



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:09 PM UTC

PDB ID : 1PFQ / pdb_00001pfq
Title : crystal structure of human apo dipeptidyl peptidase IV / CD26
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Deposited on : 2003-05-27
Resolution : 1.90 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

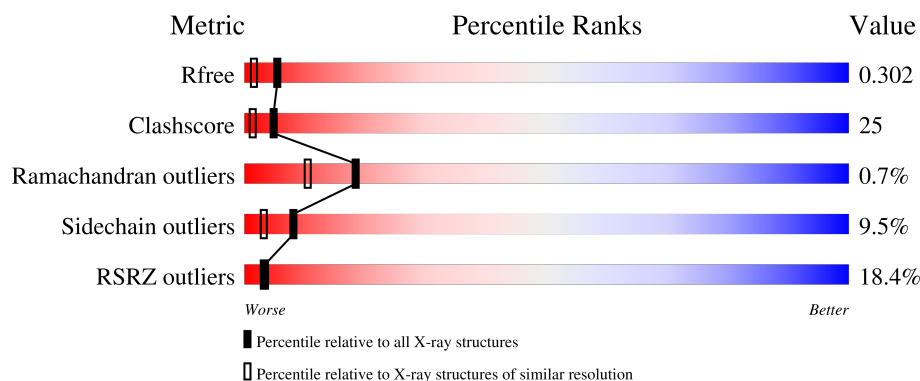
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	731	15% 65% 29% 5%
1	B	731	21% 60% 34% 5%

2 Entry composition [i](#)

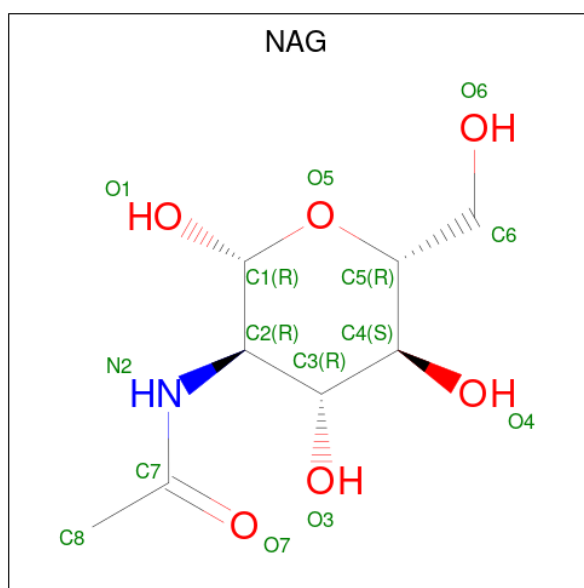
There are 3 unique types of molecules in this entry. The entry contains 12418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase IV soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			
1	B	725	Total	C	N	O	S	0	0	0
			5926	3801	977	1122	26			

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



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

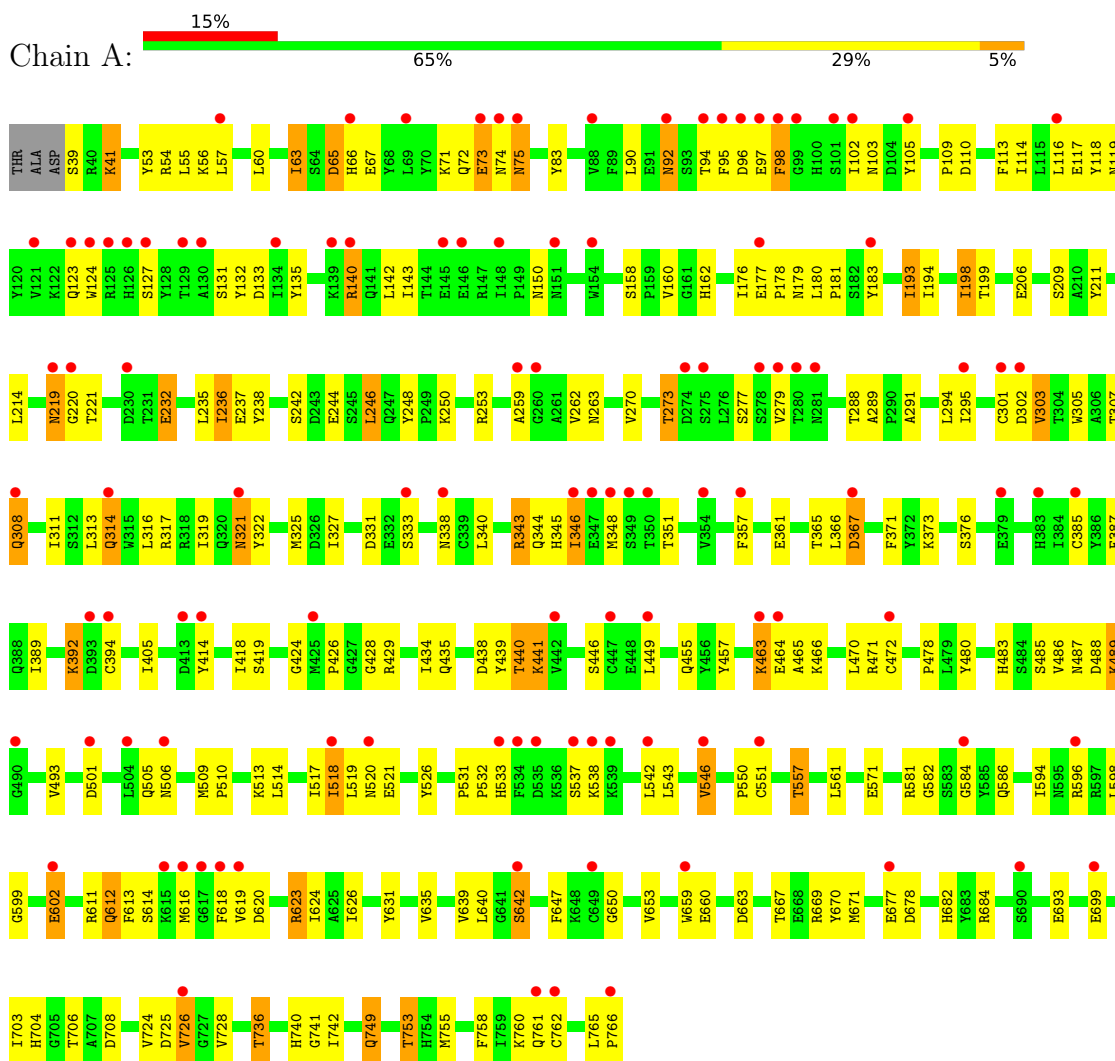
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total 268	O 268	0	0
3	B	204	Total 204	O 204	0	0

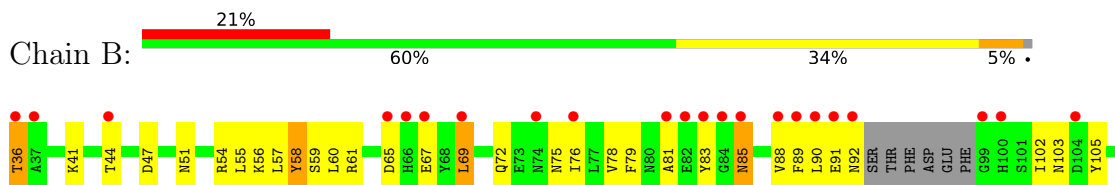
3 Residue-property plots

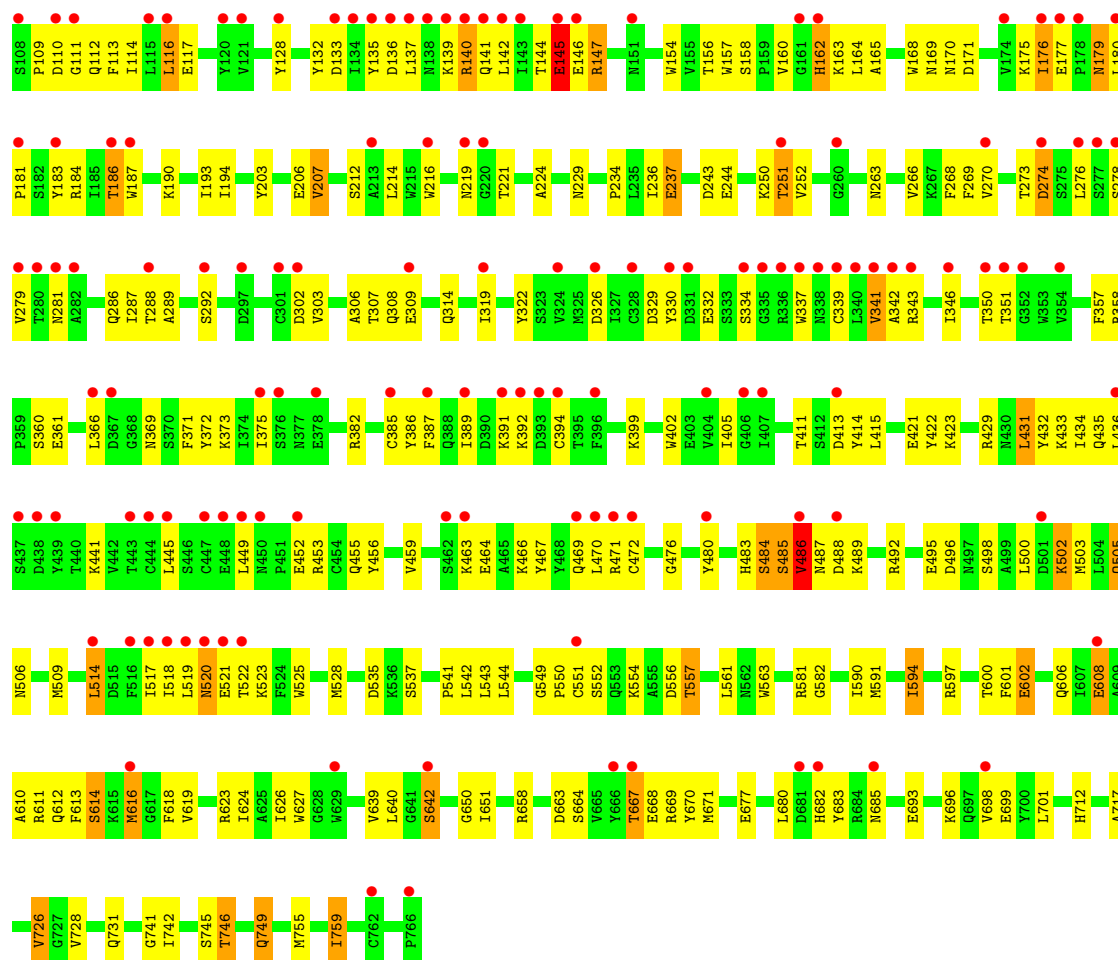
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase IV soluble form



