Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:29 AM BST

PDB ID	:	3OC0
Title	:	Structure of human DPP-IV with HTS hit (2S,3S,11bS)-3-butyl-9,10-dimethoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-2-ylamine
Authors	:	Hennig, M.; Stihle, M.; Thoma, R.
Deposited on	:	2010-08-09
Resolution	:	2.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

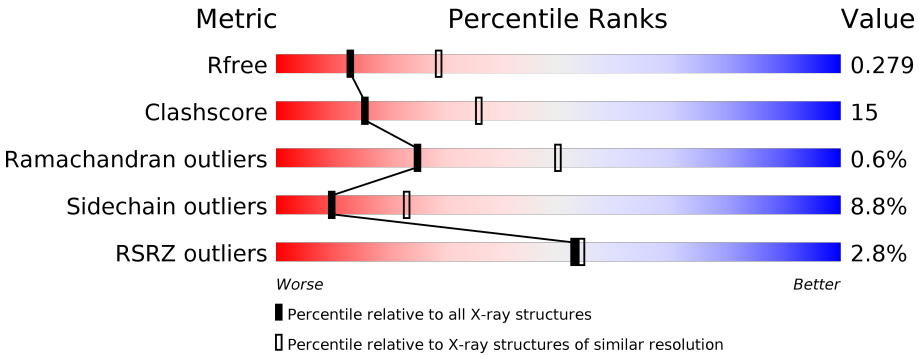
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 <=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	728	3% 69% 26% ·
1	B	728	3% 67% 27% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B2Q	A	900	X	-	-	-
3	B2Q	B	900	X	-	-	-

2 Entry composition

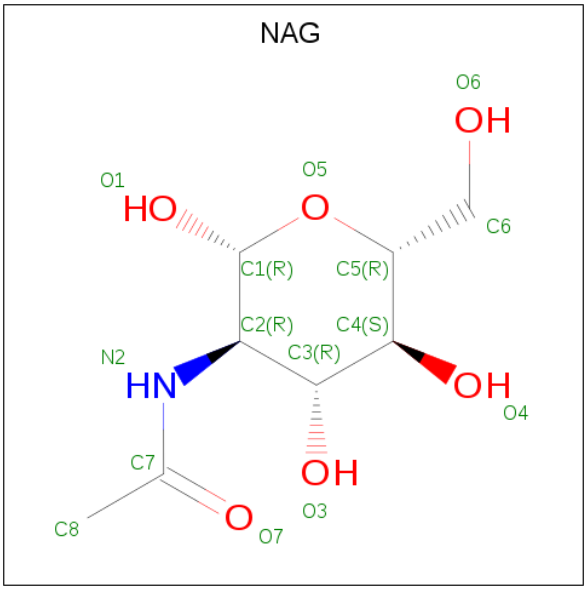
There are 4 unique types of molecules in this entry. The entry contains 12163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

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



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

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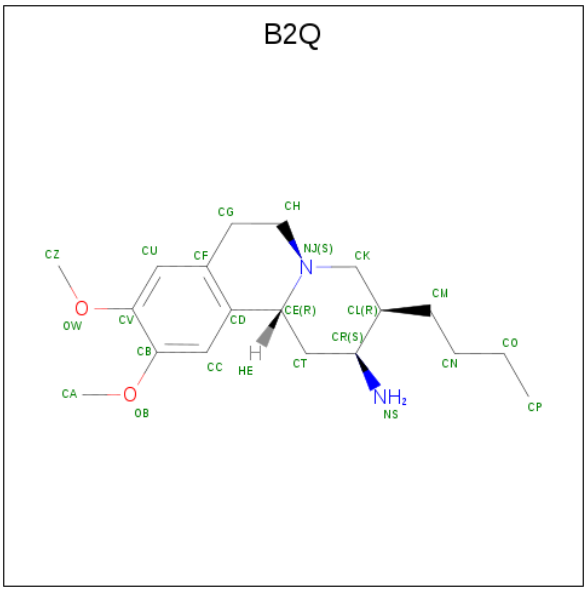
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is (2S,3R,11bR)-3-butyl-9,10-dimethoxy-1,3,4,6,7,11b-hexahydro-2H-pyrido[2,1-a]isoquinolin-2-amine (three-letter code: B2Q) (formula: $C_{19}H_{30}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 23 19 2 2	0	0
3	B	1	Total C N O 23 19 2 2	0	0

- Molecule 4 is water.

