



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 04:38 AM GMT

PDB ID : 1PFQ
Title : crystal structure of human apo dipeptidyl peptidase IV / CD26
Authors : Oefner, C.; D'Arcy, A.; Mac Sweeney, A.; Pierau, S.; Gardiner, R.; Dale, G.E.
Deposited on : 2003-05-27
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

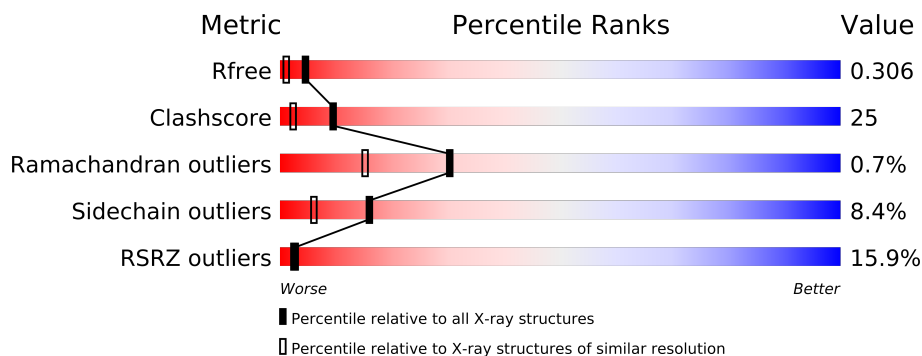
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	731	
1	B	731	

2 Entry composition i

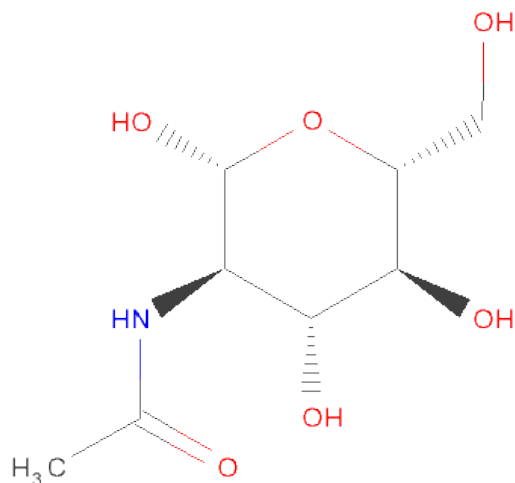
There are 3 unique types of molecules in this entry. The entry contains 12418 atoms, of which 0 are hydrogen and 0 are deuterium.

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	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	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		

- Molecule 3 is water.

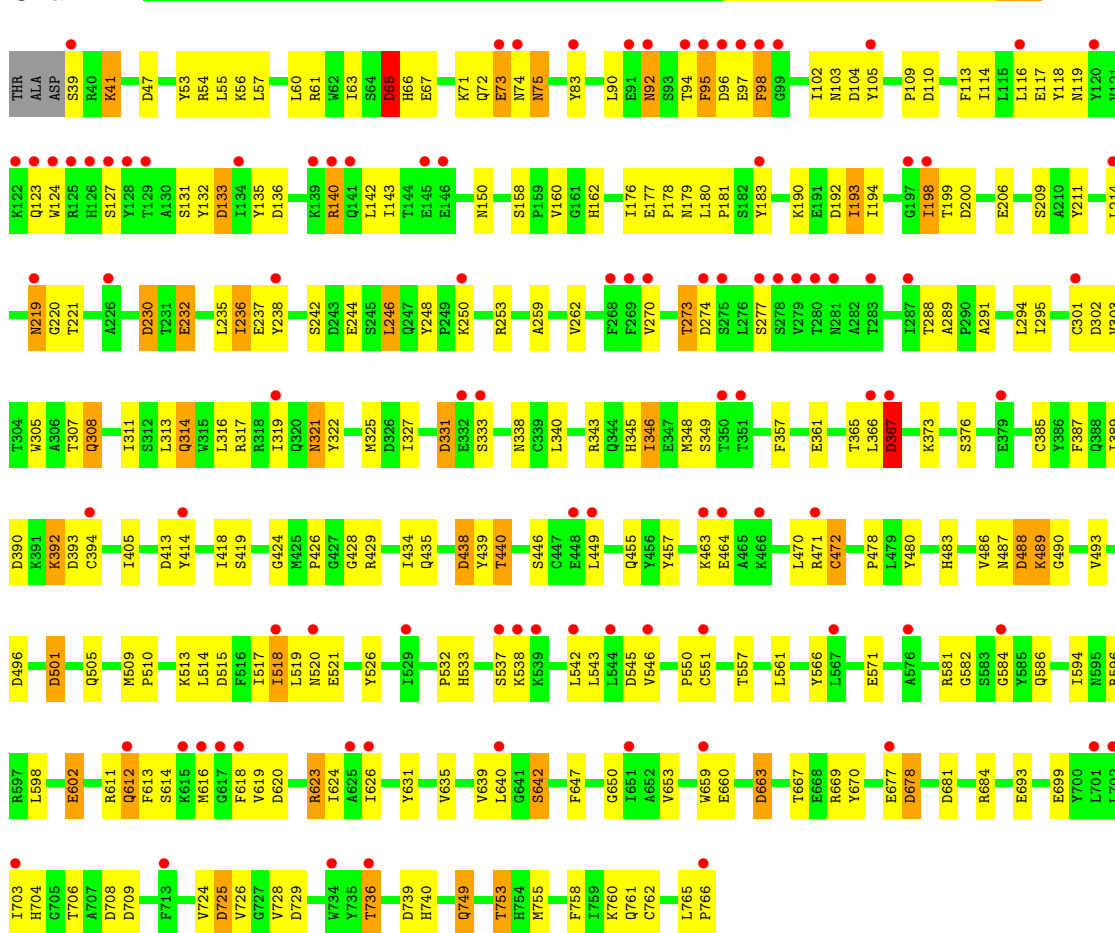
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total 268	O 268	0	0
3	B	204	Total 204	O 204	0	0

