



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:37 AM UTC

PDB ID : 8HQ2 / pdb_00008hq2
Title : Crystal structure of human ADAM22 in complex with human LGI1 mutant
Authors : Liu, H.; Lin, Z.; Xu, F.
Deposited on : 2022-12-13
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

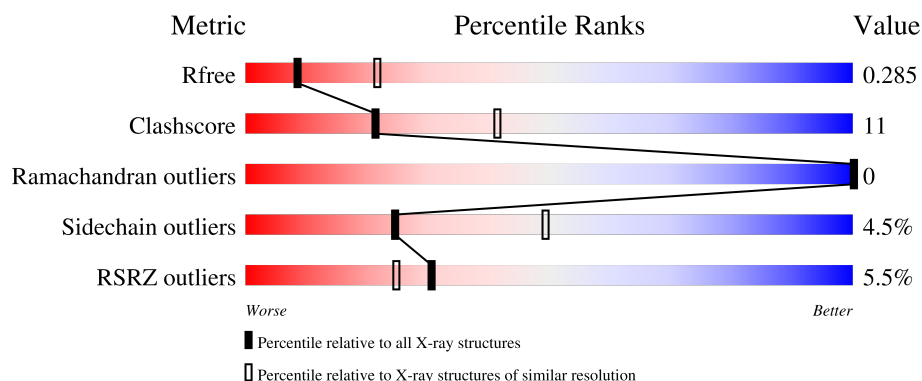
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	3% 78% 20% .
1	B	486	2% 75% 23% .
2	D	526	4% 69% 27% ..
2	E	526	11% 69% 27% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	806	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16132 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3710	2293	638	728	51			
1	B	484	Total	C	N	O	S	0	0	0
			3710	2293	638	728	51			

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	516	Total	C	N	O	S	0	0	0
			4181	2688	696	782	15			
2	E	516	Total	C	N	O	S	0	0	0
			4181	2688	696	782	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	HIS	-	expression tag	UNP O95970
D	33	HIS	-	expression tag	UNP O95970
D	34	HIS	-	expression tag	UNP O95970
D	35	HIS	-	expression tag	UNP O95970
D	36	HIS	-	expression tag	UNP O95970
D	37	HIS	-	expression tag	UNP O95970
D	38	HIS	-	expression tag	UNP O95970
D	88	ASN	LEU	engineered mutation	UNP O95970
D	89	ALA	PHE	engineered mutation	UNP O95970
D	474	GLN	ARG	engineered mutation	UNP O95970
E	32	HIS	-	expression tag	UNP O95970
E	33	HIS	-	expression tag	UNP O95970
E	34	HIS	-	expression tag	UNP O95970
E	35	HIS	-	expression tag	UNP O95970
E	36	HIS	-	expression tag	UNP O95970
E	37	HIS	-	expression tag	UNP O95970

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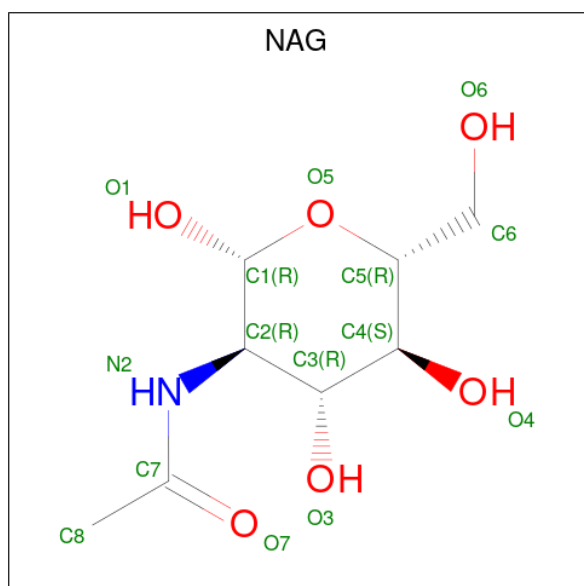
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Chain	Residue	Modelled	Actual	Comment	Reference
E	38	HIS	-	expression tag	UNP O95970
E	88	ASN	LEU	engineered mutation	UNP O95970
E	89	ALA	PHE	engineered mutation	UNP O95970
E	474	GLN	ARG	engineered mutation	UNP O95970

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	D	1	Total Ca 1 1	0	0
3	B	3	Total Ca 3 3	0	0
3	E	1	Total Ca 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

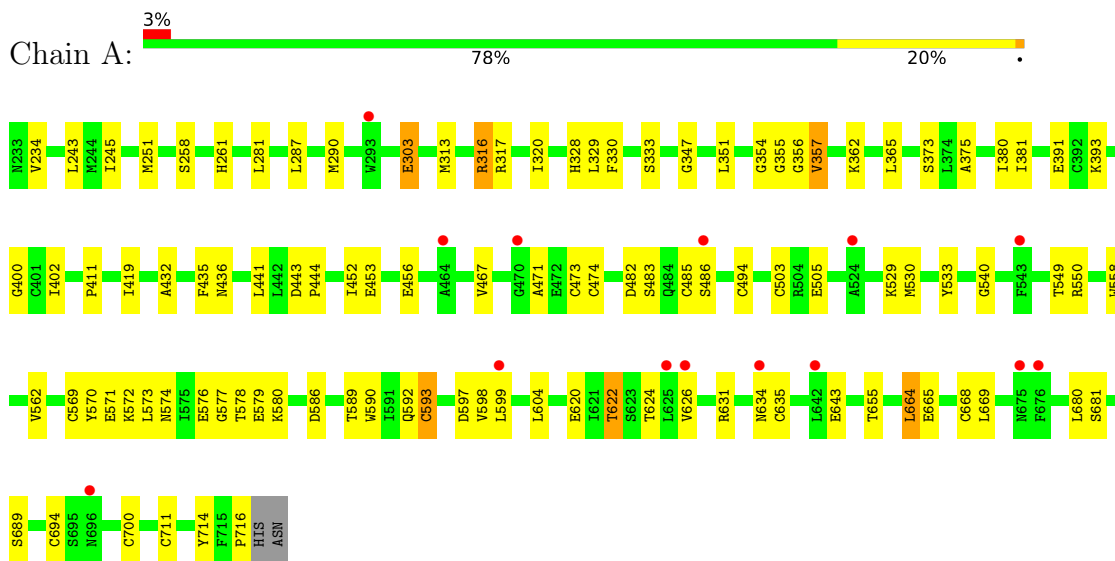
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	D	46	Total	O	0	0
			46	46		
5	B	44	Total	O	0	0
			44	44		
5	E	29	Total	O	0	0
			29	29		