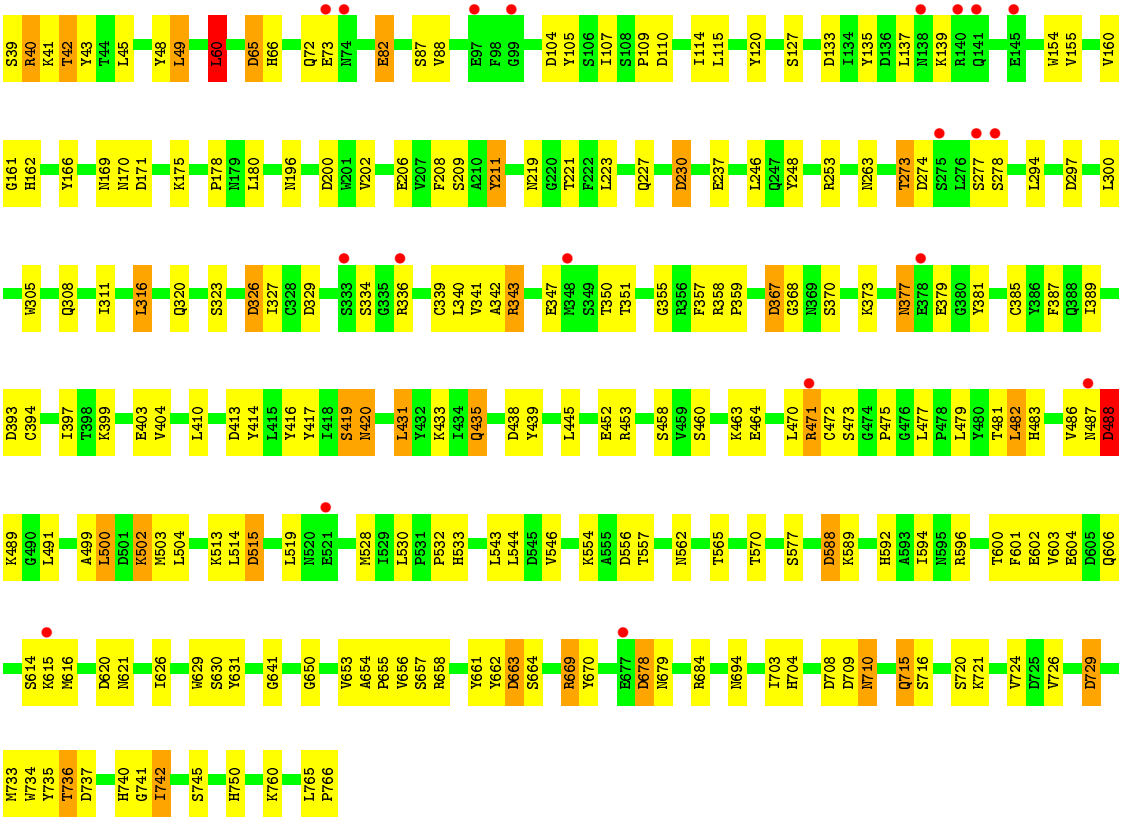
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0
4	B	38	Total O 38 38	0	0

3 Residue-property plots (i)

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.