3 Residue-property plots

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

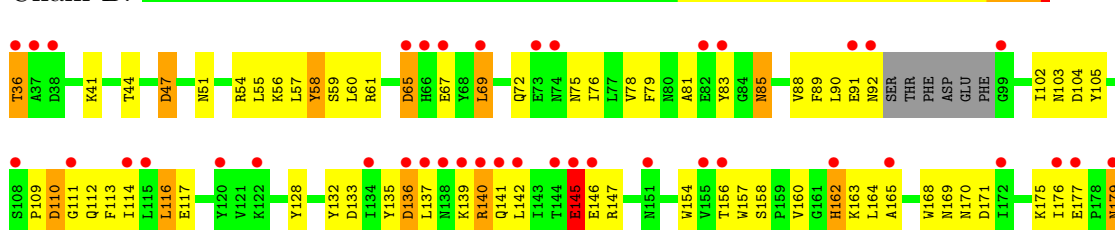
- Molecule 1: Dipeptidyl peptidase IV soluble form

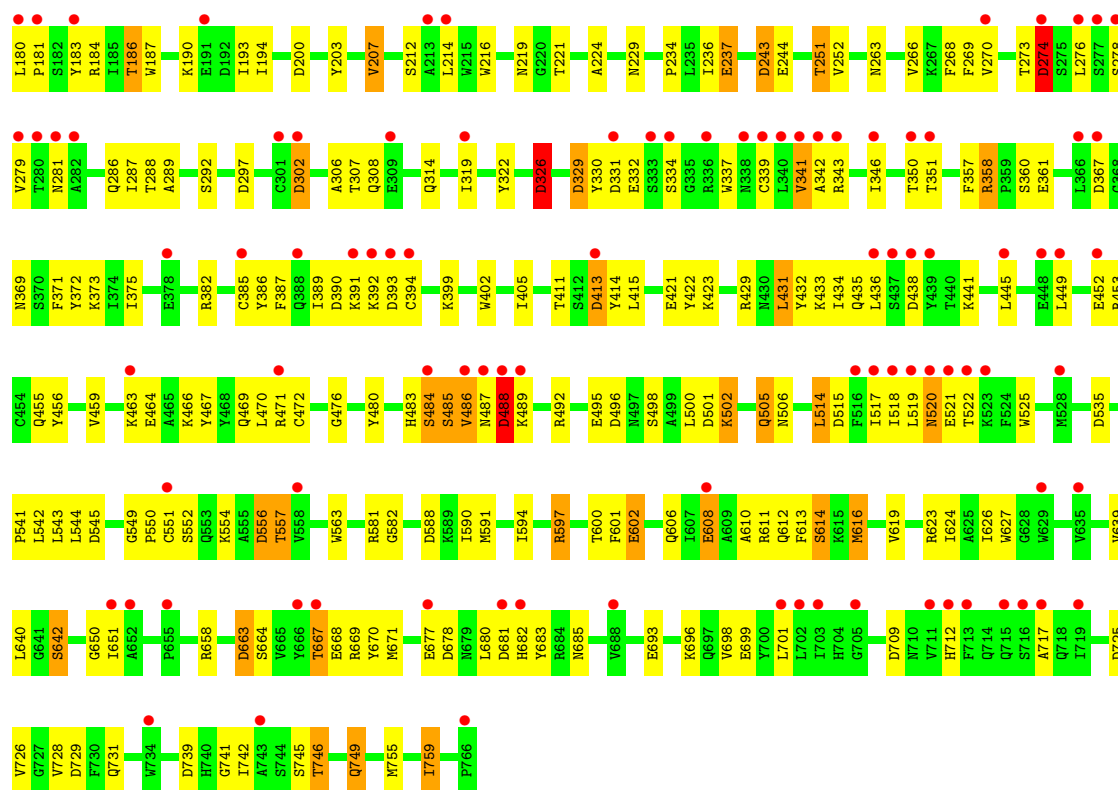
Chain A:



- Molecule 1: Dipeptidyl peptidase IV soluble form

Chain B:





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 29.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-1.90) 98.7 (29.77-1.90)	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	Depositor
R, R_{free}	0.254 , 0.298 0.265 , 0.306	Depositor DCC
R_{free} test set	6103 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 233277 reflections	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.

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/6136	0.60	27/8344 (0.3%)
1	B	0.26	0/6094	0.60	33/8287 (0.4%)
All	All	0.26	0/12230	0.60	60/16631 (0.4%)

