7	292/618 (47%)	292 (100%)	0	100	100
1	c	178/618 (29%)	178 (100%)	0	100	100
1	o	419/618 (68%)	419 (100%)	0	100	100
1	p	139/618 (22%)	139 (100%)	0	100	100
2	A	306/382 (80%)	306 (100%)	0	100	100
All	All	1748/4090 (43%)	1748 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	476	GLN
1	6	611	ASN
1	7	271	ASN
1	7	377	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7	385	ASN
1	7	648	GLN
2	A	361	GLN
2	A	369	ASN
1	c	306	ASN
1	c	611	ASN
1	c	632	HIS
1	o	328	GLN
1	o	377	GLN
1	o	424	HIS
1	o	611	ASN
1	o	680	GLN
1	o	690	GLN
1	p	377	GLN
1	p	385	ASN
1	p	388	GLN
1	p	601	GLN
1	p	644	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.