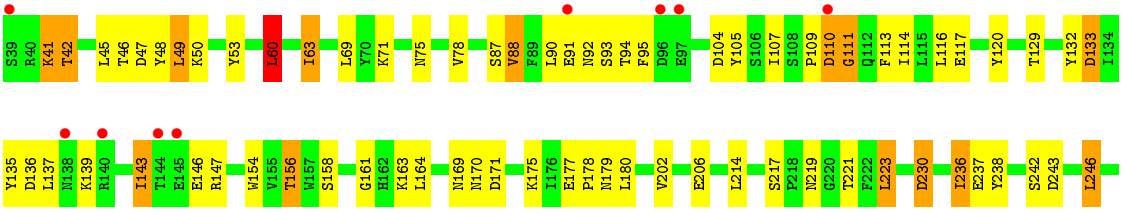
- Molecule 1: Dipeptidyl peptidase 4

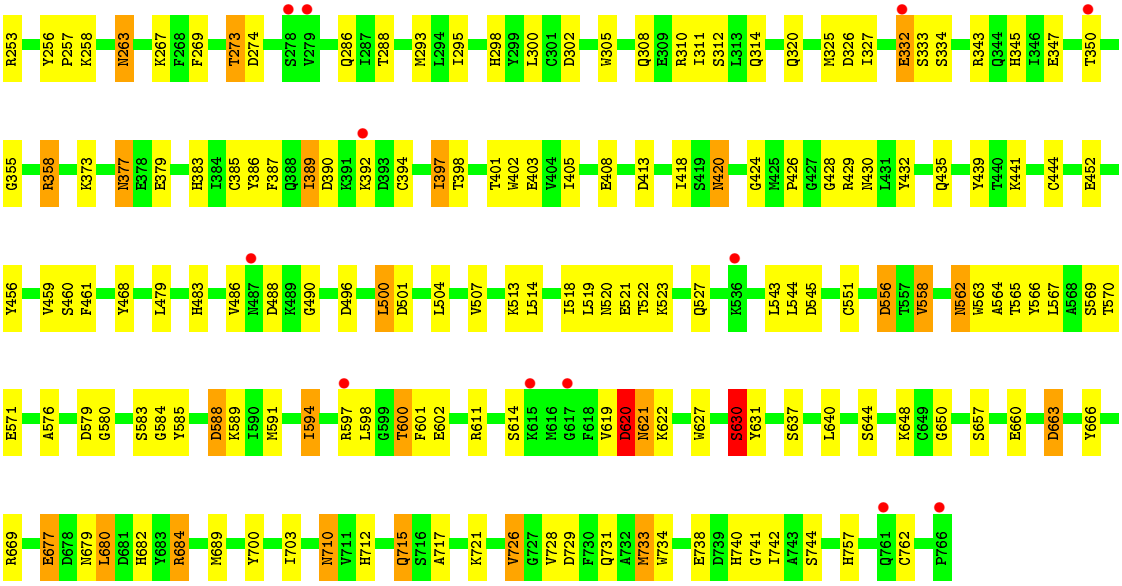
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

Chain B:




R253 Y256 P257 K258 N263 K267 F268 F269 T273 D274 S278 V279 Q286 I287 T288 M293 L294 I295 H298 Y299 L300 G301 D302 W305 Q308 E309 R310 I311 S312 L313 Q314 Q320 M325 D326 I327 E332 S333 S334 R343 Q344 H345 I346 E347 T350
G355 R358 K373 N377 E378 E379 H383 I384 C385 Y386 F387 Q388 I389 D390 K391 K392 D393 C394 I397 T398 T401 W402 E403 V404 I405 E408 D413 I418 S419 N420 G424 M425 P426 G427 G428 R429 N430 L431 Y432 Q435 Y439 T440 K441 C444 E452
Y456 V459 S460 F461 Y468 L479 H483 V486 N487 D488 K489 G490 D496 L500 D501 L504 V507 K513 L514 I518 L519 N520 E521 T522 K523 Q527 K536 L543 L544 D545 C551 D556 T557 V558 N562 W563 A564 T565 Y566 L567 A568 S569 T570
E571 A576 D579 G580 S583 G584 Y585 D588 K589 I590 M591 I594 R597 L598 G599 T600 F601 E602 R611 S614 K615 M616 G617 F618 V619 D620 N621 K622 W627 S630 Y631 S637 L640 S644 K648 C649 G650 S657 E660 D663 Y666
R669 E677 D678 N679 L680 D681 H682 Y683 R684 M689 Y700 I703 N710 V711 H712 Q715 S716 A717 K721 V726 G727 V728 D729 F730 Q731 A732 M733 W734 E738 D739 H740 G741 I742 A743 S744 H757 Q761 C762 P766

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.56Å 68.49Å 421.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70 10.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.70) 76.5 (10.01-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.85 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.236 , 0.286 0.221 , 0.279	Depositor DCC
R_{free} test set	2042 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	1.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12163	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, B2Q