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 (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	545	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	545	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	725	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	200	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	725	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	663	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	739	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	739	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	729	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	192	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	393	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	501	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	488	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	136	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	47	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	136	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	331	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	413	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	393	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	709	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	678	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	65	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	104	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	413	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	438	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	274	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	390	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	709	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	663	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	302	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	515	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	243	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	681	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	230	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	678	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	329	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	104	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	133	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	367	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	110	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	65	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	438	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	488	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	515	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	274	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	681	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	729	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	535	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	200	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	47	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	331	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	501	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	297	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	390	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	496	ASP	CB-CG-OD2	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	556	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	496	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	326	ASP	CB-CG-OD2	5.02	122.81	118.30
1	B	588	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	581	ARG	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5964	0	5683	271	3
1	B	5926	0	5650	314	3
2	A	28	0	26	1	0
2	B	28	0	26	1	0
3	A	268	0	0	26	0
3	B	204	0	0	16	2
All	All	12418	0	11385	573	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (573) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:74:ASN:HB3	1:A:92:ASN:ND2	1.59	1.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:74:ASN:HB3	1:A:92:ASN:CG	1.75	1.03
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: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
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:514:LEU:C	1:B:514:LEU:HD23	1.87	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:O	1:B:514:LEU:HD23	1.73	0.88
1:B:487:ASN:HB2	1:B:489:LYS:HZ2	1.39	0.87
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:VAL:HG22	1:A:219:ASN:O	1.73	0.87
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:B:83:TYR:O	1:B:492:ARG:NH1	2.09	0.85
1:A:65:ASP:OD1	3:A:1097:HOH:O	1.94	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:NE2	1:B:505:GLN:HA	1.90	0.84
1:A:678:ASP:OD1	3:A:1076:HOH:O	1.97	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:H	1:A:321:ASN:HD22	1.25	0.82
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.62	0.82
1:A:765:LEU:HB2	1:A:766:PRO:HD3	1.61	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:640:LEU:HD11	1:A:650:GLY:HA3	1.65	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:179:ASN:C	1:B:179:ASN:HD22	1.87	0.78