• Molecule 1: Dipeptidyl peptidase IV soluble form





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 118.14Å 184.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-1.90) 98.6 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.254 , 0.298 0.259 , 0.302	Depositor DCC
R_{free} test set	11796 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12418	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.31	0/6136	0.69	1/8344 (0.0%)
1	B	0.31	0/6094	0.69	0/8287
All	All	0.31	0/12230	0.69	1/16631 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	PRO	O-C-N	5.21	123.71	121.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	581	ARG	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5964	0	5683	280	3
1	B	5926	0	5650	324	3
2	A	28	0	26	1	0
2	B	28	0	26	1	0
3	A	268	0	0	27	0
3	B	204	0	0	17	2
All	All	12418	0	11385	592	5

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 25.

All (592) 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:A:517:ILE:HG21	1:A:612:GLN:NE2	1.28	1.45
1:A:517:ILE:CG2	1:A:612:GLN:HE22	1.37	1.36
1:A:198:ILE:HD11	1:A:211:TYR:CE2	1.73	1.22
1:B:544:LEU:HD21	1:B:606:GLN:NE2	1.56	1.20
1:A:150:ASN:ND2	3:A:1095:HOH:O	1.71	1.17
1:A:620:ASP:OD2	1:A:623:ARG:NH1	1.77	1.16
1:A:346:ILE:HD11	1:A:348:MET:HE2	1.26	1.16
1:A:74:ASN:HB3	1:A:92:ASN:ND2	1.59	1.13
1:B:81:ALA:O	1:B:492:ARG:NH2	1.81	1.13
1:B:357:PHE:CZ	1:B:551:CYS:HB2	1.86	1.10
1:A:160:VAL:CG2	1:A:219:ASN:O	2.01	1.09
1:B:484:SER:O	1:B:488:ASP:HA	1.53	1.09
1:A:74:ASN:HB3	1:A:92:ASN:CG	1.75	1.08
1:B:83:TYR:O	1:B:492:ARG:CZ	2.00	1.08
1:B:350:THR:HG23	1:B:351:THR:HG23	1.36	1.06
1:A:653:VAL:HG21	1:A:755:MET:HE1	1.37	1.05
1:A:198:ILE:HD11	1:A:211:TYR:CZ	1.94	1.03
1:B:544:LEU:CD2	1:B:606:GLN:NE2	2.22	1.03
1:A:95:PHE:HA	1:A:98:PHE:HB2	1.40	1.01
1:A:198:ILE:CD1	1:A:211:TYR:CZ	2.46	0.99
1:B:519:LEU:HD21	1:B:612:GLN:NE2	1.77	0.99
1:B:514:LEU:C	1:B:514:LEU:HD23	1.87	0.99
1:A:623:ARG:HG3	1:A:623:ARG:HH11	1.26	0.98
1:A:198:ILE:CD1	1:A:211:TYR:CE2	2.46	0.98
1:A:94:THR:HG21	1:A:102:ILE:HD12	1.45	0.98
1:B:505:GLN:HE21	1:B:505:GLN:HA	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ASN:HB2	1:B:489:LYS:HZ2	1.29	0.97
1:A:653:VAL:CG2	1:A:755:MET:HE1	1.96	0.96
1:B:749:GLN:NE2	3:B:931:HOH:O	1.97	0.96
1:A:724:VAL:HG12	1:B:746:THR:CG2	1.96	0.96
1:B:685:ASN:ND2	3:B:1022:HOH:O	1.99	0.96
1:A:103:ASN:ND2	1:A:117:GLU:OE1	1.99	0.95
1:A:71:LYS:HD2	1:A:105:TYR:OH	1.67	0.95
1:B:329:ASP:OD2	1:B:343:ARG:NH1	1.98	0.95
1:B:341:VAL:HG22	1:B:342:ALA:H	1.31	0.94
1:B:731:GLN:NE2	3:B:880:HOH:O	2.02	0.93
1:B:405:ILE:HD13	1:B:429:ARG:HD3	1.49	0.93
1:B:244:GLU:OE2	3:B:863:HOH:O	1.88	0.91
1:A:538:LYS:O	1:A:618:PHE:HA	1.72	0.90
1:A:135:TYR:OH	1:A:140:ARG:HA	1.70	0.90
1:A:160:VAL:HG21	1:A:219:ASN:O	1.71	0.90
1:A:237:GLU:OE1	1:B:251:THR:HG22	1.71	0.90
1:A:724:VAL:HG12	1:B:746:THR:HG22	1.54	0.89
1:A:176:ILE:HD12	1:A:183:TYR:HE2	1.36	0.89
1:A:72:GLN:O	1:A:73:GLU:HG2	1.72	0.89
1:B:492:ARG:HG2	3:B:939:HOH:O	1.70	0.89
1:B:519:LEU:HD21	1:B:612:GLN:HE21	1.35	0.88
1:A:660:GLU:HG2	3:A:959:HOH:O	1.71	0.88
1:A:74:ASN:HB3	1:A:92:ASN:HD21	1.34	0.88
1:B:514:LEU:HD23	1:B:514:LEU:O	1.73	0.88
1:A:405:ILE:HD12	1:A:419:SER:HA	1.55	0.87
1:A:762:CYS:HB2	3:A:1115:HOH:O	1.75	0.87
1:A:160:VAL:HG22	1:A:219:ASN:O	1.73	0.87
1:A:346:ILE:CD1	1:A:348:MET:HE2	2.05	0.86
1:B:486:VAL:HG12	1:B:487:ASN:N	1.90	0.86
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.56	0.86
1:B:459:VAL:HG12	1:B:470:LEU:HD23	1.58	0.85
1:A:65:ASP:OD1	3:A:1097:HOH:O	1.94	0.85
1:B:83:TYR:O	1:B:492:ARG:NH1	2.09	0.85
1:A:94:THR:HG21	1:A:102:ILE:CD1	2.07	0.85
1:B:326:ASP:OD2	1:B:339:CYS:HB3	1.77	0.85
1:A:749:GLN:O	1:A:753:THR:HG23	1.76	0.84
1:A:74:ASN:HB3	1:A:92:ASN:OD1	1.76	0.84
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.13	0.84
1:B:65:ASP:OD1	1:B:466:LYS:HD2	1.78	0.84
1:B:505:GLN:HA	1:B:505:GLN:NE2	1.90	0.84
1:A:678:ASP:OD1	3:A:1076:HOH:O	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LYS:NZ	3:A:977:HOH:O	2.09	0.83
1:B:179:ASN:C	1:B:179:ASN:HD22	1.87	0.83
1:A:74:ASN:CB	1:A:92:ASN:ND2	2.42	0.83
1:A:660:GLU:OE2	3:A:959:HOH:O	1.97	0.83
1:B:139:LYS:O	1:B:141:GLN:N	2.12	0.82
1:B:487:ASN:HB2	1:B:489:LYS:NZ	1.93	0.82
1:A:321:ASN:HD22	1:A:321:ASN:H	1.25	0.82
1:A:765:LEU:HB2	1:A:766:PRO:HD3	1.61	0.82
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.62	0.82
1:B:243:ASP:OD2	3:B:1058:HOH:O	1.96	0.82
1:A:438:ASP:OD2	1:A:440:THR:HB	1.79	0.81
1:B:544:LEU:CD2	1:B:606:GLN:HE21	1.93	0.81
1:A:236:ILE:HD13	1:A:237:GLU:N	1.96	0.81
1:A:291:ALA:O	1:A:295:ILE:HG13	1.79	0.81
1:A:584:GLY:O	1:A:586:GLN:NE2	2.15	0.80
1:B:463:LYS:HG2	1:B:464:GLU:HG2	1.62	0.80
1:A:135:TYR:HE1	1:A:140:ARG:O	1.64	0.80
1:A:357:PHE:CZ	1:A:551:CYS:HB2	2.17	0.80
1:B:180:LEU:HB3	1:B:181:PRO:CD	2.12	0.80
1:B:544:LEU:HD21	1:B:606:GLN:HE22	1.45	0.80
1:B:414:TYR:CE1	1:B:433:LYS:HE3	2.17	0.79
1:A:455:GLN:HB2	1:A:557:THR:HG21	1.64	0.79
1:A:623:ARG:NH1	1:A:623:ARG:HG3	1.95	0.79
1:B:314:GLN:OE1	1:B:373:LYS:NZ	2.15	0.79
1:A:703:ILE:HD12	1:A:755:MET:HE2	1.64	0.79
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.65	0.79
1:A:74:ASN:CB	1:A:92:ASN:CG	2.54	0.79
1:A:198:ILE:HD11	1:A:211:TYR:HE2	1.48	0.79
1:A:463:LYS:HB2	1:A:463:LYS:NZ	1.99	0.78
1:B:65:ASP:OD2	1:B:463:LYS:O	2.00	0.78
1:B:456:TYR:HB2	1:B:557:THR:HG22	1.65	0.78
1:A:736:THR:HG21	1:B:717:ALA:O	1.83	0.78
1:A:367:ASP:OD2	3:A:981:HOH:O	2.02	0.78
1:B:113:PHE:HE2	1:B:162:HIS:HD2	1.32	0.77
1:A:123:GLN:HB3	1:A:127:SER:HB3	1.65	0.77
1:A:236:ILE:HD13	1:A:236:ILE:C	2.09	0.77