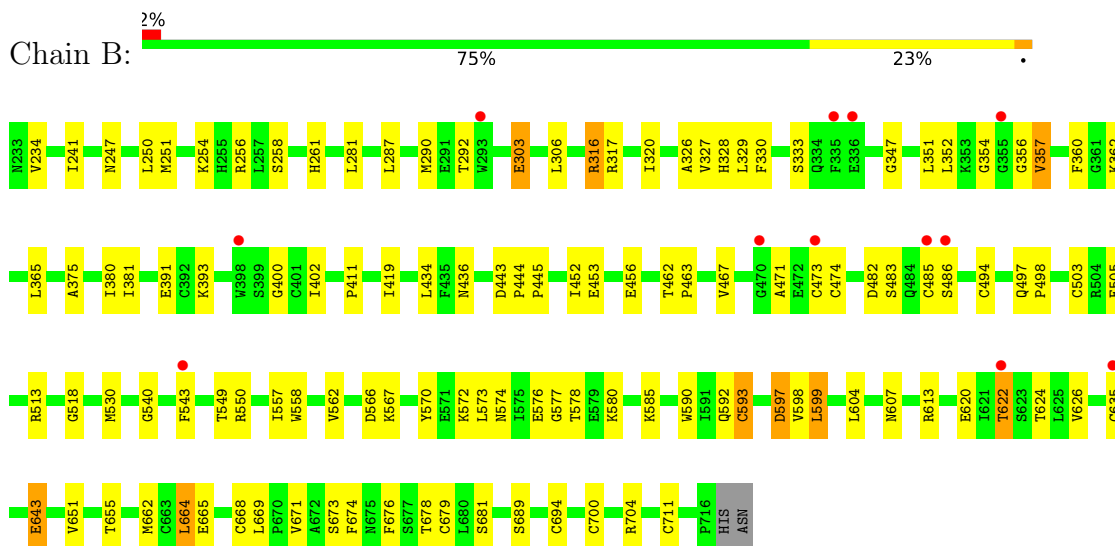
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

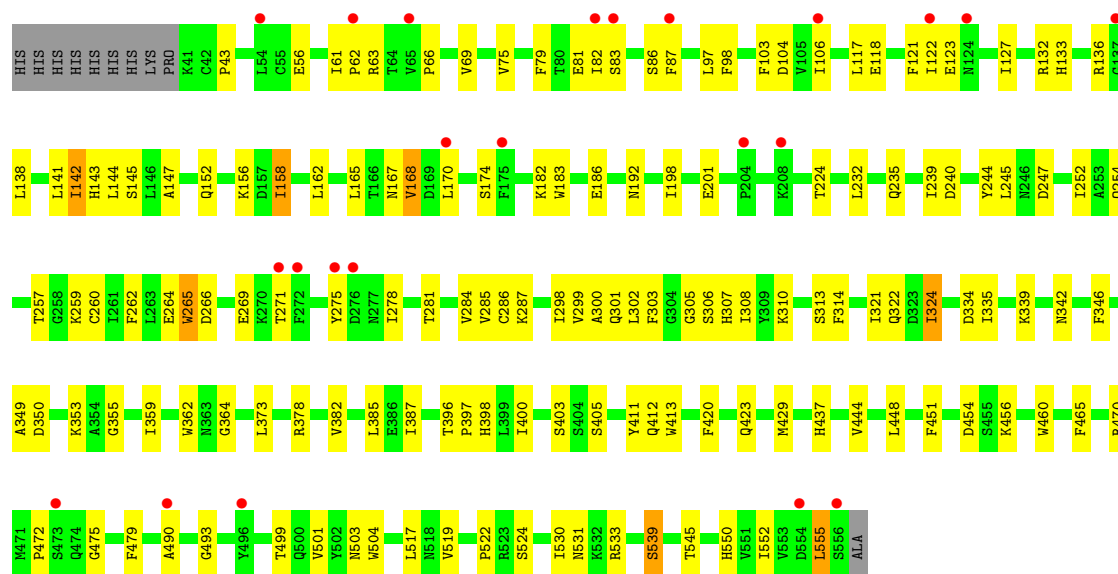


- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

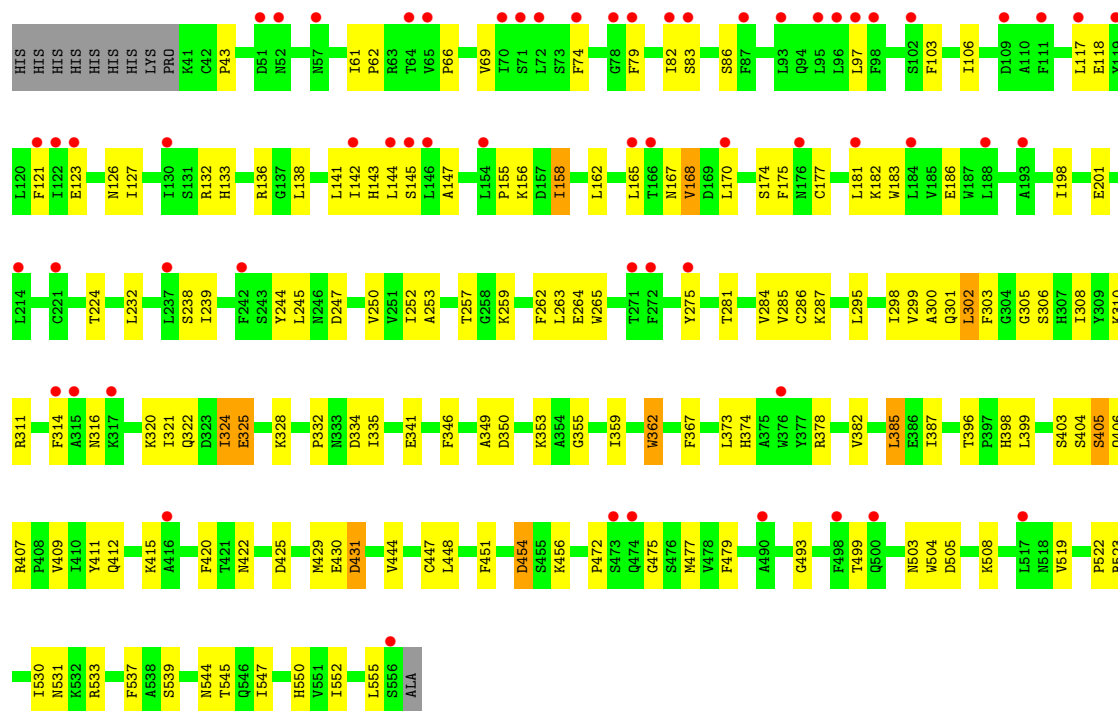


- Molecule 2: Leucine-rich glioma-inactivated protein 1





• Molecule 2: Leucine-rich glioma-inactivated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.25Å 98.85Å 131.26Å 96.21° 100.44° 91.31°	Depositor
Resolution (Å)	45.83 – 2.93 45.83 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.83-2.93) 97.4 (45.83-2.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.245 , 0.291 0.244 , 0.285	Depositor DCC
R_{free} test set	2711 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.165 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16132	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.18	0/3773	0.37	0/5079
1	B	0.22	0/3773	0.40	0/5079
2	D	0.26	0/4287	0.46	0/5818
2	E	0.21	0/4287	0.42	0/5818
All	All	0.22	0/16120	0.42	0/21794

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	A	3710	0	3566	57	0
1	B	3710	0	3567	85	0
2	D	4181	0	4092	108	0
2	E	4181	0	4092	98	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	42	0	39	10	0
4	D	42	0	39	1	0
4	E	42	0	39	0	0
5	A	55	0	0	0	0
5	B	44	0	0	0	0
5	D	46	0	0	1	0
5	E	29	0	0	2	0
All	All	16132	0	15473	341	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 11.