1:A:367:ASP:OD2	3:A:981:HOH:O	2.02	0.78
1:A:346:ILE:HD11	1:A:348:MET:CE	2.14	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: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: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
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:A:131:SER:OG	1:A:150:ASN:OD1	2.01	0.76
1:A:653:VAL:HG21	1:A:755:MET:HE1	1.67	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:A:653:VAL:CG2	1:A:755:MET:HE2	2.17	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	0.75
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:A:74:ASN:CB	1:A:92:ASN:CG	2.54	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:486:VAL:HG12	1:B:487:ASN:H	1.53	0.72
1:B:411:THR:HG22	1:B:414:TYR:H	1.51	0.72
1:A:236:ILE:C	1:A:236:ILE:HD13	2.09	0.72
1:B:179:ASN:O	1:B:179:ASN:ND2	2.21	0.72
1:B:243:ASP:CG	3:B:1058:HOH:O	2.26	0.72
1:B:60:LEU:HD11	1:B:469:GLN:OE1	1.90	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:GLN:HE22	1:A:373:LYS:HZ2	1.40	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:486:VAL:CG1	1:B:487:ASN:N	2.55	0.69
1:B:158:SER:OG	1:B:160:VAL:O	2.09	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:A:653:VAL:HG22	1:A:755:MET:HE2	1.74	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
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: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:342:ALA:HB1	1:B:391:LYS:HE3	1.74	0.67
1:B:117:GLU:HB3	1:B:132:TYR:CE1	2.31	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:405:ILE:HD13	1:A:418:ILE:HG22	1.79	0.65
1:A:346:ILE:H	1:A:392:LYS:HZ1	1.44	0.65
1:A:518:ILE:O	1:A:518:ILE:HG13	1.94	0.65
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.27	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:A:346:ILE:HD11	1:A:348:MET:HE3	1.78	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:597:ARG:HD3	1:B:600:THR:OG1	1.97	0.64
1:B:544:LEU:HD21	1:B:606:GLN:HE21	1.52	0.64
1:B:431:LEU:HD22	1:B:445:LEU:HD12	1.79	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:A:63:ILE:HD11	1:A:67:GLU:HB2	1.80	0.64
1:A:198:ILE:HD12	1:A:211:TYR:CZ	2.33	0.63
1:A:346:ILE:HD11	1:A:348:MET:HE2	1.80	0.63
1:A:124:TRP:H	1:A:127:SER:HB3	1.63	0.63
1:B:544:LEU:CD2	1:B:606:GLN:HE22	2.02	0.63
1:A:550:PRO:O	1:A:551:CYS:CB	2.47	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:B:83:TYR:O	1:B:492:ARG:NH2	2.32	0.63
1:A:557:THR:HG22	1:A:557:THR:O	1.97	0.63
1:B:557:THR:CG2	1:B:557:THR:O	2.47	0.63
1:B:455:GLN:HB2	1:B:557:THR:HG21	1.79	0.63
1:A:253:ARG:HD2	3:A:960:HOH:O	1.98	0.63
1:A:557:THR:O	1:A:557:THR:CG2	2.46	0.62
1:B:116:LEU:HD12	1:B:133:ASP:O	1.98	0.62
1:A:301:CYS:SG	1:A:316:LEU:HB2	2.39	0.62
1:B:557:THR:O	1:B:557:THR:HG23	1.99	0.62
1:A:653:VAL:HG21	1:A:755:MET:CE	2.28	0.62
1:B:67:GLU:CD	1:B:78:VAL:CG1	2.68	0.62
1:A:726:VAL:HG13	1:A:726:VAL:O	2.00	0.62
1:B:88:VAL:HG11	1:B:91:GLU:HB2	1.82	0.62
1:B:519:LEU:CD1	1:B:608:GLU:OE1	2.46	0.62
1:B:498:SER:O	1:B:502:LYS:HG2	1.99	0.62
1:B:484:SER:O	1:B:488:ASP:CA	2.41	0.62
1:B:128:TYR:HE2	1:B:132:TYR:OH	1.82	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:653:VAL:CG2	1:A:755:MET:HE1	2.30	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:HD23	1:B:276:LEU:N	2.17	0.60
1:B:128:TYR:HE2	1:B:132:TYR:HH	1.50	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:653:VAL:HG22	1:A:755:MET:CE	2.29	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
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:B:179:ASN:ND2	1:B:179:ASN:C	2.55	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:74:ASN:C	1:A:92:ASN:ND2	2.55	0.59
1:A:176:ILE:HD12	1:A:183:TYR:CE2	2.28	0.59
1:B:463:LYS:CG	1:B:464:GLU:OE2	2.50	0.59
1:A:41:LYS:HE3	1:A:53:TYR:OH	2.02	0.59
1:A:611:ARG:O	1:A:614:SER:HB2	2.02	0.59
1:A:765:LEU:CB	1:A:766:PRO:HD3	2.29	0.59
1:A:550:PRO:O	1:A:551:CYS:HB2	2.03	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:71:LYS:NZ	1:A:105:TYR:OH	2.35	0.58
1:B:44:THR:HG22	1:B:47:ASP:CG	2.23	0.58
1:A:56:LYS:HD2	3:A:999:HOH:O	2.01	0.58
1:B:171:ASP:OD1	1:B:186:THR:HG23	2.02	0.58
1:B:411:THR:HG22	1:B:414:TYR:N	2.19	0.58
1:B:273:THR:O	1:B:276:LEU:HD22	2.03	0.58
1:A:703:ILE:HD12	1:A:755:MET:CE	2.34	0.58
1:B:402:TRP:NE1	1:B:421:GLU:HG3	2.17	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:63:ILE:HD11	1:A:67:GLU:CB	2.34	0.58
1:B:514:LEU:CD2	1:B:514:LEU:O	2.50	0.58
1:A:758:PHE:O	1:A:761:GLN:HG3	2.03	0.58
1:B:67:GLU:CD	1:B:78:VAL:HG11	2.23	0.58
1:B:498:SER:O	1:B:502:LYS:CG	2.52	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:487:ASN:CG	1:B:489:LYS:HZ1	2.07	0.57
1:A:760:LYS:HB3	1:A:766:PRO:CG	2.34	0.57
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.04	0.57
1:B:431:LEU:CD2	1:B:432:TYR:N	2.68	0.57
1:B:402:TRP:CE2	1:B:421:GLU:HG3	2.40	0.57
1:B:518:ILE:HG13	1:B:518:ILE:O	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:A:114:ILE:HG23	1:A:135:TYR:HB3	1.86	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
1:B:640:LEU:HD22	1:B:698:VAL:HG11	1.87	0.56
1:B:745:SER:O	1:B:749:GLN:NE2	2.39	0.56
1:A:387:PHE:CE2	1:A:394:CYS:CB	2.87	0.56