1:B:519:LEU:HD13	1:B:608:GLU:OE1	1.84	0.77
1:B:183:TYR:HE1	1:B:279:VAL:HG12	1.50	0.77
1:B:243:ASP:CG	3:B:1058:HOH:O	2.26	0.77
1:A:725:ASP:HA	1:B:746:THR:HG21	1.66	0.76
1:A:596:ARG:NE	3:A:957:HOH:O	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HD2	1:B:193:ILE:HD12	1.68	0.76
1:B:273:THR:O	1:B:276:LEU:CD2	2.33	0.76
1:B:287:ILE:CG2	1:B:339:CYS:SG	2.75	0.75
1:A:760:LYS:HE3	1:A:766:PRO:HG3	1.65	0.75
1:B:357:PHE:CZ	1:B:551:CYS:CB	2.66	0.75
1:B:519:LEU:CD2	1:B:612:GLN:NE2	2.49	0.75
1:A:653:VAL:CG2	1:A:755:MET:CE	2.65	0.74
1:A:346:ILE:HD11	1:A:348:MET:CE	2.14	0.74
1:B:44:THR:HG23	1:B:47:ASP:H	1.52	0.74
1:A:405:ILE:HD12	1:A:419:SER:CA	2.18	0.73
1:A:71:LYS:CD	1:A:105:TYR:OH	2.36	0.73
1:B:171:ASP:OD1	1:B:186:THR:CG2	2.35	0.73
1:A:198:ILE:CG1	1:A:211:TYR:CE2	2.71	0.73
1:A:135:TYR:CE1	1:A:140:ARG:O	2.41	0.73
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.69	0.73
1:B:411:THR:HG22	1:B:414:TYR:H	1.51	0.72
1:B:486:VAL:HG12	1:B:487:ASN:H	1.53	0.72
1:B:179:ASN:ND2	1:B:179:ASN:O	2.21	0.72
1:B:60:LEU:HD11	1:B:469:GLN:OE1	1.90	0.72
1:B:514:LEU:C	1:B:514:LEU:CD2	2.62	0.72
1:B:135:TYR:CZ	1:B:142:LEU:HD12	2.25	0.72
1:A:343:ARG:HG3	1:A:389:ILE:O	1.91	0.71
1:A:131:SER:OG	1:A:150:ASN:OD1	2.01	0.71
1:B:113:PHE:HE2	1:B:162:HIS:CD2	2.07	0.71
1:A:724:VAL:CG1	1:B:746:THR:HG22	2.20	0.71
1:B:613:PHE:O	1:B:616:MET:HG3	1.90	0.71
1:B:405:ILE:HD13	1:B:429:ARG:CD	2.21	0.70
1:A:434:ILE:HD11	1:A:439:TYR:O	1.91	0.70
1:A:317:ARG:NH2	3:A:875:HOH:O	2.25	0.70
1:A:73:GLU:HG3	1:A:74:ASN:N	2.07	0.70
1:B:156:THR:HG23	1:B:216:TRP:HE1	1.57	0.70
1:B:287:ILE:HG23	1:B:339:CYS:SG	2.32	0.70
1:B:158:SER:OG	1:B:160:VAL:O	2.09	0.69
1:B:486:VAL:CG1	1:B:487:ASN:N	2.55	0.69
1:B:250:LYS:NZ	3:B:942:HOH:O	2.14	0.69
1:B:505:GLN:HE21	1:B:505:GLN:CA	1.98	0.69
1:A:117:GLU:HB3	1:A:132:TYR:CE1	2.28	0.69
1:B:597:ARG:HA	1:B:682:HIS:CD2	2.28	0.69
1:A:463:LYS:HB2	1:A:463:LYS:HZ2	1.57	0.69
1:B:114:ILE:HG21	1:B:140:ARG:HH12	1.57	0.68
1:B:135:TYR:OH	1:B:142:LEU:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:CB	1:A:92:ASN:OD1	2.41	0.68
1:A:314:GLN:HE22	1:A:373:LYS:NZ	1.92	0.68
1:B:431:LEU:HD23	1:B:432:TYR:N	2.09	0.68
1:A:602:GLU:OE2	1:A:631:TYR:OH	2.11	0.67
1:B:180:LEU:HB3	1:B:181:PRO:HD2	1.75	0.67
1:B:663:ASP:O	1:B:667:THR:HG23	1.95	0.67
1:B:67:GLU:CD	1:B:78:VAL:CG1	2.68	0.67
1:B:243:ASP:OD1	3:B:1058:HOH:O	2.12	0.67
1:A:760:LYS:CE	1:A:766:PRO:HG3	2.25	0.67
1:B:117:GLU:HB3	1:B:132:TYR:CE1	2.31	0.67
1:B:342:ALA:HB1	1:B:391:LYS:HE3	1.74	0.67
1:A:198:ILE:HG12	1:A:199:THR:N	2.09	0.66
1:A:244:GLU:OE2	3:A:1116:HOH:O	2.13	0.66
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.25	0.66
1:A:322:TYR:HD2	1:A:348:MET:HG2	1.59	0.66
1:B:341:VAL:HG22	1:B:342:ALA:N	2.08	0.66
1:A:493:VAL:O	3:A:997:HOH:O	2.13	0.66
1:B:65:ASP:OD1	1:B:466:LYS:CD	2.43	0.65
1:B:102:ILE:HD13	1:B:105:TYR:OH	1.96	0.65
1:A:57:LEU:O	3:A:992:HOH:O	2.13	0.65
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.78	0.65
1:A:346:ILE:H	1:A:392:LYS:HZ1	1.44	0.65
1:A:405:ILE:HD13	1:A:418:ILE:HG22	1.79	0.65
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.27	0.65
1:A:518:ILE:HG13	1:A:518:ILE:O	1.94	0.65
1:A:198:ILE:CD1	1:A:211:TYR:OH	2.44	0.65
1:B:520:ASN:O	1:B:521:GLU:HB2	1.95	0.65
1:A:571:GLU:OE2	3:A:917:HOH:O	2.14	0.65
1:A:73:GLU:HG3	1:A:74:ASN:H	1.62	0.64
1:A:237:GLU:OE1	1:B:251:THR:CG2	2.44	0.64
1:B:597:ARG:HD3	1:B:600:THR:OG1	1.97	0.64
1:A:74:ASN:C	1:A:92:ASN:ND2	2.55	0.64
1:B:431:LEU:HD22	1:B:445:LEU:HD12	1.79	0.64
1:B:544:LEU:HD21	1:B:606:GLN:HE21	1.52	0.64
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.32	0.64
1:B:411:THR:HG23	1:B:413:ASP:H	1.62	0.64
1:B:663:ASP:O	1:B:667:THR:CG2	2.45	0.64
1:B:44:THR:HG22	1:B:47:ASP:CG	2.23	0.64
1:A:63:ILE:HD11	1:A:67:GLU:HB2	1.80	0.64
1:A:124:TRP:H	1:A:127:SER:HB3	1.63	0.63
1:A:198:ILE:HD12	1:A:211:TYR:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:PRO:O	1:A:551:CYS:CB	2.47	0.63
1:B:544:LEU:CD2	1:B:606:GLN:HE22	2.02	0.63
1:A:726:VAL:O	1:A:726:VAL:CG1	2.46	0.63
1:B:610:ALA:O	1:B:614:SER:HB2	1.98	0.63
1:A:236:ILE:HD12	1:A:238:TYR:HD2	1.64	0.63
1:A:471:ARG:HG3	1:A:480:TYR:CE2	2.34	0.63
1:A:253:ARG:HD2	3:A:960:HOH:O	1.98	0.63
1:A:557:THR:HG22	1:A:557:THR:O	1.97	0.63
1:B:83:TYR:O	1:B:492:ARG:NH2	2.32	0.63
1:B:455:GLN:HB2	1:B:557:THR:HG21	1.79	0.63
1:B:500:LEU:HA	1:B:503:MET:HE3	1.80	0.63
1:B:557:THR:O	1:B:557:THR:CG2	2.47	0.63
1:A:301:CYS:SG	1:A:316:LEU:HB2	2.39	0.62
1:A:557:THR:O	1:A:557:THR:CG2	2.46	0.62
1:B:67:GLU:CD	1:B:78:VAL:HG11	2.23	0.62
1:B:116:LEU:HD12	1:B:133:ASP:O	1.98	0.62
1:B:557:THR:O	1:B:557:THR:HG23	1.99	0.62
1:A:726:VAL:O	1:A:726:VAL:HG13	2.00	0.62
1:B:88:VAL:HG11	1:B:91:GLU:HB2	1.82	0.62
1:B:498:SER:O	1:B:502:LYS:HG2	1.99	0.62
1:B:519:LEU:CD1	1:B:608:GLU:OE1	2.46	0.62
1:A:653:VAL:HG22	1:A:755:MET:CE	2.29	0.62
1:B:128:TYR:HE2	1:B:132:TYR:OH	1.82	0.62
1:B:484:SER:O	1:B:488:ASP:CA	2.41	0.62
1:B:350:THR:HG23	1:B:351:THR:CG2	2.24	0.61
1:A:94:THR:CG2	1:A:102:ILE:CD1	2.77	0.61
1:B:273:THR:HA	1:B:276:LEU:HD22	1.83	0.61
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.82	0.61
1:A:761:GLN:NE2	3:A:1115:HOH:O	2.33	0.61
1:B:229:ASN:HB2	3:B:1038:HOH:O	1.99	0.61
1:A:71:LYS:HD2	1:A:105:TYR:HH	1.64	0.61
1:A:236:ILE:CD1	1:A:238:TYR:HD2	2.14	0.61
1:A:198:ILE:HD11	1:A:211:TYR:OH	1.99	0.61
1:B:463:LYS:HG2	1:B:464:GLU:OE2	2.01	0.61
1:B:471:ARG:HG2	1:B:480:TYR:CE2	2.35	0.61
1:B:405:ILE:CD1	1:B:429:ARG:HD3	2.26	0.60
1:B:276:LEU:N	1:B:276:LEU:HD23	2.17	0.60
1:A:724:VAL:O	1:B:746:THR:HG23	2.00	0.60