All (341) 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:673:SER:HA	4:B:806:NAG:H5	1.11	1.07
2:D:265:TRP:HA	2:D:271:THR:HG22	1.43	1.00
1:B:483:SER:HB3	1:B:494:CYS:HB3	1.51	0.92
1:B:664:LEU:HD12	1:B:665:GLU:N	1.87	0.89
2:D:265:TRP:CB	2:D:271:THR:CG2	2.51	0.88
1:A:586:ASP:HB3	1:A:589:THR:OG1	1.72	0.87
2:D:240:ASP:OD2	2:D:287:LYS:HD2	1.74	0.87
1:B:673:SER:O	4:B:806:NAG:H3	1.73	0.86
2:D:264:GLU:HB3	2:D:275:TYR:CD1	2.12	0.85
1:A:483:SER:HB3	1:A:494:CYS:HB3	1.60	0.83
1:B:673:SER:HA	4:B:806:NAG:C5	2.05	0.82
2:D:284:VAL:HG12	2:D:285:VAL:HG23	1.64	0.80
2:D:247:ASP:OD2	2:D:265:TRP:HZ2	1.64	0.79
2:E:284:VAL:HG12	2:E:285:VAL:HG23	1.66	0.78
2:D:265:TRP:CA	2:D:271:THR:HG22	2.13	0.78
2:D:265:TRP:HB2	2:D:271:THR:HG23	1.69	0.75
2:D:411:TYR:HB3	2:D:420:PHE:HB3	1.70	0.74
1:B:597:ASP:HB3	1:B:668:CYS:H	1.53	0.72
2:D:257:THR:HG23	2:D:259:LYS:H	1.55	0.72
2:D:265:TRP:HA	2:D:271:THR:CG2	2.17	0.72
2:D:306:SER:HB3	2:D:324:ILE:HB	1.72	0.72
1:B:580:LYS:HA	1:B:622:THR:HG21	1.69	0.72
1:B:673:SER:CA	4:B:806:NAG:H5	2.06	0.72
2:E:306:SER:HB3	2:E:324:ILE:HB	1.72	0.71
1:B:664:LEU:HD12	1:B:664:LEU:C	2.14	0.71
2:D:265:TRP:CA	2:D:271:THR:CG2	2.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:MET:HE3	1:B:671:VAL:HG23	1.71	0.71
2:D:349:ALA:HB2	2:D:382:VAL:HG23	1.73	0.71
1:A:580:LYS:HA	1:A:622:THR:HG21	1.72	0.70
2:D:265:TRP:HB2	2:D:271:THR:CG2	2.20	0.70
2:E:349:ALA:HB2	2:E:382:VAL:HG23	1.74	0.68
2:E:132:ARG:HG2	2:E:155:PRO:HB2	1.74	0.68
1:A:573:LEU:HD21	1:A:624:THR:HB	1.77	0.66
1:A:597:ASP:HB3	1:A:668:CYS:H	1.59	0.66
2:E:257:THR:HG23	2:E:259:LYS:H	1.59	0.66
2:E:411:TYR:HB3	2:E:420:PHE:HB3	1.76	0.66
1:B:573:LEU:HD21	1:B:624:THR:HB	1.76	0.66
1:B:473:CYS:CB	1:B:486:SER:HA	2.26	0.66
1:B:362:LYS:HE2	2:E:431:ASP:OD1	1.97	0.65
2:D:429:MET:HE3	2:D:448:LEU:HD22	1.78	0.65
1:A:664:LEU:HB3	1:A:669:LEU:HD13	1.79	0.65
1:A:664:LEU:HD22	1:A:665:GLU:N	2.13	0.64
2:D:387:ILE:HG22	2:D:444:VAL:HG21	1.79	0.63
1:B:673:SER:HB3	4:B:806:NAG:O4	2.00	0.62
1:B:577:GLY:HA3	1:B:592:GLN:HG2	1.81	0.61
2:D:247:ASP:CG	2:D:265:TRP:HZ2	2.07	0.61
1:A:573:LEU:HD22	1:A:604:LEU:HD21	1.82	0.61
1:A:473:CYS:CB	1:A:486:SER:HA	2.30	0.61
1:B:473:CYS:HB2	1:B:486:SER:HA	1.80	0.61
2:D:265:TRP:CB	2:D:271:THR:HG23	2.26	0.61
2:E:454:ASP:HA	2:E:472:PRO:HA	1.83	0.60
2:E:239:ILE:HD13	2:E:537:PHE:HB3	1.84	0.60
2:E:239:ILE:HG12	2:E:252:ILE:HG12	1.82	0.60
1:A:577:GLY:HA3	1:A:592:GLN:HG2	1.84	0.59
1:B:306:LEU:HD13	1:B:643:GLU:HG3	1.84	0.59
1:A:474:CYS:HB2	1:A:486:SER:OG	2.02	0.59
1:A:473:CYS:HB2	1:A:486:SER:HA	1.84	0.59
2:D:260:CYS:HB3	2:D:278:ILE:HB	1.85	0.58
1:B:287:LEU:HD21	1:B:290:MET:HE2	1.86	0.58
2:E:387:ILE:HG22	2:E:444:VAL:HG21	1.85	0.58
2:E:409:VAL:HG12	2:E:425:ASP:HB3	1.84	0.58
2:D:310:LYS:HB3	2:D:321:ILE:HG13	1.84	0.57
1:B:550:ARG:HG3	1:B:655:THR:HG21	1.85	0.57
1:A:443:ASP:OD1	1:A:444:PRO:HD2	2.04	0.57
1:A:281:LEU:HD23	1:A:419:ILE:HD13	1.86	0.57
2:D:123:GLU:HB2	2:D:147:ALA:O	2.03	0.57
1:A:365:LEU:HD21	2:D:378:ARG:NH1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:HD23	1:B:419:ILE:HD13	1.85	0.57
2:E:429:MET:HE3	2:E:448:LEU:HD22	1.85	0.57
1:A:287:LEU:HD21	1:A:290:MET:HE2	1.87	0.57
1:A:604:LEU:HD23	1:A:635:CYS:HB2	1.87	0.57
2:D:454:ASP:HA	2:D:472:PRO:HA	1.86	0.57
1:B:443:ASP:OD1	1:B:444:PRO:HD2	2.04	0.57
2:D:239:ILE:HG12	2:D:252:ILE:HG12	1.87	0.57
1:B:365:LEU:HD21	2:E:378:ARG:NH1	2.20	0.57
2:E:43:PRO:HG3	2:E:62:PRO:HB3	1.86	0.57
2:E:403:SER:HB2	2:E:406:GLN:HB3	1.86	0.56
1:B:445:PRO:HA	1:B:453:GLU:OE2	2.05	0.56
2:E:253:ALA:HB2	2:E:286:CYS:SG	2.45	0.56
2:D:83:SER:HB3	2:D:86:SER:HB2	1.87	0.56
1:B:673:SER:O	4:B:806:NAG:C3	2.50	0.56
2:E:522:PRO:HA	2:E:539:SER:O	2.05	0.56
2:E:97:LEU:HA	2:E:121:PHE:O	2.06	0.56
2:D:265:TRP:HB3	2:D:271:THR:CG2	2.36	0.56
2:D:265:TRP:H	2:D:265:TRP:CD1	2.22	0.56
2:D:359:ILE:HD11	2:D:373:LEU:HD11	1.88	0.56
2:D:265:TRP:CB	2:D:271:THR:HG22	2.34	0.56