1:B:287:ILE:HG21	1:B:339:CYS:SG	2.45	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:A:235:LEU:N	1:A:235:LEU:HD22	2.21	0.56
1:A:724:VAL:CG1	1:B:746:THR:CG2	2.78	0.56
1:A:703:ILE:HD12	1:A:755:MET:HE3	1.88	0.55
1:B:273:THR:C	1:B:276:LEU:HD22	2.26	0.55
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:471:ARG:CG	1:B:480:TYR:CE2	2.90	0.55
1:B:371:PHE:CE2	1:B:387:PHE:CD1	2.95	0.55
1:B:514:LEU:CD2	1:B:514:LEU:C	2.62	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:B:487:ASN:CB	1:B:489:LYS:NZ	2.69	0.54
1:A:749:GLN:O	1:A:753:THR:CG2	2.53	0.54
1:A:594:ILE:HD12	1:A:598:LEU:CD2	2.37	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:A:325:MET:HE1	1:A:327:ILE:HD11	1.90	0.54
1:B:544:LEU:CG	1:B:606:GLN:HE22	2.20	0.54
1:B:346:ILE:HG12	3:B:899:HOH:O	2.06	0.54
1:B:519:LEU:CD2	1:B:612:GLN:HE21	2.12	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:544:LEU:HD23	1:B:606:GLN:HE21	1.70	0.54
1:B:563:TRP:CH2	1:B:755:MET:HE2	2.43	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:391:LYS:O	1:B:392:LYS:HB2	2.08	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:291:ALA:O	1:A:295:ILE:CG1	2.52	0.53
1:B:180:LEU:CB	1:B:181:PRO:CD	2.80	0.53
1:B:61:ARG:NH2	1:B:105:TYR:O	2.41	0.53
1:A:206:GLU:OE2	1:A:663:ASP:OD1	2.25	0.53
1:B:276:LEU:HD23	1:B:276:LEU:H	1.72	0.53
1:B:56:LYS:HD3	1:B:495:GLU:OE1	2.08	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:341:VAL:HG13	1:B:342:ALA:N	2.24	0.53
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.90	0.53
1:A:75:ASN:HB2	1:A:90:LEU:O	2.09	0.52
1:A:659:TRP:CE3	1:A:667:THR:HG23	2.44	0.52
1:A:232:GLU:O	1:A:232:GLU:OE1	2.27	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:236:ILE:CD1	1:A:236:ILE:C	2.78	0.52
1:A:288:THR:CG2	1:A:294:LEU:HD11	2.40	0.52
1:A:331:ASP:HB2	1:A:338:ASN:HD21	1.75	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:B:594:ILE:CD1	1:B:602:GLU:HG3	2.41	0.51
1:B:357:PHE:O	1:B:358:ARG:HB3	2.11	0.51
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.46	0.51
1:A:325:MET:HE2	1:A:345:HIS:ND1	2.26	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: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: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:B:276:LEU:O	1:B:276:LEU:HG	2.11	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:626:ILE:O	1:A:650:GLY:HA2	2.11	0.49
1:B:626:ILE:O	1:B:650:GLY:HA2	2.12	0.49
1:A:109:PRO:HG2	1:A:158:SER:O	2.11	0.49
1:A:703:ILE:CD1	1:A:755:MET:HE3	2.43	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: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:B:415:LEU:C	1:B:415:LEU:HD23	2.34	0.48
1:B:550:PRO:O	1:B:551:CYS:CB	2.59	0.48
1:B:65:ASP:OD2	1:B:464:GLU:HB2	2.13	0.48
1:B:667:THR:O	1:B:671:MET:HB2	2.12	0.48
1:A:262:VAL:HA	3:A:1005:HOH:O	2.12	0.48
1:A:180:LEU:HB3	1:A:181:PRO:HD2	1.94	0.48
1:B:90:LEU:HD22	1:B:140:ARG:HH21	1.77	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:708:ASP:OD2	1:A:740:HIS:HD2	1.96	0.48
1:A:94:THR:O	1:A:94:THR:HG22	2.14	0.48
1:B:110:ASP:CG	1:B:112:GLN:HG3	2.34	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:91:GLU:O	1:B:92:ASN:C	2.52	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: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:A:618:PHE:CD1	1:A:619:VAL:HG23	2.49	0.47
1:B:698:VAL:CG1	1:B:699:GLU:N	2.77	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:519:LEU:HD13	1:B:608:GLU:CD	2.34	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:A:96:ASP:O	1:A:142:LEU:HD11	2.15	0.47
1:A:346:ILE:HD12	1:A:346:ILE:C	2.35	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: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:B:350:THR:HG21	3:B:866:HOH:O	2.15	0.47
1:B:341:VAL:HG13	1:B:343:ARG:H	1.80	0.47
1:B:171:ASP:CB	1:B:186:THR:HG22	2.43	0.47
1:B:542:LEU:HD12	1:B:619:VAL:HG11	1.97	0.47
1:B:145:GLU:HG2	1:B:145:GLU:H	1.49	0.47
1:A:639:VAL:O	1:A:642:SER:HB2	2.15	0.47
1:B:693:GLU:O	1:B:696:LYS:HD3	2.15	0.47
1:A:60:LEU:HD12	1:A:60:LEU:O	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:B:556:ASP:C	1:B:556:ASP:OD1	2.54	0.47
1:B:514:LEU:HD21	1:B:525:TRP:CZ3	2.51	0.46
1:A:135:TYR:CE1	1:A:140:ARG:C	2.89	0.46
1:A:179:ASN:C	1:A:180:LEU:HD12	2.35	0.46
1:A:505:GLN:HE21	1:A:505:GLN:HA	1.79	0.46
1:B:219:ASN:HB3	1:B:221:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:357:PHE:CE2	1:B:551:CYS:HB2	2.46	0.46
1:A:405:ILE:CD1	1:A:418:ILE:HG22	2.44	0.46
1:B:518:ILE:HA	1:B:522:THR:O	2.15	0.46
1:B:36:THR:HG22	3:B:1026:HOH:O	2.15	0.46
1:A:449:LEU:HA	1:A:449:LEU:HD23	1.82	0.46
1:A:346:ILE:H	1:A:392:LYS:NZ	2.12	0.46
1:A:288:THR:HG22	1:A:289:ALA:O	2.15	0.46
1:A:340:LEU:H	1:A:340:LEU:HD12	1.81	0.46
1:B:759:ILE:HA	1:B:759:ILE:HD13	1.80	0.46
1:B:431:LEU:C	1:B:431:LEU:CD2	2.83	0.46
1:A:602:GLU:CD	1:A:631:TYR:HH	2.18	0.46
1:A:325:MET:CE	1:A:345:HIS:ND1	2.78	0.46
1:B:563:TRP:CH2	1:B:755:MET:CE	2.99	0.46
1:B:292:SER:OG	1:B:322:TYR:HE1	1.98	0.46
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.49	0.46
1:B:463:LYS:HG3	1:B:464:GLU:OE2	2.15	0.46
1:B:113:PHE:CE2	1:B:162:HIS:CD2	2.96	0.46