1:B:342:ALA:HB1	1:B:391:LYS:CE	2.32	0.60
1:A:598:LEU:HD13	1:A:659:TRP:CZ2	2.36	0.60
1:B:288:THR:HG22	1:B:289:ALA:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:MET:HE1	1:B:616:MET:HE1	1.83	0.60
1:B:273:THR:C	1:B:276:LEU:HD22	2.26	0.60
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.84	0.60
1:B:459:VAL:HG12	1:B:470:LEU:CD2	2.32	0.59
1:A:517:ILE:HG21	1:A:612:GLN:HE22	0.51	0.59
1:A:198:ILE:HG13	1:A:211:TYR:CE2	2.37	0.59
1:A:41:LYS:HE3	1:A:53:TYR:OH	2.02	0.59
1:A:176:ILE:HD12	1:A:183:TYR:CE2	2.28	0.59
1:A:611:ARG:O	1:A:614:SER:HB2	2.02	0.59
1:B:463:LYS:CG	1:B:464:GLU:OE2	2.50	0.59
1:A:550:PRO:O	1:A:551:CYS:HB2	2.03	0.59
1:A:765:LEU:CB	1:A:766:PRO:HD3	2.29	0.59
1:A:72:GLN:O	1:A:73:GLU:CG	2.47	0.59
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.03	0.59
1:A:56:LYS:HD2	3:A:999:HOH:O	2.01	0.58
1:A:71:LYS:NZ	1:A:105:TYR:OH	2.35	0.58
1:B:171:ASP:OD1	1:B:186:THR:HG23	2.02	0.58
1:B:273:THR:O	1:B:276:LEU:HD22	2.03	0.58
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.17	0.58
1:B:411:THR:HG22	1:B:414:TYR:N	2.19	0.58
1:A:703:ILE:HD12	1:A:755:MET:CE	2.34	0.58
1:A:63:ILE:HD11	1:A:67:GLU:CB	2.34	0.58
1:A:405:ILE:CD1	1:A:419:SER:HA	2.31	0.58
1:B:463:LYS:HG2	1:B:464:GLU:CG	2.34	0.58
1:A:758:PHE:O	1:A:761:GLN:HG3	2.03	0.58
1:B:498:SER:O	1:B:502:LYS:CG	2.52	0.58
1:B:514:LEU:O	1:B:514:LEU:CD2	2.50	0.58
1:A:63:ILE:CD1	1:A:67:GLU:HB2	2.34	0.58
1:B:171:ASP:OD1	1:B:186:THR:HG22	2.03	0.58
1:A:760:LYS:HB3	1:A:766:PRO:CG	2.34	0.57
1:B:308:GLN:HA	1:B:308:GLN:OE1	2.04	0.57
1:B:110:ASP:OD1	1:B:112:GLN:HG3	2.03	0.57
1:B:146:GLU:O	1:B:175:LYS:HE3	2.05	0.57
1:B:402:TRP:CE2	1:B:421:GLU:HG3	2.40	0.57
1:B:431:LEU:CD2	1:B:432:TYR:N	2.68	0.57
1:B:518:ILE:O	1:B:518:ILE:HG13	2.04	0.57
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.86	0.57
1:A:236:ILE:C	1:A:236:ILE:CD1	2.78	0.57
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.20	0.57
1:A:143:ILE:HD11	1:A:178:PRO:HB2	1.87	0.56
1:A:135:TYR:OH	1:A:140:ARG:CA	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:TRP:CH2	1:B:755:MET:HE2	2.40	0.56
1:B:640:LEU:HD22	1:B:698:VAL:HG11	1.87	0.56
1:A:387:PHE:CE2	1:A:394:CYS:CB	2.87	0.56
1:B:745:SER:O	1:B:749:GLN:NE2	2.39	0.56
1:B:103:ASN:ND2	1:B:117:GLU:OE1	2.32	0.56
1:B:128:TYR:CE2	1:B:132:TYR:OH	2.59	0.56
1:B:184:ARG:HD3	1:B:187:TRP:CZ2	2.40	0.56
1:B:287:ILE:HG21	1:B:339:CYS:SG	2.45	0.56
1:A:235:LEU:HD22	1:A:235:LEU:N	2.21	0.56
1:A:724:VAL:CG1	1:B:746:THR:CG2	2.78	0.56
1:A:96:ASP:O	1:A:142:LEU:CD1	2.55	0.55
1:A:71:LYS:CD	1:A:105:TYR:HH	2.19	0.55
1:A:660:GLU:CG	3:A:959:HOH:O	2.42	0.55
1:A:463:LYS:HD2	3:A:1097:HOH:O	2.05	0.55
1:B:371:PHE:CE2	1:B:387:PHE:CD1	2.95	0.55
1:B:471:ARG:CG	1:B:480:TYR:CE2	2.90	0.55
1:A:365:THR:HB	3:A:981:HOH:O	2.06	0.55
1:A:435:GLN:O	1:A:439:TYR:HA	2.07	0.55
1:B:342:ALA:CB	1:B:391:LYS:HE3	2.37	0.55
1:A:594:ILE:HD12	1:A:598:LEU:CD2	2.37	0.54
1:A:749:GLN:O	1:A:753:THR:CG2	2.53	0.54
1:B:487:ASN:CB	1:B:489:LYS:NZ	2.69	0.54
1:A:219:ASN:N	1:A:220:GLY:HA2	2.21	0.54
1:B:453:ARG:HG3	1:B:476:GLY:HA3	1.89	0.54
1:B:346:ILE:HG12	3:B:899:HOH:O	2.06	0.54
1:B:544:LEU:CG	1:B:606:GLN:HE22	2.20	0.54
1:B:519:LEU:CD2	1:B:612:GLN:HE21	2.12	0.54
1:B:544:LEU:HD23	1:B:606:GLN:HE21	1.70	0.54
1:B:184:ARG:HD3	1:B:187:TRP:CE2	2.43	0.54
1:B:169:ASN:O	1:B:170:ASN:HB2	2.08	0.54
1:B:36:THR:CG2	3:B:1026:HOH:O	2.56	0.54
1:A:346:ILE:CD1	1:A:348:MET:HG3	2.38	0.53
2:B:855:NAG:O3	3:B:1017:HOH:O	2.19	0.53
1:B:60:LEU:CD1	1:B:469:GLN:OE1	2.57	0.53
1:A:357:PHE:CZ	1:A:551:CYS:CB	2.91	0.53
1:A:206:GLU:OE2	1:A:663:ASP:OD1	2.25	0.53
1:A:291:ALA:O	1:A:295:ILE:CG1	2.52	0.53
1:B:61:ARG:NH2	1:B:105:TYR:O	2.41	0.53
1:B:180:LEU:CB	1:B:181:PRO:CD	2.80	0.53
1:B:56:LYS:HD3	1:B:495:GLU:OE1	2.08	0.53
1:B:110:ASP:CG	1:B:112:GLN:HG3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HD23	1:B:276:LEU:H	1.72	0.53
1:B:487:ASN:CG	1:B:489:LYS:HZ1	2.16	0.53
1:B:639:VAL:O	1:B:642:SER:HB2	2.09	0.53
1:A:760:LYS:HB3	1:A:766:PRO:CD	2.38	0.53
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.44	0.53
1:A:198:ILE:HD12	1:A:211:TYR:OH	2.09	0.53
1:A:322:TYR:CD2	1:A:348:MET:HG2	2.43	0.53
1:A:546:VAL:HG21	1:A:635:VAL:HG11	1.90	0.53
1:B:91:GLU:O	1:B:92:ASN:C	2.52	0.53
1:B:415:LEU:C	1:B:415:LEU:HD23	2.34	0.53
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.90	0.53
1:B:341:VAL:HG13	1:B:342:ALA:N	2.24	0.53
1:A:75:ASN:HB2	1:A:90:LEU:O	2.09	0.52
1:A:232:GLU:OE1	1:A:232:GLU:O	2.27	0.52
1:A:659:TRP:CE3	1:A:667:THR:HG23	2.44	0.52
1:A:219:ASN:HB2	1:A:308:GLN:HG2	1.90	0.52
1:A:486:VAL:HG12	1:A:487:ASN:ND2	2.24	0.52
1:A:726:VAL:CG1	1:A:728:VAL:HG23	2.33	0.52
1:B:67:GLU:HG3	1:B:79:PHE:O	2.09	0.52
1:A:74:ASN:CB	1:A:92:ASN:HD21	2.14	0.52
1:A:288:THR:CG2	1:A:294:LEU:HD11	2.40	0.52
1:A:314:GLN:HE22	1:A:373:LYS:HZ2	1.56	0.52
1:B:128:TYR:HE2	1:B:132:TYR:HH	1.55	0.52
1:B:519:LEU:HD13	1:B:608:GLU:CD	2.34	0.52
1:A:331:ASP:HB2	1:A:338:ASN:HD21	1.75	0.52
1:A:346:ILE:C	1:A:346:ILE:HD12	2.35	0.52
1:B:391:LYS:O	1:B:392:LYS:HB2	2.08	0.52
1:A:760:LYS:HB3	1:A:766:PRO:HD3	1.90	0.52
1:B:431:LEU:HD23	1:B:432:TYR:H	1.73	0.52
1:B:698:VAL:HG12	1:B:699:GLU:N	2.25	0.51
1:A:305:TRP:CZ2	1:A:311:ILE:HD12	2.46	0.51
1:A:325:MET:HE2	1:A:345:HIS:ND1	2.25	0.51
1:B:594:ILE:CD1	1:B:602:GLU:HG3	2.41	0.51
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.91	0.51
1:B:357:PHE:O	1:B:358:ARG:HB3	2.11	0.51
1:A:760:LYS:NZ	1:A:766:PRO:HG3	2.25	0.51
1:B:273:THR:CA	1:B:276:LEU:HD22	2.40	0.51
1:A:135:TYR:CE1	1:A:140:ARG:C	2.89	0.51