2:D:301:GLN:HB2	2:D:305:GLY:HA3	1.87	0.55
1:B:485:CYS:O	1:B:494:CYS:HA	2.05	0.55
2:E:141:LEU:HD21	2:E:144:LEU:HB2	1.88	0.55
1:B:570:TYR:HB3	1:B:598:VAL:HG12	1.89	0.55
2:E:310:LYS:HB3	2:E:321:ILE:HG13	1.89	0.55
2:E:325:GLU:OE2	2:E:328:LYS:HG3	2.05	0.55
2:E:295:LEU:HD23	2:E:311:ARG:HD2	1.88	0.55
2:D:43:PRO:HG3	2:D:62:PRO:HB3	1.89	0.54
1:B:258:SER:HB3	1:B:261:HIS:HB2	1.90	0.54
1:A:251:MET:HE3	1:A:330:PHE:HB3	1.88	0.54
2:D:97:LEU:HA	2:D:121:PHE:O	2.07	0.54
1:B:558:TRP:HB2	1:B:562:VAL:HG21	1.89	0.54
1:B:664:LEU:CD1	1:B:665:GLU:N	2.67	0.54
1:A:328:HIS:CE1	1:A:356:GLY:HA3	2.42	0.54
1:B:328:HIS:CE1	1:B:356:GLY:HA3	2.43	0.54
1:B:393:LYS:HE3	2:E:303:PHE:HZ	1.71	0.54
1:A:530:MET:HG2	1:A:694:CYS:HB3	1.89	0.54
2:E:123:GLU:HB2	2:E:147:ALA:O	2.08	0.53
1:B:573:LEU:HD22	1:B:604:LEU:HD21	1.91	0.53
2:E:321:ILE:HG22	2:E:322:GLN:HG3	1.89	0.53
2:E:398:HIS:NE2	2:E:412:GLN:HG3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ASP:OD2	2:D:355:GLY:HA3	2.09	0.53
1:A:681:SER:HB2	1:A:689:SER:H	1.74	0.53
1:A:558:TRP:HB2	1:A:562:VAL:HG21	1.91	0.52
2:D:165:LEU:HD21	2:D:168:VAL:HG23	1.90	0.52
1:B:250:LEU:HD22	1:B:333:SER:HB3	1.90	0.52
1:B:673:SER:CB	4:B:806:NAG:O4	2.58	0.52
1:A:329:LEU:HD23	1:A:357:VAL:HG22	1.92	0.52
2:D:493:GLY:HA2	2:D:499:THR:HG23	1.92	0.52
1:B:513:ARG:HH22	1:B:704:ARG:HH21	1.57	0.52
1:A:574:ASN:O	1:A:593:CYS:HB2	2.10	0.52
1:B:576:GLU:HB3	1:B:578:THR:HG23	1.92	0.52
2:E:83:SER:HB3	2:E:86:SER:HB2	1.92	0.52
2:E:298:ILE:HG22	2:E:335:ILE:HD13	1.92	0.52
2:D:265:TRP:CD1	2:D:265:TRP:N	2.73	0.51
2:D:451:PHE:CE1	2:D:475:GLY:HA2	2.45	0.51
2:E:311:ARG:HH21	2:E:316:ASN:HB3	1.75	0.51
1:B:664:LEU:C	1:B:664:LEU:CD1	2.83	0.51
1:A:483:SER:CB	1:A:494:CYS:HB3	2.37	0.51
2:D:174:SER:HA	2:D:201:GLU:HG3	1.93	0.51
2:E:103:PHE:HB2	2:E:127:ILE:HG12	1.92	0.51
2:E:117:LEU:HD23	2:E:138:LEU:HD13	1.93	0.51
2:E:301:GLN:HB2	2:E:305:GLY:HA3	1.91	0.51
2:D:522:PRO:HA	2:D:539:SER:O	2.11	0.51
2:D:262:PHE:HB3	2:D:275:TYR:CE1	2.45	0.51
2:E:165:LEU:HD21	2:E:168:VAL:HG23	1.93	0.51
2:D:247:ASP:OD2	2:D:265:TRP:CZ2	2.54	0.50
2:D:550:HIS:NE2	2:D:552:ILE:HD11	2.26	0.50
2:E:141:LEU:HD22	2:E:162:LEU:HD23	1.94	0.50
2:E:262:PHE:HB3	2:E:275:TYR:CE1	2.46	0.50
2:E:143:HIS:CD2	2:E:167:ASN:HB2	2.46	0.50
2:E:550:HIS:NE2	2:E:552:ILE:HD11	2.27	0.50
1:B:673:SER:HB3	4:B:806:NAG:H3	1.94	0.50
2:E:247:ASP:HB3	2:E:265:TRP:HH2	1.77	0.50
2:E:493:GLY:HA2	2:E:499:THR:HG23	1.93	0.50
2:D:82:ILE:HG21	2:D:106:ILE:HG23	1.94	0.50
1:B:329:LEU:HD23	1:B:357:VAL:HG22	1.94	0.50
2:E:396:THR:HB	2:E:398:HIS:HE1	1.76	0.50
2:D:244:TYR:O	2:D:247:ASP:HB2	2.12	0.50
2:D:339:LYS:NZ	2:D:342:ASN:HA	2.25	0.50
1:A:714:TYR:CZ	1:A:716:PRO:HG3	2.46	0.50
2:E:298:ILE:HG13	2:E:308:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:ILE:HG21	2:E:106:ILE:HG23	1.93	0.49
1:A:441:LEU:HD13	1:A:453:GLU:OE1	2.12	0.49
1:B:585:LYS:HB2	1:B:590:TRP:CZ3	2.47	0.49
2:D:385:LEU:HD12	2:D:398:HIS:HB2	1.94	0.49
2:D:141:LEU:HD21	2:D:144:LEU:HB2	1.93	0.49
2:D:396:THR:HB	2:D:398:HIS:HE1	1.78	0.49
2:E:247:ASP:HB3	2:E:265:TRP:CH2	2.48	0.49
1:B:483:SER:CB	1:B:494:CYS:HB3	2.33	0.49
1:B:326:ALA:HA	1:B:354:GLY:O	2.13	0.48
2:E:262:PHE:HB3	2:E:275:TYR:CZ	2.48	0.48
2:D:141:LEU:HD22	2:D:162:LEU:HD23	1.95	0.48
2:D:156:LYS:HA	2:D:183:TRP:CD2	2.48	0.48
2:E:144:LEU:O	2:E:168:VAL:HA	2.13	0.48
1:A:485:CYS:O	1:A:494:CYS:HA	2.13	0.48
2:D:298:ILE:HG22	2:D:335:ILE:HD13	1.96	0.48
2:E:385:LEU:HD12	2:E:398:HIS:HB2	1.96	0.48
1:A:680:LEU:HD12	1:A:680:LEU:H	1.78	0.48
2:D:142:ILE:HG23	2:D:143:HIS:H	1.79	0.48
2:D:143:HIS:CD2	2:D:167:ASN:HB2	2.48	0.48
2:E:156:LYS:HA	2:E:183:TRP:CD2	2.49	0.48
2:E:244:TYR:HE2	2:E:311:ARG:HD3	1.79	0.48
2:D:387:ILE:HD12	2:D:460:TRP:CE2	2.49	0.48
2:E:244:TYR:CE2	2:E:311:ARG:HD3	2.49	0.48
2:D:298:ILE:HG13	2:D:308:ILE:HG12	1.96	0.48
2:E:232:LEU:HB2	2:E:545:THR:HB	1.95	0.48
2:E:142:ILE:HG23	2:E:143:HIS:H	1.79	0.48
2:D:530:ILE:HG22	2:D:531:ASN:H	1.78	0.47