1:B:582:GLY:HA2	1:B:590:ILE:O	2.16	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:411:THR:HG23	1:B:413:ASP:N	2.29	0.45
1:B:90:LEU:CD2	1:B:140:ARG:HH21	2.30	0.45
1:B:302:ASP:N	1:B:302:ASP:OD1	2.49	0.45
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.49	0.45
1:B:44:THR:HG22	1:B:47:ASP:OD1	2.16	0.45
1:B:664:SER:HB2	1:B:668:GLU:OE2	2.16	0.45
1:A:532:PRO:O	1:A:533:HIS:HB2	2.17	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: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: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: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:487:ASN:OD1	1:B:489:LYS:NZ	2.42	0.44
1:B:306:ALA:O	1:B:307:THR:HG22	2.17	0.44
1:B:110:ASP:C	1:B:110:ASP:OD1	2.56	0.44
1:B:435:GLN:HG3	1:B:441:LYS:CB	2.47	0.44
1:A:194:ILE:HD12	2:A:853:NAG:H82	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:350:THR:HG23	1:B:351:THR:N	2.31	0.44
1:A:301:CYS:SG	1:A:316:LEU:CB	3.05	0.44
1:B:492:ARG:CG	3:B:939:HOH:O	2.46	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: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:CG	1:A:623:ARG:NH1	2.71	0.44
1:B:550:PRO:O	1:B:551:CYS:HB2	2.17	0.44
1:B:350:THR:CG2	1:B:351:THR:HG23	2.27	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:111:GLY:C	1:B:137:LEU:HD12	2.37	0.44
1:A:463:LYS:CB	1:A:463:LYS:NZ	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:B:214:LEU:HD12	1:B:214:LEU:C	2.38	0.43
1:A:143:ILE:CD1	1:A:178:PRO:CB	2.96	0.43
1:A:60:LEU:HD12	1:A:60:LEU:C	2.38	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:624:ILE:HG22	1:A:647:PHE:CD1	2.53	0.43
1:A:623:ARG:CG	1:A:623:ARG:HH11	2.09	0.43
1:A:703:ILE:HD12	1:A:755:MET:HE2	2.01	0.43
1:A:532:PRO:O	1:A:533:HIS:CB	2.67	0.43
1:B:466:LYS:HG2	1:B:467:TYR:CE2	2.53	0.43
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.54	0.43
1:A:725:ASP:HA	1:B:746:THR:CG2	2.44	0.43
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.53	0.43
1:B:69:LEU:HD21	1:B:76:ILE:HG21	2.01	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.53	0.43
1:B:391:LYS:O	1:B:392:LYS:CB	2.67	0.43
1:B:369:ASN:O	1:B:389:ILE:HG12	2.19	0.43
1:A:303:VAL:HB	1:A:313:LEU:HD23	2.01	0.43
1:A:307:THR:HB	3:A:982:HOH:O	2.18	0.43
1:B:341:VAL:HG13	1:B:343:ARG:N	2.34	0.43
1:B:190:LYS:HD2	1:B:193:ILE:CD1	2.45	0.43
1:B:411:THR:C	1:B:413:ASP:H	2.23	0.42
1:A:706:THR:OG1	1:A:736:THR:HA	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:GLY:O	1:A:426:PRO:HD3	2.18	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:HD3	1:A:489:LYS:HA	1.84	0.42
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.55	0.42
1:B:180:LEU:CB	1:B:181:PRO:HD3	2.49	0.42
1:A:244:GLU:OE2	1:B:658:ARG:NH2	2.49	0.42
1:B:375:ILE:HD11	1:B:387:PHE:HZ	1.85	0.42
1:B:485:SER:O	1:B:486:VAL:C	2.58	0.42
1:B:60:LEU:CG	1:B:469:GLN:OE1	2.68	0.42
1:B:114:ILE:CG2	1:B:140:ARG:HH12	2.29	0.42
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.49	0.42
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.49	0.42
1:A:514:LEU:HD12	1:A:526:TYR:O	2.20	0.42
1:B:563:TRP:CZ3	1:B:755:MET:CE	3.03	0.42
1:A:366:LEU:HD23	1:A:366:LEU:C	2.40	0.42
1:B:88:VAL:CG1	1:B:91:GLU:HB2	2.49	0.42
1:B:341:VAL:CG2	1:B:342:ALA:N	2.77	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.20	0.42
1:B:582:GLY:HA3	1:B:591:MET:HA	2.02	0.41
1:A:581:ARG:HA	1:A:582:GLY:HA2	1.75	0.41
1:A:509:MET:HA	1:A:510:PRO:HD3	1.90	0.41
1:B:431:LEU:CD2	1:B:445:LEU:HD12	2.48	0.41
1:B:382:ARG:HH21	1:B:591:MET:HE2	1.85	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:428:GLY:C	1:A:429:ARG:HG2	2.40	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:B:369:ASN:HB2	1:B:389:ILE:HG12	2.02	0.41
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.55	0.41
1:B:375:ILE:HD11	1:B:387:PHE:CZ	2.56	0.41
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.36	0.41
1:B:57:LEU:O	1:B:58:TYR:C	2.58	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:483:HIS:HD1	1:A:490:GLY:HA2	1.86	0.41
1:B:498:SER:O	1:B:502:LYS:HG3	2.21	0.41
1:B:693:GLU:HA	1:B:726:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:330:TYR:HE2	1:B:332:GLU:HG2	1.86	0.41
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.85	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:B:158:SER:HB3	1:B:163:LYS:HB3	2.02	0.41
1:A:41:LYS:CE	1:A:53:TYR:OH	2.67	0.41
1:B:422:TYR:O	1:B:423:LYS:HB2	2.20	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: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:B:741:GLY:O	1:B:742:ILE:C	2.60	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: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:680:LEU:O	1:B:683:TYR:HB2	2.22	0.40
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.79	0.40
1:A:361:GLU:OE1	3:A:855:HOH:O	2.22	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	Distance(Å)	Clash(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
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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/731 (99%)	678 (93%)	45 (6%)	3 (0%)	43	29
1	B	721/731 (99%)	667 (92%)	47 (6%)	7 (1%)	22	8
All	All	1447/1462 (99%)	1345 (93%)	92 (6%)	10 (1%)	30	15