1:A:179:ASN:C	1:A:180:LEU:HD12	2.35	0.51
1:B:91:GLU:HG2	1:B:92:ASN:OD1	2.11	0.51
1:A:73:GLU:CG	1:A:74:ASN:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.46	0.51
1:A:97:GLU:OE1	1:A:133:ASP:OD1	2.29	0.51
1:A:463:LYS:HG2	1:A:464:GLU:HG2	1.92	0.51
1:B:549:GLY:O	1:B:552:SER:HB3	2.11	0.51
1:A:73:GLU:CG	1:A:74:ASN:H	2.23	0.51
1:A:340:LEU:N	1:A:340:LEU:HD12	2.26	0.51
1:A:602:GLU:CD	1:A:631:TYR:HH	2.18	0.51
1:B:431:LEU:CD2	1:B:431:LEU:C	2.83	0.51
1:A:221:THR:O	1:A:273:THR:HB	2.10	0.50
1:A:519:LEU:O	1:A:520:ASN:HB2	2.11	0.50
1:B:357:PHE:CE1	1:B:551:CYS:CB	2.95	0.50
1:B:44:THR:O	1:B:47:ASP:HB2	2.11	0.50
1:B:67:GLU:HG2	1:B:78:VAL:HG13	1.93	0.50
1:A:179:ASN:O	1:A:180:LEU:HD12	2.11	0.50
1:B:616:MET:HE3	1:B:618:PHE:CE1	2.46	0.50
1:B:556:ASP:C	1:B:556:ASP:OD1	2.54	0.50
1:A:198:ILE:HG13	1:A:211:TYR:CD2	2.46	0.50
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.94	0.50
1:A:55:LEU:CD1	1:A:561:LEU:HD12	2.42	0.50
1:B:582:GLY:CA	1:B:590:ILE:O	2.60	0.50
1:A:109:PRO:HG2	1:A:158:SER:O	2.11	0.49
1:A:626:ILE:O	1:A:650:GLY:HA2	2.11	0.49
1:B:276:LEU:O	1:B:276:LEU:HG	2.11	0.49
1:B:626:ILE:O	1:B:650:GLY:HA2	2.12	0.49
1:A:501:ASP:O	1:A:505:GLN:HG2	2.12	0.49
1:A:232:GLU:HB3	1:A:262:VAL:HG11	1.93	0.49
1:B:110:ASP:OD1	1:B:110:ASP:C	2.56	0.49
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.47	0.49
1:A:113:PHE:CE1	1:A:178:PRO:HG2	2.47	0.49
1:A:331:ASP:HB2	1:A:338:ASN:ND2	2.27	0.49
1:A:405:ILE:CD1	1:A:419:SER:CA	2.90	0.49
1:B:664:SER:O	1:B:668:GLU:HB2	2.12	0.49
1:A:317:ARG:HG2	3:A:1019:HOH:O	2.12	0.49
1:B:176:ILE:O	1:B:177:GLU:HG3	2.13	0.49
1:A:180:LEU:HB3	1:A:181:PRO:HD2	1.94	0.48
1:A:262:VAL:HA	3:A:1005:HOH:O	2.12	0.48
1:B:65:ASP:OD2	1:B:464:GLU:HB2	2.13	0.48
1:B:550:PRO:O	1:B:551:CYS:CB	2.59	0.48
1:B:667:THR:O	1:B:671:MET:HB2	2.12	0.48
1:A:708:ASP:OD2	1:A:740:HIS:HD2	1.96	0.48
1:B:90:LEU:HD22	1:B:140:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:C	1:B:137:LEU:HD12	2.37	0.48
1:B:214:LEU:HD12	1:B:214:LEU:C	2.38	0.48
1:A:94:THR:HG22	1:A:94:THR:O	2.14	0.48
1:A:60:LEU:HD12	1:A:60:LEU:C	2.38	0.48
1:A:671:MET:HE1	1:A:682:HIS:CD2	2.49	0.48
1:B:41:LYS:NZ	1:B:47:ASP:OD1	2.47	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.48
1:B:372:TYR:OH	1:B:436:LEU:HD11	2.14	0.48
1:A:463:LYS:HB2	1:A:463:LYS:HZ3	1.77	0.48
1:B:372:TYR:CZ	1:B:386:TYR:HD1	2.32	0.48
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.96	0.48
1:A:584:GLY:C	1:A:586:GLN:HE21	2.17	0.48
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.43	0.48
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.47	0.48
1:B:528:MET:HE1	1:B:616:MET:CE	2.44	0.48
1:A:618:PHE:CD1	1:A:619:VAL:HG23	2.49	0.47
1:B:435:GLN:HG3	1:B:441:LYS:HB3	1.95	0.47
1:B:542:LEU:HD12	1:B:619:VAL:CG1	2.44	0.47
1:B:698:VAL:CG1	1:B:699:GLU:N	2.77	0.47
1:A:96:ASP:O	1:A:142:LEU:HD11	2.15	0.47
1:A:405:ILE:HD13	1:A:429:ARG:HD3	1.95	0.47
1:B:156:THR:HG21	1:B:214:LEU:CD1	2.44	0.47
1:B:411:THR:C	1:B:413:ASP:H	2.23	0.47
1:B:145:GLU:O	1:B:147:ARG:HG3	2.13	0.47
1:A:321:ASN:H	1:A:321:ASN:ND2	2.04	0.47
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.49	0.47
1:B:411:THR:CG2	1:B:414:TYR:H	2.22	0.47
1:B:726:VAL:O	1:B:726:VAL:CG1	2.63	0.47
1:A:517:ILE:HG22	1:A:518:ILE:N	2.28	0.47
1:A:639:VAL:O	1:A:642:SER:HB2	2.15	0.47
1:B:145:GLU:H	1:B:145:GLU:HG2	1.49	0.47
1:B:171:ASP:CB	1:B:186:THR:HG22	2.43	0.47
1:B:341:VAL:HG13	1:B:343:ARG:H	1.80	0.47
1:B:350:THR:HG21	3:B:866:HOH:O	2.15	0.47
1:B:542:LEU:HD12	1:B:619:VAL:HG11	1.97	0.47
1:A:60:LEU:HD12	1:A:60:LEU:O	2.15	0.47
1:B:485:SER:O	1:B:486:VAL:C	2.58	0.47
1:B:693:GLU:O	1:B:696:LYS:HD3	2.15	0.47
1:A:598:LEU:CD1	1:A:659:TRP:CZ2	2.98	0.47
1:A:236:ILE:HD12	1:A:238:TYR:CD2	2.47	0.47
1:A:505:GLN:HE21	1:A:505:GLN:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:LEU:HD21	1:B:525:TRP:CZ3	2.51	0.46
1:B:219:ASN:HB3	1:B:221:THR:OG1	2.16	0.46
1:A:405:ILE:CD1	1:A:418:ILE:HG22	2.44	0.46
1:A:449:LEU:HD23	1:A:449:LEU:HA	1.82	0.46
1:B:36:THR:HG22	3:B:1026:HOH:O	2.15	0.46
1:B:357:PHE:CE2	1:B:551:CYS:HB2	2.46	0.46
1:B:518:ILE:HA	1:B:522:THR:O	2.15	0.46
1:A:288:THR:HG22	1:A:289:ALA:O	2.15	0.46
1:A:346:ILE:H	1:A:392:LYS:NZ	2.12	0.46
1:A:340:LEU:HD12	1:A:340:LEU:H	1.81	0.46
1:A:366:LEU:C	1:A:366:LEU:HD23	2.40	0.46
1:B:759:ILE:HD13	1:B:759:ILE:HA	1.80	0.46
1:A:325:MET:CE	1:A:345:HIS:ND1	2.78	0.46
1:A:428:GLY:C	1:A:429:ARG:HG2	2.40	0.46
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.49	0.46
1:B:292:SER:OG	1:B:322:TYR:HE1	1.98	0.46
1:B:563:TRP:CH2	1:B:755:MET:CE	2.99	0.46
1:B:57:LEU:O	1:B:58:TYR:C	2.58	0.46
1:B:113:PHE:CE2	1:B:162:HIS:CD2	2.96	0.46
1:B:463:LYS:HG3	1:B:464:GLU:OE2	2.15	0.46
1:B:582:GLY:HA2	1:B:590:ILE:O	2.16	0.46
1:A:314:GLN:HE22	1:A:373:LYS:HZ1	1.64	0.46
1:A:317:ARG:CZ	3:A:875:HOH:O	2.62	0.46
1:B:518:ILE:O	1:B:518:ILE:CG1	2.64	0.46
1:B:90:LEU:CD2	1:B:140:ARG:HH21	2.30	0.45
1:B:411:THR:HG23	1:B:413:ASP:N	2.29	0.45
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.49	0.45
1:A:653:VAL:HG22	1:A:755:MET:HE2	1.98	0.45
1:B:44:THR:HG22	1:B:47:ASP:OD1	2.16	0.45
1:A:532:PRO:O	1:A:533:HIS:HB2	2.17	0.45
1:B:664:SER:HB2	1:B:668:GLU:OE2	2.16	0.45
1:B:357:PHE:CE1	1:B:551:CYS:HB3	2.51	0.45
1:B:372:TYR:OH	1:B:436:LEU:CD1	2.64	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.60	0.45
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.99	0.45
1:A:65:ASP:OD2	1:A:66:HIS:HD2	2.00	0.45
1:A:319:ILE:O	1:A:321:ASN:ND2	2.47	0.45
1:B:292:SER:HG	1:B:322:TYR:HE1	1.65	0.45
1:B:330:TYR:HB2	1:B:337:TRP:CZ3	2.52	0.45