1:B:664:LEU:HB3	1:B:669:LEU:HD22	1.96	0.47
2:E:224:THR:HG22	2:E:552:ILE:HD12	1.96	0.47
2:D:460:TRP:HE3	2:D:465:PHE:CE1	2.32	0.47
1:B:251:MET:HE3	1:B:330:PHE:HB3	1.97	0.47
1:B:540:GLY:HA3	1:B:549:THR:HG22	1.95	0.47
1:A:571:GLU:HA	1:A:598:VAL:HG11	1.95	0.47
1:A:576:GLU:HB3	1:A:578:THR:HG23	1.97	0.47
2:D:362:TRP:CH2	2:D:364:GLY:HA2	2.49	0.47
1:B:558:TRP:CB	1:B:562:VAL:HG21	2.45	0.47
2:E:429:MET:SD	2:E:456:LYS:HE3	2.54	0.47
2:D:232:LEU:HB2	2:D:545:THR:HB	1.95	0.47
2:D:429:MET:SD	2:D:456:LYS:HE3	2.55	0.47
2:E:324:ILE:HD11	2:E:346:PHE:HZ	1.80	0.47
1:B:453:GLU:O	1:B:456:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:285:VAL:HG12	2:E:287:LYS:HG2	1.97	0.46
2:E:407:ARG:HG3	2:E:430:GLU:HG3	1.97	0.46
1:A:258:SER:HB3	1:A:261:HIS:HB2	1.98	0.46
2:D:265:TRP:CA	2:D:271:THR:HG23	2.45	0.46
1:B:662:MET:HE1	1:B:676:PHE:HE2	1.80	0.46
2:D:321:ILE:HG22	2:D:322:GLN:HG3	1.96	0.46
2:D:362:TRP:CZ3	2:D:364:GLY:HA2	2.50	0.46
1:B:673:SER:O	4:B:806:NAG:C1	2.64	0.46
2:D:132:ARG:O	2:D:158:ILE:HD12	2.15	0.46
1:A:570:TYR:HB3	1:A:598:VAL:HG12	1.96	0.46
2:D:423:GLN:HG3	2:D:423:GLN:O	2.14	0.46
1:A:316:ARG:HB2	1:A:320:ILE:HD12	1.96	0.46
2:E:121:PHE:HD1	2:E:145:SER:HB3	1.81	0.46
2:D:170:LEU:HB2	2:D:198:ILE:HG21	1.98	0.46
2:D:117:LEU:HD23	2:D:138:LEU:HD13	1.98	0.46
1:B:317:ARG:HG3	1:B:351:LEU:HD21	1.98	0.46
1:B:375:ALA:HB1	1:B:380:ILE:HB	1.98	0.46
1:B:574:ASN:O	1:B:593:CYS:HB2	2.16	0.46
1:B:604:LEU:HD23	1:B:635:CYS:HB3	1.98	0.46
2:D:98:PHE:HD1	2:D:122:ILE:HG12	1.81	0.45
1:A:540:GLY:HA3	1:A:549:THR:HG22	1.98	0.45
1:B:497:GLN:O	1:B:518:GLY:HA2	2.16	0.45
2:E:177:CYS:HA	2:E:181:LEU:HD12	1.97	0.45
1:B:530:MET:HE1	1:B:678:THR:HG23	1.98	0.45
1:A:631:ARG:HD2	1:A:631:ARG:HA	1.64	0.45
2:D:144:LEU:O	2:D:168:VAL:HA	2.16	0.45
2:D:235:GLN:O	2:D:254:GLN:HG3	2.16	0.45
2:E:350:ASP:OD2	2:E:355:GLY:HA3	2.17	0.45
1:A:579:GLU:HG2	1:A:590:TRP:CZ2	2.51	0.45
1:B:530:MET:HG2	1:B:694:CYS:HB3	1.97	0.45
2:E:287:LYS:HG3	2:E:335:ILE:HB	1.99	0.45
2:E:396:THR:HB	2:E:398:HIS:CE1	2.51	0.45
2:D:81:GLU:OE1	2:D:104:ASP:HB2	2.17	0.45
1:B:393:LYS:HE3	2:E:303:PHE:CZ	2.49	0.45
2:E:530:ILE:HG22	2:E:531:ASN:H	1.82	0.45
1:A:328:HIS:HE1	1:A:373:SER:HB3	1.81	0.45
2:D:79:PHE:HB2	2:D:103:PHE:HE1	1.82	0.45
2:D:285:VAL:HG21	2:D:334:ASP:HA	1.98	0.45
2:D:103:PHE:HB2	2:D:127:ILE:HG12	1.99	0.45
2:D:412:GLN:NE2	5:D:703:HOH:O	2.50	0.45
2:E:451:PHE:CE1	2:E:475:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:TRP:CB	1:A:562:VAL:HG21	2.47	0.44
2:D:224:THR:HG22	2:D:552:ILE:HD12	2.00	0.44
2:D:339:LYS:HZ1	2:D:342:ASN:HA	1.82	0.44
2:E:79:PHE:HB2	2:E:103:PHE:HE1	1.83	0.44
1:A:572:LYS:HD3	1:A:626:VAL:HG11	1.98	0.44
2:D:133:HIS:HB3	2:D:136:ARG:HE	1.83	0.44
1:B:400:GLY:O	1:B:411:PRO:HB3	2.18	0.44
2:E:359:ILE:HD11	2:E:373:LEU:HD11	2.00	0.44
1:A:375:ALA:HB1	1:A:380:ILE:HB	2.00	0.44
1:A:700:CYS:HB3	1:A:711:CYS:SG	2.57	0.44
2:E:531:ASN:C	2:E:533:ARG:H	2.26	0.44
2:E:61:ILE:HG23	2:E:74:PHE:HZ	1.81	0.44
2:E:281:THR:O	2:E:301:GLN:HB3	2.17	0.44
2:E:170:LEU:HB2	2:E:198:ILE:HG21	2.00	0.44
1:A:400:GLY:O	1:A:411:PRO:HB3	2.18	0.44
1:B:597:ASP:CB	1:B:668:CYS:H	2.28	0.44
1:B:700:CYS:HB3	1:B:711:CYS:SG	2.58	0.44
2:E:285:VAL:HG21	2:E:334:ASP:HA	1.99	0.44
2:D:182:LYS:O	2:D:186:GLU:HG2	2.18	0.44
2:E:265:TRP:H	2:E:265:TRP:HE3	1.63	0.44
1:A:453:GLU:O	1:A:456:GLU:HB2	2.18	0.43
2:D:265:TRP:CD1	2:D:265:TRP:O	2.71	0.43
1:A:243:LEU:HD21	1:A:245:ILE:HD11	2.00	0.43
1:A:362:LYS:HG3	2:D:405:SER:OG	2.18	0.43
1:B:347:GLY:O	1:B:354:GLY:HA2	2.18	0.43
1:B:673:SER:O	4:B:806:NAG:C2	2.67	0.43
2:E:133:HIS:HB3	2:E:136:ARG:HE	1.82	0.43
2:D:281:THR:O	2:D:301:GLN:HB3	2.18	0.43
2:D:396:THR:HB	2:D:398:HIS:CE1	2.53	0.43
1:B:241:ILE:HG12	1:B:434:LEU:HD22	1.99	0.43
1:B:467:VAL:HA	1:B:471:ALA:HB2	2.00	0.43
2:E:232:LEU:HD11	2:E:547:ILE:HD11	2.00	0.43
2:E:132:ARG:O	2:E:158:ILE:HD12	2.18	0.43
2:E:405:SER:HB2	5:E:701:HOH:O	2.17	0.43