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 ⓘ

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%)	596 (91%)	57 (9%)	15	6
1	B	647/655 (99%)	595 (92%)	52 (8%)	17	7
All	All	1300/1310 (99%)	1191 (92%)	109 (8%)	16	6

All (109) 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	61	ARG
1	A	65	ASP
1	A	75	ASN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	95	PHE
1	A	116	LEU
1	A	190	LYS
1	A	193	ILE
1	A	198	ILE
1	A	209	SER
1	A	214	LEU
1	A	219	ASN
1	A	230	ASP
1	A	232	GLU
1	A	236	ILE
1	A	246	LEU
1	A	250	LYS
1	A	270	VAL
1	A	273	THR
1	A	277	SER
1	A	302	ASP
1	A	308	GLN
1	A	314	GLN
1	A	321	ASN
1	A	333	SER
1	A	346	ILE
1	A	349	SER
1	A	367	ASP
1	A	376	SER
1	A	385	CYS
1	A	392	LYS
1	A	414	TYR
1	A	440	THR
1	A	472	CYS
1	A	488	ASP
1	A	489	LYS
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	566	TYR
1	A	602	GLU
1	A	612	GLN
1	A	623	ARG

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Mol	Chain	Res	Type
1	A	642	SER
1	A	684	ARG
1	A	693	GLU
1	A	699	GLU
1	A	704	HIS
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	145	GLU
1	B	162	HIS
1	B	179	ASN
1	B	186	THR
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	319	ILE
1	B	326	ASP
1	B	334	SER
1	B	358	ARG
1	B	360	SER
1	B	361	GLU
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	488	ASP
1	B	502	LYS
1	B	505	GLN

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Mol	Chain	Res	Type
1	B	506	ASN
1	B	514	LEU
1	B	517	ILE
1	B	543	LEU
1	B	554	LYS
1	B	557	THR
1	B	597	ARG
1	B	602	GLU
1	B	608	GLU
1	B	614	SER
1	B	616	MET
1	B	642	SER
1	B	667	THR
1	B	677	GLU
1	B	701	LEU
1	B	746	THR
1	B	749	GLN
1	B	759	ILE