1:A:74:ASN:O	1:A:92:ASN:ND2	2.50	0.45
1:A:131:SER:HG	1:A:150:ASN:CG	2.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:TRP:HE3	1:A:667:THR:HG23	1.82	0.45
1:A:71:LYS:CE	1:A:105:TYR:OH	2.65	0.45
1:B:471:ARG:HG3	1:B:480:TYR:HE2	1.81	0.45
1:B:302:ASP:OD1	1:B:302:ASP:N	2.49	0.44
1:B:306:ALA:O	1:B:307:THR:HG22	2.17	0.44
1:B:487:ASN:OD1	1:B:489:LYS:NZ	2.42	0.44
1:B:535:ASP:C	1:B:535:ASP:OD1	2.60	0.44
1:A:194:ILE:HD12	2:A:853:NAG:H82	1.99	0.44
1:B:435:GLN:HG3	1:B:441:LYS:CB	2.47	0.44
1:A:301:CYS:SG	1:A:316:LEU:CB	3.05	0.44
1:B:350:THR:HG23	1:B:351:THR:N	2.31	0.44
1:A:96:ASP:O	1:A:142:LEU:HD12	2.18	0.44
1:A:118:TYR:O	1:A:119:ASN:HB2	2.18	0.44
1:B:492:ARG:CG	3:B:939:HOH:O	2.46	0.44
1:A:94:THR:CG2	1:A:102:ILE:HD11	2.45	0.44
1:B:75:ASN:OD1	1:B:91:GLU:HG3	2.17	0.44
1:B:219:ASN:HB3	1:B:221:THR:H	1.82	0.44
1:B:369:ASN:HB3	1:B:389:ILE:CD1	2.48	0.44
1:B:608:GLU:HA	1:B:611:ARG:HB2	2.00	0.44
1:A:623:ARG:NH1	1:A:623:ARG:CG	2.71	0.44
1:B:136:ASP:HB2	1:B:139:LYS:O	2.18	0.44
1:B:165:ALA:HB2	1:B:216:TRP:CZ2	2.52	0.44
1:B:350:THR:CG2	1:B:351:THR:HG23	2.27	0.44
1:B:550:PRO:O	1:B:551:CYS:HB2	2.17	0.44
1:A:463:LYS:NZ	1:A:463:LYS:CB	2.69	0.44
1:B:44:THR:CG2	1:B:47:ASP:H	2.26	0.43
1:B:614:SER:OG	1:B:624:ILE:HD11	2.17	0.43
1:A:143:ILE:CD1	1:A:178:PRO:CB	2.96	0.43
1:A:624:ILE:HG22	1:A:647:PHE:CD1	2.53	0.43
1:A:724:VAL:HG12	1:B:746:THR:HG21	1.95	0.43
1:B:434:ILE:HA	1:B:441:LYS:O	2.19	0.43
1:A:623:ARG:HH11	1:A:623:ARG:CG	2.09	0.43
1:A:532:PRO:O	1:A:533:HIS:CB	2.67	0.43
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.54	0.43
1:B:466:LYS:HG2	1:B:467:TYR:CE2	2.53	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.53	0.43
1:A:325:MET:HE3	1:A:327:ILE:HD11	2.00	0.43
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.53	0.43
1:A:725:ASP:HA	1:B:746:THR:CG2	2.44	0.43
1:B:69:LEU:HD21	1:B:76:ILE:HG21	2.01	0.43
1:A:303:VAL:HB	1:A:313:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:THR:HB	3:A:982:HOH:O	2.18	0.43
1:A:438:ASP:C	1:A:440:THR:N	2.77	0.43
1:B:369:ASN:O	1:B:389:ILE:HG12	2.19	0.43
1:B:391:LYS:O	1:B:392:LYS:CB	2.67	0.43
1:B:190:LYS:HD2	1:B:193:ILE:CD1	2.45	0.43
1:B:341:VAL:HG13	1:B:343:ARG:N	2.34	0.43
1:A:424:GLY:O	1:A:426:PRO:HD3	2.18	0.42
1:A:438:ASP:C	1:A:440:THR:H	2.26	0.42
1:A:706:THR:OG1	1:A:736:THR:HA	2.19	0.42
1:B:278:SER:HB3	1:B:281:ASN:O	2.19	0.42
1:B:422:TYR:CE1	1:B:423:LYS:HG3	2.54	0.42
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.42
1:A:489:LYS:HA	1:A:489:LYS:HD3	1.84	0.42
1:B:535:ASP:C	1:B:537:SER:H	2.27	0.42
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.55	0.42
1:A:244:GLU:OE2	1:B:658:ARG:NH2	2.49	0.42
1:B:180:LEU:CB	1:B:181:PRO:HD3	2.49	0.42
1:B:375:ILE:HD11	1:B:387:PHE:HZ	1.85	0.42
1:A:741:GLY:O	1:A:742:ILE:C	2.61	0.42
1:B:60:LEU:CG	1:B:469:GLN:OE1	2.68	0.42
1:B:496:ASP:CG	1:B:498:SER:HG	2.27	0.42
1:A:72:GLN:C	1:A:73:GLU:HG2	2.44	0.42
1:A:514:LEU:HD12	1:A:526:TYR:O	2.20	0.42
1:B:114:ILE:CG2	1:B:140:ARG:HH12	2.29	0.42
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.49	0.42
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.49	0.42
1:B:563:TRP:CZ3	1:B:755:MET:CE	3.03	0.42
1:B:88:VAL:CG1	1:B:91:GLU:HB2	2.49	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.20	0.42
1:A:509:MET:HA	1:A:510:PRO:HD3	1.90	0.41
1:A:581:ARG:HA	1:A:582:GLY:HA2	1.75	0.41
1:B:582:GLY:HA3	1:B:591:MET:HA	2.02	0.41
1:B:382:ARG:NH2	1:B:591:MET:HE1	2.35	0.41
1:B:431:LEU:CD2	1:B:445:LEU:HD12	2.48	0.41
1:B:60:LEU:HD12	1:B:60:LEU:O	2.20	0.41
1:B:306:ALA:O	1:B:307:THR:CG2	2.68	0.41
1:B:422:TYR:CD1	1:B:423:LYS:HG3	2.55	0.41
1:A:317:ARG:NE	3:A:875:HOH:O	2.53	0.41
1:B:594:ILE:HD12	1:B:594:ILE:HA	1.94	0.41
1:A:463:LYS:C	1:A:465:ALA:H	2.29	0.41
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ASN:HB2	1:B:389:ILE:HG12	2.02	0.41
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.36	0.41
1:B:375:ILE:HD11	1:B:387:PHE:CZ	2.56	0.41
1:A:219:ASN:CB	1:A:220:GLY:HA2	2.51	0.41
1:B:156:THR:HG23	1:B:156:THR:O	2.19	0.41
1:B:471:ARG:HG3	1:B:480:TYR:CE2	2.56	0.41
1:A:485:SER:O	1:A:486:VAL:C	2.64	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:B:330:TYR:HE2	1:B:332:GLU:HG2	1.86	0.41
1:B:449:LEU:HA	1:B:449:LEU:HD23	1.85	0.41
1:B:498:SER:O	1:B:502:LYS:HG3	2.21	0.41
1:B:509:MET:HE1	1:B:561:LEU:CD2	2.50	0.41
1:B:693:GLU:HA	1:B:726:VAL:HG11	2.03	0.41
1:A:41:LYS:CE	1:A:53:TYR:OH	2.67	0.41
1:A:613:PHE:O	1:A:616:MET:HG2	2.21	0.41
1:B:157:TRP:CE3	1:B:164:LEU:HG	2.55	0.41
1:B:158:SER:HB3	1:B:163:LYS:HB3	2.02	0.41
1:B:422:TYR:O	1:B:423:LYS:HB2	2.20	0.41
1:B:487:ASN:O	1:B:488:ASP:C	2.62	0.41
1:B:369:ASN:HB3	1:B:389:ILE:HD11	2.02	0.41
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.40
1:A:599:GLY:H	1:A:602:GLU:CD	2.30	0.40
1:A:671:MET:HE1	1:A:682:HIS:HD2	1.86	0.40
1:B:528:MET:CE	1:B:616:MET:HE1	2.51	0.40
1:A:193:ILE:HD12	3:A:1071:HOH:O	2.20	0.40
1:B:452:GLU:H	1:B:452:GLU:HG3	1.71	0.40
1:B:492:ARG:HD3	3:B:939:HOH:O	2.20	0.40
1:B:597:ARG:HA	1:B:682:HIS:NE2	2.35	0.40
1:B:680:LEU:O	1:B:683:TYR:HB2	2.22	0.40
1:A:361:GLU:OE1	3:A:855:HOH:O	2.22	0.40
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.79	0.40
1:A:760:LYS:HE3	1:A:766:PRO:CG	2.45	0.40
1:B:214:LEU:HD12	1:B:214:LEU:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1043:HOH:O	3:B:1054:HOH:O[3_555]	1.53	0.67
1:A:98:PHE:CZ	1:B:168:TRP:CZ3[1_455]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:CD1	1:A:677:GLU:OE1[1_455]	1.89	0.31
1:B:642:SER:O	3:B:1017:HOH:O[1_455]	1.91	0.29
1:A:98:PHE:CZ	1:B:168:TRP:CH2[1_455]	2.12	0.08