2:E:523:ARG:HA	2:E:523:ARG:HD3	1.85	0.43
2:D:300:ALA:HB2	2:D:335:ILE:HD11	2.01	0.43
1:B:247:ASN:HB2	1:B:292:THR:HG23	1.99	0.43
2:D:397:PRO:HG2	2:D:413:TRP:HB3	1.99	0.43
2:E:302:LEU:HD12	2:E:332:PRO:HD2	2.00	0.43
1:B:462:THR:HG22	1:B:463:PRO:HD2	2.01	0.43
1:B:679:CYS:HB3	1:B:700:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:GLU:HB3	2:E:275:TYR:CD1	2.54	0.43
1:A:313:MET:SD	1:A:355:GLY:HA3	2.58	0.43
1:B:352:LEU:HD12	1:B:352:LEU:H	1.84	0.43
2:D:531:ASN:C	2:D:533:ARG:H	2.27	0.42
1:B:254:LYS:HE2	1:B:360:PHE:CE2	2.54	0.42
2:E:250:VAL:HB	2:E:263:LEU:HB2	2.01	0.42
2:E:503:ASN:OD1	2:E:504:TRP:N	2.52	0.42
1:B:566:ASP:OD1	1:B:567:LYS:N	2.52	0.42
2:E:409:VAL:HA	2:E:425:ASP:HA	2.00	0.42
2:D:192:ASN:HD22	4:D:604:NAG:C7	2.31	0.42
1:B:316:ARG:HG3	1:B:317:ARG:N	2.31	0.42
1:B:543:PHE:HZ	1:B:662:MET:SD	2.42	0.42
1:B:572:LYS:HD3	1:B:626:VAL:HG11	2.02	0.42
1:A:303:GLU:CD	1:A:303:GLU:H	2.26	0.42
2:D:262:PHE:HB3	2:D:275:TYR:CZ	2.54	0.42
1:B:681:SER:HB2	1:B:689:SER:H	1.85	0.42
1:A:634:ASN:HD22	4:A:804:NAG:H83	1.84	0.42
1:B:473:CYS:SG	1:B:486:SER:HA	2.60	0.42
2:E:174:SER:HA	2:E:201:GLU:HG3	2.02	0.42
1:A:681:SER:CB	1:A:689:SER:H	2.32	0.42
2:D:555:LEU:HD22	2:D:555:LEU:HA	1.95	0.42
1:B:557:ILE:O	1:B:613:ARG:HB2	2.19	0.42
2:E:156:LYS:HA	2:E:183:TRP:CE2	2.55	0.42
2:D:503:ASN:OD1	2:D:504:TRP:N	2.53	0.42
1:B:562:VAL:HG22	1:B:607:ASN:O	2.19	0.42
2:D:324:ILE:HD11	2:D:346:PHE:HZ	1.85	0.42
2:E:182:LYS:O	2:E:186:GLU:HG2	2.20	0.42
2:D:61:ILE:HD13	2:D:87:PHE:CE1	2.55	0.42
2:D:66:PRO:HB2	2:D:69:VAL:HG23	2.02	0.42
2:D:385:LEU:HB3	2:D:437:HIS:CD2	2.55	0.42
2:D:501:VAL:HG21	2:D:517:LEU:HD13	2.00	0.42
2:E:399:LEU:HB2	2:E:411:TYR:HB2	2.02	0.42
2:D:479:PHE:CE1	2:D:490:ALA:HB1	2.54	0.41
1:B:316:ARG:HB2	1:B:320:ILE:HD12	2.01	0.41
1:A:393:LYS:HE3	2:D:303:PHE:HZ	1.85	0.41
1:A:550:ARG:HG3	1:A:655:THR:HG21	2.02	0.41
2:D:121:PHE:HD1	2:D:145:SER:HB3	1.85	0.41
2:D:301:GLN:HE21	2:D:307:HIS:HD2	1.68	0.41
2:E:362:TRP:HB2	2:E:367:PHE:CE1	2.55	0.41
2:E:505:ASP:HB3	2:E:508:LYS:HB2	2.01	0.41
2:D:56:GLU:HG3	2:D:75:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:LEU:HD22	1:B:674:PHE:CZ	2.55	0.41
2:D:152:GLN:HA	2:D:174:SER:O	2.21	0.41
1:B:474:CYS:HB2	1:B:486:SER:HB2	2.01	0.41
2:E:118:GLU:HB3	2:E:142:ILE:HG22	2.02	0.41
1:A:317:ARG:HG3	1:A:351:LEU:HD21	2.02	0.41
2:D:519:VAL:HG13	2:D:522:PRO:HD3	2.03	0.41
1:B:303:GLU:CD	1:B:303:GLU:H	2.29	0.41
1:A:347:GLY:O	1:A:354:GLY:HA2	2.21	0.41
2:E:66:PRO:HB2	2:E:69:VAL:HG23	2.02	0.41
2:E:300:ALA:HB2	2:E:335:ILE:HD11	2.02	0.41
2:E:519:VAL:HG13	2:E:522:PRO:HD3	2.02	0.41
1:B:316:ARG:HD2	1:B:327:VAL:HB	2.03	0.41
2:E:477:MET:HG3	2:E:523:ARG:CZ	2.51	0.41
2:D:142:ILE:HG23	2:D:143:HIS:N	2.36	0.41
2:E:422:ASN:HD22	2:E:422:ASN:HA	1.74	0.41
2:E:447:CYS:HB3	2:E:479:PHE:CD2	2.56	0.41
1:A:432:ALA:O	1:A:435:PHE:HD2	2.04	0.40
2:D:118:GLU:HB3	2:D:142:ILE:HG22	2.01	0.40
2:E:374:HIS:HE1	5:E:721:HOH:O	2.03	0.40
2:D:429:MET:HE1	2:D:456:LYS:HG3	2.03	0.40
1:B:662:MET:HE1	1:B:676:PHE:CE2	2.56	0.40
1:A:467:VAL:HA	1:A:471:ALA:HB2	2.03	0.40
1:A:529:LYS:HB3	1:A:533:TYR:CD2	2.56	0.40
2:D:385:LEU:HD21	2:D:400:ILE:HD12	2.03	0.40
1:B:599:LEU:O	1:B:651:VAL:HG21	2.22	0.40
1:B:497:GLN:HG3	1:B:498:PRO:HD2	2.04	0.40
2:E:341:GLU:OE2	2:E:415:LYS:HD3	2.21	0.40
2:D:266:ASP:H	2:D:271:THR:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/486 (99%)	474 (98%)	8 (2%)	0	100	100
1	B	482/486 (99%)	472 (98%)	10 (2%)	0	100	100
2	D	514/526 (98%)	496 (96%)	18 (4%)	0	100	100
2	E	514/526 (98%)	497 (97%)	17 (3%)	0	100	100
All	All	1992/2024 (98%)	1939 (97%)	53 (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 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	418/420 (100%)	398 (95%)	20 (5%)	23	47
1	B	418/420 (100%)	398 (95%)	20 (5%)	23	47
2	D	473/482 (98%)	454 (96%)	19 (4%)	28	53
2	E	473/482 (98%)	452 (96%)	21 (4%)	25	50
All	All	1782/1804 (99%)	1702 (96%)	80 (4%)	24	49