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

Mol	Chain	Res	Type
1	A	66	HIS
1	A	92	ASN
1	A	112	GLN
1	A	179	ASN
1	A	263	ASN
1	A	314	GLN
1	A	321	ASN
1	A	338	ASN
1	A	383	HIS
1	A	388	GLN
1	A	435	GLN
1	A	487	ASN
1	A	505	GLN
1	A	572	ASN
1	A	595	ASN
1	A	612	GLN
1	A	740	HIS
1	B	51	ASN
1	B	112	GLN
1	B	119	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	263	ASN
1	B	298	HIS
1	B	320	GLN
1	B	338	ASN
1	B	383	HIS
1	B	435	GLN
1	B	455	GLN
1	B	505	GLN
1	B	606	GLN
1	B	612	GLN
1	B	712	HIS
1	B	749	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	851	1	12,14,15	0.75	1 (8%)	15,19,21	1.26	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	853	1	12,14,15	0.67	0	15,19,21	0.80	0
2	NAG	B	852	1	12,14,15	0.71	0	15,19,21	1.15	1 (6%)
2	NAG	B	855	1	12,14,15	0.71	1 (8%)	15,19,21	0.90	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	851	1	-	0/6/23/26	0/1/1/1
2	NAG	A	853	1	-	0/6/23/26	0/1/1/1
2	NAG	B	852	1	-	0/6/23/26	0/1/1/1
2	NAG	B	855	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	851	NAG	O5-C5	-2.22	1.41	1.45
2	B	855	NAG	O5-C5	-2.11	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	851	NAG	O5-C5-C6	3.49	110.64	106.98
2	B	852	NAG	O5-C5-C6	3.43	110.58	106.98
2	B	855	NAG	O5-C5-C6	2.07	109.15	106.98
2	A	851	NAG	C3-C2-N2	-2.04	108.65	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	1.00	97 (13%) 4 3	14, 40, 55, 60	0
1	B	725/731 (99%)	1.22	134 (18%) 2 2	17, 43, 64, 72	0
All	All	1453/1462 (99%)	1.11	231 (15%) 3 2	14, 41, 59, 72	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	10.8
1	A	96	ASP	10.4
1	A	95	PHE	10.2
1	A	766	PRO	9.1
1	B	278	SER	8.5
1	B	99	GLY	8.4
1	B	279	VAL	8.2
1	A	94	THR	6.5
1	B	436	LEU	6.4
1	B	137	LEU	6.4
1	A	280	THR	6.2
1	A	98	PHE	6.0
1	B	342	ALA	5.7
1	B	336	ARG	5.6
1	B	140	ARG	5.4
1	B	517	ILE	5.4
1	B	83	TYR	5.4
1	B	391	LYS	5.1
1	B	334	SER	5.1
1	A	279	VAL	5.0
1	B	378	GLU	5.0
1	A	125	ARG	5.0
1	B	138	ASN	4.9
1	B	766	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	414	TYR	4.9
1	B	521	GLU	4.8
1	B	341	VAL	4.8
1	A	74	ASN	4.8
1	B	392	LYS	4.7
1	B	92	ASN	4.7
1	B	183	TYR	4.6
1	A	140	ARG	4.5
1	B	37	ALA	4.5
1	A	278	SER	4.5
1	B	519	LEU	4.4
1	B	393	ASP	4.4
1	B	734	TRP	4.4
1	B	520	ASN	4.3
1	A	73	GLU	4.3
1	A	584	GLY	4.3
1	B	176	ILE	4.3
1	B	36	THR	4.2
1	B	713	PHE	4.2
1	B	66	HIS	4.1
1	A	120	TYR	4.1
1	A	127	SER	4.0
1	B	74	ASN	4.0
1	B	280	THR	4.0
1	A	734	TRP	4.0
1	A	333	SER	3.9
1	B	522	THR	3.8
1	A	449	LEU	3.8
1	A	626	ILE	3.8
1	A	281	ASN	3.8
1	B	91	GLU	3.8
1	B	114	ILE	3.7
1	B	367	ASP	3.7
1	A	99	GLY	3.7
1	A	105	TYR	3.7
1	B	180	LEU	3.6
1	B	463	LYS	3.6
1	A	97	GLU	3.6
1	B	136	ASP	3.6
1	A	274	ASP	3.6
1	B	274	ASP	3.6
1	A	518	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	488	ASP	3.5
1	B	449	LEU	3.5
1	B	144	THR	3.5
1	B	717	ALA	3.4
1	B	339	CYS	3.4
1	B	145	GLU	3.3
1	B	452	GLU	3.3
1	A	703	ILE	3.2
1	A	301	CYS	3.2
1	B	120	TYR	3.2
1	A	367	ASP	3.2
1	A	126	HIS	3.2
1	B	162	HIS	3.2
1	B	471	ARG	3.1
1	B	276	LEU	3.1
1	A	145	GLU	3.1
1	A	122	LYS	3.1
1	A	615	LYS	3.1
1	B	703	ILE	3.1
1	B	366	LEU	3.1
1	A	124	TRP	3.1
1	A	702	LEU	3.1
1	B	82	GLU	3.1
1	B	134	ILE	3.1
1	B	523	LYS	3.0
1	B	394	CYS	3.0
1	A	520	ASN	3.0
1	A	146	GLU	3.0
1	B	333	SER	3.0
1	A	612	GLN	3.0
1	A	618	PHE	3.0
1	B	73	GLU	3.0
1	A	551	CYS	2.9
1	A	464	GLU	2.9
1	A	539	LYS	2.9
1	A	275	SER	2.9
1	B	487	ASN	2.9
1	B	608	GLU	2.9
1	B	281	ASN	2.9
1	A	92	ASN	2.8
1	A	379	GLU	2.8
1	B	652	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	38	ASP	2.8
1	B	67	GLU	2.8
1	A	198	ILE	2.8
1	B	142	LEU	2.8
1	B	667	THR	2.8
1	A	39	SER	2.8
1	B	350	THR	2.7
1	A	91	GLU	2.7
1	B	309	GLU	2.7
1	A	538	LYS	2.7
1	A	616	MET	2.7
1	A	123	GLN	2.7
1	B	69	LEU	2.7
1	B	115	LEU	2.7
1	A	129	THR	2.7
1	A	677	GLU	2.7
1	B	711	VAL	2.7
1	A	128	TYR	2.6
1	B	165	ALA	2.6
1	B	701	LEU	2.6
1	A	270	VAL	2.6
1	A	134	ILE	2.6
1	B	122	LYS	2.6
1	B	155	VAL	2.6
1	A	576	ALA	2.5
1	B	351	THR	2.5
1	A	183	TYR	2.5
1	B	179	ASN	2.5
1	B	177	GLU	2.5
1	A	537	SER	2.5
1	A	659	TRP	2.5
1	A	701	LEU	2.5
1	B	139	LYS	2.5
1	A	640	LEU	2.5
1	B	445	LEU	2.5
1	B	712	HIS	2.5
1	A	471	ARG	2.4
1	B	191	GLU	2.4
1	B	319	ILE	2.4
1	A	226	ALA	2.4
1	A	448	GLU	2.4
1	B	213	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	546	VAL	2.4
1	B	385	CYS	2.4
1	B	551	CYS	2.4
1	A	351	THR	2.4
1	B	489	LYS	2.4
1	B	346	ILE	2.4
1	A	268	PHE	2.4
1	B	715	GLN	2.4
1	A	625	ALA	2.3
1	A	466	LYS	2.3
1	A	713	PHE	2.3
1	B	629	TRP	2.3
1	B	682	HIS	2.3
1	A	463	LYS	2.3
1	A	214	LEU	2.3
1	B	437	SER	2.3
1	A	366	LEU	2.3
1	B	156	THR	2.3
1	B	172	ILE	2.3
1	B	108	SER	2.3
1	B	277	SER	2.3
1	B	719	ILE	2.3
1	B	151	ASN	2.2
1	B	331	ASP	2.2
1	B	681	ASP	2.2
1	A	277	SER	2.2
1	B	635	VAL	2.2
1	B	743	ALA	2.2
1	B	518	ILE	2.2
1	B	301	CYS	2.2
1	B	181	PRO	2.2
1	A	651	ILE	2.2
1	B	302	ASP	2.2
1	B	413	ASP	2.2
1	B	438	ASP	2.2
1	A	139	LYS	2.2
1	B	270	VAL	2.2
1	B	688	VAL	2.2
1	A	332	GLU	2.2
1	A	736	THR	2.2
1	A	617	GLY	2.2
1	A	529	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	282	ALA	2.2
1	B	677	GLU	2.2
1	B	716	SER	2.2
1	A	283	THR	2.2
1	A	544	LEU	2.2
1	B	439	TYR	2.1
1	B	448	GLU	2.1
1	B	702	LEU	2.1
1	A	287	ILE	2.1
1	B	146	GLU	2.1
1	A	269	PHE	2.1
1	A	116	LEU	2.1
1	B	214	LEU	2.1
1	B	338	ASN	2.1
1	B	141	GLN	2.1
1	B	388	GLN	2.1
1	A	250	LYS	2.1
1	A	350	THR	2.1
1	B	666	TYR	2.1
1	A	141	GLN	2.1
1	A	567	LEU	2.1
1	A	197	GLY	2.1
1	B	528	MET	2.1
1	B	65	ASP	2.1
1	B	484	SER	2.1
1	B	655	PRO	2.1
1	B	343	ARG	2.1
1	A	394	CYS	2.1
1	A	542	LEU	2.0
1	A	83	TYR	2.0
1	A	238	TYR	2.0
1	B	516	PHE	2.0
1	A	219	ASN	2.0
1	A	319	ILE	2.0
1	B	486	VAL	2.0
1	B	558	VAL	2.0
1	B	651	ILE	2.0
1	B	111	GLY	2.0
1	B	705	GLY	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	855	14/15	0.25	0.82	68,69,69,69	0
2	NAG	B	852	14/15	0.16	-0.13	42,42,44,45	0
2	NAG	A	853	14/15	0.15	-0.41	42,43,43,44	0
2	NAG	A	851	14/15	0.10	-1.00	48,48,49,49	0

6.5 Other polymers

There are no such residues in this entry.