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	726/731 (99%)	678 (93%)	45 (6%)	3 (0%)	30	22
1	B	721/731 (99%)	667 (92%)	47 (6%)	7 (1%)	12	5
All	All	1447/1462 (99%)	1345 (93%)	92 (6%)	10 (1%)	18	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	B	140	ARG
1	B	341	VAL
1	A	98	PHE
1	B	274	ASP
1	A	73	GLU
1	B	58	TYR
1	B	145	GLU
1	B	520	ASN
1	B	486	VAL

5.3.2 Protein sidechains [i](#)

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	653/655 (100%)	589 (90%)	64 (10%)	7	3
1	B	647/655 (99%)	588 (91%)	59 (9%)	9	3
All	All	1300/1310 (99%)	1177 (90%)	123 (10%)	8	3

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	41	LYS
1	A	54	ARG
1	A	63	ILE
1	A	65	ASP
1	A	75	ASN
1	A	92	ASN
1	A	116	LEU
1	A	193	ILE
1	A	198	ILE
1	A	209	SER
1	A	214	LEU
1	A	219	ASN
1	A	232	GLU
1	A	236	ILE
1	A	246	LEU
1	A	250	LYS
1	A	263	ASN
1	A	270	VAL
1	A	273	THR
1	A	277	SER
1	A	279	VAL
1	A	302	ASP
1	A	303	VAL
1	A	308	GLN
1	A	314	GLN
1	A	321	ASN
1	A	333	SER
1	A	343	ARG
1	A	344	GLN
1	A	346	ILE
1	A	351	THR
1	A	367	ASP

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Mol	Chain	Res	Type
1	A	376	SER
1	A	385	CYS
1	A	392	LYS
1	A	414	TYR
1	A	440	THR
1	A	441	LYS
1	A	463	LYS
1	A	466	LYS
1	A	488	ASP
1	A	489	LYS
1	A	506	ASN
1	A	513	LYS
1	A	518	ILE
1	A	521	GLU
1	A	537	SER
1	A	542	LEU
1	A	543	LEU
1	A	546	VAL
1	A	557	THR
1	A	602	GLU
1	A	612	GLN
1	A	623	ARG
1	A	642	SER
1	A	684	ARG
1	A	693	GLU
1	A	699	GLU
1	A	704	HIS
1	A	726	VAL
1	A	736	THR
1	A	749	GLN
1	A	753	THR
1	B	36	THR
1	B	51	ASN
1	B	54	ARG
1	B	59	SER
1	B	69	LEU
1	B	72	GLN
1	B	85	ASN
1	B	116	LEU
1	B	144	THR
1	B	145	GLU
1	B	147	ARG

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Mol	Chain	Res	Type
1	B	162	HIS
1	B	176	ILE
1	B	179	ASN
1	B	186	THR
1	B	206	GLU
1	B	207	VAL
1	B	237	GLU
1	B	251	THR
1	B	263	ASN
1	B	266	VAL
1	B	270	VAL
1	B	274	ASP
1	B	303	VAL
1	B	309	GLU
1	B	319	ILE
1	B	334	SER
1	B	360	SER
1	B	361	GLU
1	B	366	LEU
1	B	385	CYS
1	B	399	LYS
1	B	431	LEU
1	B	472	CYS
1	B	484	SER
1	B	485	SER
1	B	486	VAL
1	B	502	LYS
1	B	505	GLN
1	B	506	ASN
1	B	514	LEU
1	B	517	ILE
1	B	523	LYS
1	B	543	LEU
1	B	554	LYS
1	B	557	THR
1	B	594	ILE
1	B	602	GLU
1	B	608	GLU
1	B	614	SER
1	B	616	MET
1	B	642	SER
1	B	667	THR

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Mol	Chain	Res	Type
1	B	677	GLU
1	B	701	LEU
1	B	726	VAL
1	B	746	THR
1	B	749	GLN
1	B	759	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	92	ASN
1	A	112	GLN
1	A	126	HIS
1	A	179	ASN
1	A	196	ASN
1	A	263	ASN
1	A	314	GLN
1	A	320	GLN
1	A	321	ASN
1	A	338	ASN
1	A	344	GLN
1	A	383	HIS
1	A	388	GLN
1	A	435	GLN
1	A	487	ASN
1	A	505	GLN
1	A	533	HIS
1	A	572	ASN
1	A	595	ASN
1	A	612	GLN
1	A	740	HIS
1	B	112	GLN
1	B	119	ASN
1	B	179	ASN
1	B	263	ASN
1	B	298	HIS
1	B	320	GLN
1	B	383	HIS
1	B	388	GLN
1	B	450	ASN
1	B	455	GLN