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	VAL
1	A	303	GLU
1	A	316	ARG
1	A	333	SER
1	A	357	VAL
1	A	381	ILE
1	A	391	GLU
1	A	402	ILE
1	A	436	ASN
1	A	452	ILE
1	A	482	ASP
1	A	503	CYS
1	A	505	GLU

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Mol	Chain	Res	Type
1	A	569	CYS
1	A	593	CYS
1	A	599	LEU
1	A	620	GLU
1	A	622	THR
1	A	643	GLU
1	A	664	LEU
2	D	63	ARG
2	D	142	ILE
2	D	158	ILE
2	D	168	VAL
2	D	245	LEU
2	D	265	TRP
2	D	269	GLU
2	D	286	CYS
2	D	299	VAL
2	D	302	LEU
2	D	313	SER
2	D	314	PHE
2	D	324	ILE
2	D	353	LYS
2	D	403	SER
2	D	470	ARG
2	D	524	SER
2	D	539	SER
2	D	555	LEU
1	B	234	VAL
1	B	256	ARG
1	B	303	GLU
1	B	316	ARG
1	B	357	VAL
1	B	381	ILE
1	B	391	GLU
1	B	402	ILE
1	B	436	ASN
1	B	452	ILE
1	B	482	ASP
1	B	503	CYS
1	B	505	GLU
1	B	593	CYS
1	B	597	ASP
1	B	599	LEU