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Mol	Chain	Res	Type
1	B	505	GLN
1	B	572	ASN
1	B	606	GLN
1	B	612	GLN
1	B	731	GLN
1	B	748	HIS
1	B	749	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	852	1	14,14,15	0.55	0	17,19,21	0.73	0
2	NAG	A	853	1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
2	NAG	A	851	1	14,14,15	0.60	0	17,19,21	0.75	0
2	NAG	B	855	1	14,14,15	0.55	0	17,19,21	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	852	1	-	0/6/23/26	0/1/1/1
2	NAG	A	853	1	-	2/6/23/26	0/1/1/1
2	NAG	A	851	1	-	0/6/23/26	0/1/1/1
2	NAG	B	855	1	-	2/6/23/26	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	853	NAG	O5-C1-C2	-2.50	107.42	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	855	NAG	C4-C5-C6-O6
2	B	855	NAG	O5-C5-C6-O6
2	A	853	NAG	C4-C5-C6-O6
2	A	853	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	853	NAG	1	0
2	B	855	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	728/731 (99%)	1.11	110 (15%) 5 5	14, 40, 55, 60	0
1	B	725/731 (99%)	1.30	157 (21%) 2 2	17, 43, 64, 72	0
All	All	1453/1462 (99%)	1.20	267 (18%) 3 3	14, 41, 59, 72	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ASP	11.8
1	A	95	PHE	11.1
1	A	94	THR	8.7
1	A	766	PRO	6.8
1	B	340	LEU	6.5
1	A	98	PHE	6.2
1	B	279	VAL	6.2
1	B	341	VAL	6.1
1	A	127	SER	6.0
1	B	436	LEU	5.9
1	B	99	GLY	5.7
1	A	414	TYR	5.6
1	A	584	GLY	5.4
1	B	278	SER	5.2
1	B	385	CYS	5.0
1	A	121	VAL	4.9
1	B	339	CYS	4.9
1	A	74	ASN	4.8
1	B	137	LEU	4.8
1	A	99	GLY	4.8
1	B	134	ILE	4.6
1	B	342	ALA	4.5
1	A	301	CYS	4.5
1	B	608	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	334	SER	4.4
1	A	280	THR	4.3
1	A	97	GLU	4.3
1	B	183	TYR	4.3
1	A	333	SER	4.3
1	A	449	LEU	4.3
1	B	449	LEU	4.2
1	B	486	VAL	4.2
1	B	92	ASN	4.1
1	B	142	LEU	4.1
1	B	337	TRP	4.1
1	B	83	TYR	4.1
1	B	140	ARG	4.0
1	B	378	GLU	4.0
1	B	551	CYS	4.0
1	B	394	CYS	4.0
1	B	517	ILE	4.0
1	B	74	ASN	4.0
1	B	393	ASP	3.9
1	B	520	ASN	3.9
1	A	551	CYS	3.9
1	A	602	GLU	3.9
1	B	367	ASP	3.9
1	B	667	THR	3.9
1	B	351	THR	3.9
1	A	274	ASP	3.8
1	B	67	GLU	3.8
1	B	471	ARG	3.7
1	A	659	TRP	3.7
1	B	488	ASP	3.7
1	B	301	CYS	3.7
1	B	136	ASP	3.7
1	A	259	ALA	3.6
1	A	105	TYR	3.6
1	A	616	MET	3.6
1	B	452	GLU	3.6
1	B	143	ILE	3.5
1	B	84	GLY	3.5
1	B	447	CYS	3.5
1	A	146	GLU	3.5
1	B	220	GLY	3.5
1	B	276	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	385	CYS	3.4
1	B	138	ASN	3.4
1	A	129	THR	3.4
1	B	444	CYS	3.4
1	A	145	GLU	3.4
1	B	108	SER	3.4
1	A	278	SER	3.3
1	B	437	SER	3.3
1	B	518	ILE	3.3
1	A	535	ASP	3.3
1	A	677	GLU	3.3
1	B	69	LEU	3.3
1	A	134	ILE	3.2
1	B	88	VAL	3.2
1	B	309	GLU	3.2
1	A	615	LYS	3.2
1	B	111	GLY	3.2
1	B	335	GLY	3.2
1	A	762	CYS	3.2
1	B	762	CYS	3.2
1	A	295	ILE	3.2
1	B	176	ILE	3.2
1	A	472	CYS	3.2
1	A	123	GLN	3.1
1	B	350	THR	3.1
1	A	275	SER	3.1
1	A	140	ARG	3.1
1	B	162	HIS	3.1
1	B	445	LEU	3.0
1	B	682	HIS	3.0
1	B	387	PHE	3.0
1	B	186	THR	3.0
1	A	220	GLY	3.0
1	B	463	LYS	3.0
1	B	116	LEU	2.9
1	B	181	PRO	2.9
1	B	389	ILE	2.9
1	A	73	GLU	2.9
1	A	124	TRP	2.9
1	B	391	LYS	2.9
1	A	413	ASP	2.9
1	B	438	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	642	SER	2.9
1	B	120	TYR	2.9
1	A	126	HIS	2.9
1	B	376	SER	2.9
1	A	463	LYS	2.8
1	A	518	ILE	2.8
1	A	617	GLY	2.8
1	B	187	TRP	2.8
1	B	216	TRP	2.8
1	B	330	TYR	2.8
1	A	219	ASN	2.8
1	B	281	ASN	2.8
1	B	44	THR	2.8
1	B	519	LEU	2.8
1	B	65	ASP	2.8
1	B	274	ASP	2.8
1	A	279	VAL	2.8
1	B	104	ASP	2.7
1	B	121	VAL	2.7
1	B	629	TRP	2.7
1	A	379	GLU	2.7
1	A	116	LEU	2.7
1	A	151	ASN	2.7
1	B	151	ASN	2.7
1	B	66	HIS	2.7
1	A	183	TYR	2.6
1	A	501	ASP	2.6
1	B	135	TYR	2.6
1	B	331	ASP	2.6
1	A	394	CYS	2.6
1	B	522	THR	2.6
1	A	139	LYS	2.6
1	B	277	SER	2.6
1	A	130	ALA	2.6
1	B	133	ASP	2.6
1	B	336	ARG	2.6
1	A	367	ASP	2.6
1	A	761	GLN	2.6
1	B	413	ASP	2.6
1	B	282	ALA	2.6
1	B	219	ASN	2.6
1	B	91	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	685	ASN	2.6
1	B	346	ILE	2.5
1	A	537	SER	2.5
1	B	698	VAL	2.5
1	A	447	CYS	2.5
1	B	480	TYR	2.5
1	B	666	TYR	2.5
1	B	392	LYS	2.5
1	B	366	LEU	2.5
1	A	66	HIS	2.5
1	B	146	GLU	2.5
1	B	354	VAL	2.5
1	A	542	LEU	2.5
1	A	75	ASN	2.5
1	B	448	GLU	2.5
1	B	338	ASN	2.4
1	A	346	ILE	2.4
1	B	81	ALA	2.4
1	B	297	ASP	2.4
1	B	328	CYS	2.4
1	B	472	CYS	2.4
1	A	348	MET	2.4
1	B	180	LEU	2.4
1	B	616	MET	2.4
1	B	110	ASP	2.4
1	B	324	VAL	2.4
1	B	115	LEU	2.4
1	B	89	PHE	2.4
1	B	213	ALA	2.4
1	B	145	GLU	2.4
1	B	100	HIS	2.4
1	B	462	SER	2.4
1	B	396	PHE	2.3
1	B	177	GLU	2.3
1	B	280	THR	2.3
1	A	314	GLN	2.3
1	A	101	SER	2.3
1	B	270	VAL	2.3
1	A	393	ASP	2.3
1	A	308	GLN	2.3
1	B	516	PHE	2.3
1	A	281	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	85	ASN	2.3
1	B	76	ILE	2.3
1	B	319	ILE	2.3
1	B	766	PRO	2.3
1	A	699	GLU	2.3
1	A	383	HIS	2.3
1	A	539	LYS	2.3
1	B	178	PRO	2.3
1	B	161	GLY	2.3
1	A	230	ASP	2.3
1	A	520	ASN	2.3
1	B	450	ASN	2.3
1	B	139	LYS	2.3
1	B	292	SER	2.2
1	B	407	ILE	2.2
1	A	88	VAL	2.2
1	A	726	VAL	2.2
1	A	125	ARG	2.2
1	B	302	ASP	2.2
1	A	618	PHE	2.2
1	B	128	TYR	2.2
1	A	425	MET	2.2
1	A	504	LEU	2.2
1	A	534	PHE	2.2
1	A	102	ILE	2.2
1	A	464	GLU	2.2
1	A	442	VAL	2.2
1	B	469	GLN	2.2
1	A	350	THR	2.2
1	B	501	ASP	2.2
1	A	642	SER	2.2
1	A	490	GLY	2.2
1	B	514	LEU	2.2
1	A	506	ASN	2.1
1	B	82	GLU	2.1
1	A	154	TRP	2.1
1	B	288	THR	2.1
1	B	404	VAL	2.1
1	A	596	ARG	2.1
1	B	470	LEU	2.1
1	A	92	ASN	2.1
1	B	326	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	36	THR	2.1
1	A	619	VAL	2.1
1	A	177	GLU	2.1
1	B	375	ILE	2.1
1	B	681	ASP	2.1
1	A	538	LYS	2.1
1	B	251	THR	2.1
1	A	260	GLY	2.1
1	B	260	GLY	2.1
1	B	352	GLY	2.1
1	B	174	VAL	2.1
1	A	57	LEU	2.1
1	B	90	LEU	2.1
1	A	148	ILE	2.0
1	A	347	GLU	2.0
1	A	357	PHE	2.0
1	B	521	GLU	2.0
1	B	439	TYR	2.0
1	B	443	THR	2.0
1	A	533	HIS	2.0
1	A	546	VAL	2.0
1	A	69	LEU	2.0
1	A	649	CYS	2.0
1	B	37	ALA	2.0
1	A	302	ASP	2.0
1	A	349	SER	2.0
1	A	690	SER	2.0
1	B	141	GLN	2.0
1	A	321	ASN	2.0
1	A	338	ASN	2.0
1	B	406	GLY	2.0
1	A	354	VAL	2.0
1	B	343	ARG	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
2	NAG	B	855	14/15	0.63	0.20	68,69,69,69	0
2	NAG	B	852	14/15	0.80	0.11	42,42,44,45	0
2	NAG	A	853	14/15	0.80	0.11	42,43,43,44	0
2	NAG	A	851	14/15	0.88	0.09	48,48,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.