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Mol	Chain	Res	Type
1	B	620	GLU
1	B	622	THR
1	B	643	GLU
1	B	664	LEU
2	E	126	ASN
2	E	158	ILE
2	E	168	VAL
2	E	175	PHE
2	E	238	SER
2	E	245	LEU
2	E	299	VAL
2	E	302	LEU
2	E	314	PHE
2	E	320	LYS
2	E	324	ILE
2	E	325	GLU
2	E	353	LYS
2	E	362	TRP
2	E	385	LEU
2	E	404	SER
2	E	405	SER
2	E	431	ASP
2	E	454	ASP
2	E	544	ASN
2	E	555	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	377	ASN
1	A	691	ASN
2	D	143	HIS
2	D	176	ASN
2	D	333	ASN
2	D	412	GLN
2	D	486	ASN
2	D	488	GLN
1	B	334	GLN
1	B	639	HIS
1	B	691	ASN
2	E	143	HIS

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Mol	Chain	Res	Type
2	E	176	ASN
2	E	333	ASN
2	E	412	GLN
2	E	486	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	804	1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	E	602	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	B	805	1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	B	806	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	B	804	1	14,14,15	0.18	0	17,19,21	0.66	0
4	NAG	D	604	2	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	E	603	2	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	A	805	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	E	604	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	D	603	2	14,14,15	0.21	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	806	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	D	602	2	14,14,15	0.22	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	804	1	-	4/6/23/26	0/1/1/1
4	NAG	E	602	2	-	4/6/23/26	0/1/1/1
4	NAG	B	805	1	-	4/6/23/26	0/1/1/1
4	NAG	B	806	1	-	3/6/23/26	0/1/1/1
4	NAG	B	804	1	-	4/6/23/26	0/1/1/1
4	NAG	D	604	2	-	0/6/23/26	0/1/1/1
4	NAG	E	603	2	-	2/6/23/26	0/1/1/1
4	NAG	A	805	1	-	4/6/23/26	0/1/1/1
4	NAG	E	604	2	-	0/6/23/26	0/1/1/1
4	NAG	D	603	2	-	0/6/23/26	0/1/1/1
4	NAG	A	806	1	-	0/6/23/26	0/1/1/1
4	NAG	D	602	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	NAG	O5-C5-C6-O6
4	B	804	NAG	O5-C5-C6-O6
4	B	806	NAG	O5-C5-C6-O6
4	B	804	NAG	C4-C5-C6-O6
4	E	602	NAG	O5-C5-C6-O6
4	A	804	NAG	C8-C7-N2-C2
4	A	804	NAG	O7-C7-N2-C2
4	A	805	NAG	C8-C7-N2-C2
4	A	805	NAG	O7-C7-N2-C2
4	D	602	NAG	C8-C7-N2-C2
4	D	602	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	805	NAG	C8-C7-N2-C2
4	B	805	NAG	O7-C7-N2-C2
4	E	602	NAG	C8-C7-N2-C2
4	E	602	NAG	O7-C7-N2-C2
4	B	806	NAG	C4-C5-C6-O6
4	A	804	NAG	C4-C5-C6-O6
4	E	603	NAG	O5-C5-C6-O6
4	A	805	NAG	O5-C5-C6-O6
4	B	805	NAG	O5-C5-C6-O6
4	E	602	NAG	C4-C5-C6-O6
4	E	603	NAG	C4-C5-C6-O6
4	A	805	NAG	C4-C5-C6-O6
4	B	804	NAG	C3-C2-N2-C7
4	B	805	NAG	C4-C5-C6-O6
4	B	804	NAG	C1-C2-N2-C7
4	B	806	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	NAG	1	0
4	B	806	NAG	10	0
4	D	604	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/486 (99%)	0.35	14 (2%) 53 44	50, 82, 131, 193	0
1	B	484/486 (99%)	0.43	12 (2%) 58 49	46, 76, 123, 162	0
2	D	516/526 (98%)	0.53	23 (4%) 38 30	52, 92, 205, 245	0
2	E	516/526 (98%)	0.89	60 (11%) 9 9	60, 105, 246, 279	0
All	All	2000/2024 (98%)	0.56	109 (5%) 30 25	46, 87, 211, 279	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	122	ILE	6.0
2	D	54	LEU	4.5
2	E	416	ALA	4.5
2	E	78	GLY	4.3
2	E	96	LEU	4.0
2	E	117	LEU	4.0
2	D	496	TYR	4.0
2	E	188	LEU	4.0
2	E	97	LEU	3.9
2	E	93	LEU	3.8
2	E	170	LEU	3.8
2	E	71	SER	3.7
1	B	398	TRP	3.6
1	B	543	PHE	3.4
2	E	98	PHE	3.4
2	D	208	LYS	3.4
1	B	635	CYS	3.4
2	E	473	SER	3.3
2	E	142	ILE	3.3
1	B	293	TRP	3.3
2	E	65	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	E	165	LEU	3.0
1	A	524	ALA	3.0
2	E	490	ALA	3.0
2	E	271	THR	3.0
2	E	146	LEU	3.0
1	A	470	GLY	2.9
2	E	315	ALA	2.9
2	E	184	LEU	2.9
2	E	111	PHE	2.8
1	A	486	SER	2.8
2	E	376	TRP	2.8
2	E	144	LEU	2.7
1	A	625	LEU	2.7
2	E	214	LEU	2.7
2	D	275	TYR	2.7
2	E	556	SER	2.7
2	E	121	PHE	2.6
2	E	272	PHE	2.6
2	D	87	PHE	2.6
2	D	272	PHE	2.6
2	D	271	THR	2.6
2	D	473	SER	2.5
2	E	474	GLN	2.5
2	D	276	ASP	2.5
2	E	51	ASP	2.5
2	E	95	LEU	2.5
2	D	106	ILE	2.5
1	B	485	CYS	2.5
2	E	109	ASP	2.5
2	E	517	LEU	2.5
2	E	154	LEU	2.4
2	E	74	PHE	2.4
2	D	556	SER	2.4
1	A	676	PHE	2.4
2	E	83	SER	2.4
2	E	181	LEU	2.4
2	E	52	ASN	2.3
2	E	317	LYS	2.3
1	B	355	GLY	2.3
2	E	87	PHE	2.3
2	E	102	SER	2.3
2	D	175	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	490	ALA	2.3
2	E	193	ALA	2.3
1	A	599	LEU	2.3
2	E	166	THR	2.3
1	A	626	VAL	2.3
2	D	65	VAL	2.3
2	D	204	PRO	2.3
2	D	137	GLY	2.3
2	D	170	LEU	2.3
2	D	122	ILE	2.3
2	E	221	CYS	2.3
1	B	486	SER	2.3
2	D	62	PRO	2.3
1	B	470	GLY	2.3
2	D	82	ILE	2.2
2	D	83	SER	2.2
2	E	57	ASN	2.2
1	A	293	TRP	2.2
1	A	675	ASN	2.2
1	A	696	ASN	2.2
2	E	176	ASN	2.2
1	B	622	THR	2.2
2	E	79	PHE	2.1
2	E	242	PHE	2.1
1	B	473	CYS	2.1
2	E	145	SER	2.1
2	E	500	GLN	2.1
1	A	642	LEU	2.1
1	B	335	PHE	2.1
2	E	498	PHE	2.1
2	E	119	TYR	2.1
2	D	124	ASN	2.1
2	E	314	PHE	2.1
2	E	82	ILE	2.1
2	E	275	TYR	2.1
1	A	543	PHE	2.1
2	D	554	ASP	2.1
2	E	64	THR	2.1
2	E	70	ILE	2.1
1	B	336	GLU	2.1
2	E	72	LEU	2.0
2	E	123	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	237	LEU	2.0
1	A	634	ASN	2.0
2	E	130	ILE	2.0
1	A	464	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	806	14/15	-0.35	0.23	134,140,144,145	0
4	NAG	A	806	14/15	0.13	0.23	170,187,194,196	0
4	NAG	D	604	14/15	0.16	0.12	181,195,208,221	0
4	NAG	E	603	14/15	0.19	0.14	207,215,221,221	0
4	NAG	D	603	14/15	0.26	0.18	153,161,168,170	0
4	NAG	B	805	14/15	0.38	0.20	142,149,152,153	0
4	NAG	E	604	14/15	0.50	0.15	152,159,167,168	0
4	NAG	A	805	14/15	0.59	0.15	112,122,125,128	0
4	NAG	E	602	14/15	0.68	0.14	120,131,141,142	0
4	NAG	D	602	14/15	0.77	0.12	87,102,111,113	0
4	NAG	B	804	14/15	0.85	0.10	87,97,103,104	0
3	CA	E	601	1/1	0.87	0.09	114,114,114,114	0
4	NAG	A	804	14/15	0.88	0.10	109,113,121,130	0
3	CA	B	801	1/1	0.92	0.06	105,105,105,105	0
3	CA	A	801	1/1	0.93	0.07	92,92,92,92	0
3	CA	D	601	1/1	0.93	0.10	97,97,97,97	0
3	CA	B	803	1/1	0.96	0.06	124,124,124,124	0
3	CA	A	802	1/1	0.97	0.04	115,115,115,115	0
3	CA	B	802	1/1	0.98	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	803	1/1	0.99	0.04	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.