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	0.76	0/6135	0.94	21/8344 (0.3%)
1	B	0.77	0/6135	0.96	24/8344 (0.3%)
All	All	0.76	0/12270	0.95	45/16688 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	678	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	110	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	729	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	501	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	133	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	663	ASP	CB-CG-OD2	6.74	124.37	118.30
1	A	588	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	230	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	620	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	274	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	579	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	297	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	737	ASP	CB-CG-OD2	6.29	123.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	588	ASP	CB-CG-OD2	6.23	123.90	118.30
1	B	390	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	111	GLY	N-CA-C	6.13	128.43	113.10
1	A	171	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	329	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	620	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	515	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	133	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	243	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	47	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	413	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	230	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	721	LYS	CD-CE-NZ	5.41	124.13	111.70
1	A	488	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	200	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	60	LEU	CA-CB-CG	5.35	127.60	115.30
1	B	60	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	104	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	171	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	104	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	496	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	488	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	358	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	709	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	413	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	65	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	556	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	274	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	729	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	40	ARG	N-CA-C	5.01	124.52	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	40	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5681	146	0
1	B	5963	0	5680	198	0
2	A	56	0	52	2	0
2	B	56	0	52	3	0
3	A	23	0	30	2	0
3	B	23	0	30	4	0
4	A	41	0	0	5	0
4	B	38	0	0	13	0
All	All	12163	0	11525	346	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:THR:HG22	1:B:601:PHE:H	1.13	1.12
1:B:267:LYS:HE3	4:B:772:HOH:O	1.56	1.06
1:B:543:LEU:HD21	1:B:627:TRP:HD1	1.22	1.02
1:A:347:GLU:OE2	1:A:373:LYS:NZ	2.01	0.94
1:B:600:THR:HG22	1:B:601:PHE:N	1.83	0.93
1:B:221:THR:O	1:B:273:THR:HB	1.71	0.91
1:A:377:ASN:C	1:A:377:ASN:HD22	1.74	0.90
1:A:160:VAL:HG12	1:A:160:VAL:O	1.68	0.90
1:B:377:ASN:HD22	1:B:377:ASN:C	1.74	0.89
1:B:620:ASP:OD1	1:B:620:ASP:C	2.10	0.88
1:B:267:LYS:CE	4:B:772:HOH:O	2.14	0.87
1:B:680:LEU:HD22	1:B:684:ARG:HD3	1.58	0.86
1:A:704:HIS:HD1	1:A:716:SER:HG	0.87	0.84
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.60	0.84
1:B:253:ARG:HD2	4:B:767:HOH:O	1.77	0.84
1:B:87:SER:OG	2:B:794:NAG:O7	1.97	0.81
1:B:267:LYS:HD2	1:B:286:GLN:NE2	1.95	0.80
1:B:117:GLU:HG3	1:B:132:TYR:CE1	2.17	0.79
1:B:75:ASN:OD1	1:B:92:ASN:HB3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:SER:H	1:B:715:GLN:NE2	1.81	0.79
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.83	0.78
1:B:347:GLU:OE2	1:B:373:LYS:NZ	2.14	0.78
3:B:900:B2Q:HH	4:B:11:HOH:O	1.81	0.78
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.16	0.78
1:B:46:THR:HG22	1:B:50:LYS:HD3	1.66	0.78
1:B:731:GLN:NE2	4:B:779:HOH:O	2.16	0.78
1:B:600:THR:CG2	1:B:601:PHE:H	1.96	0.77
1:B:562:ASN:HD22	1:B:562:ASN:C	1.90	0.75
1:A:487:ASN:O	1:A:489:LYS:N	2.20	0.74
1:A:403:GLU:H	1:A:420:ASN:HD21	1.33	0.74
1:B:175:LYS:NZ	1:B:178:PRO:O	2.21	0.74
1:B:600:THR:CG2	1:B:601:PHE:N	2.49	0.73
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.23	0.73
1:B:543:LEU:HD21	1:B:627:TRP:CD1	2.15	0.72
1:A:414:TYR:CE1	1:A:435:GLN:HG3	2.24	0.72
1:B:242:SER:OG	1:B:246:LEU:HD12	1.88	0.72
1:B:621:ASN:HD22	1:B:622:LYS:N	1.88	0.72
1:A:109:PRO:HD2	1:A:161:GLY:O	1.91	0.71
1:B:236:ILE:HD12	1:B:712:HIS:CD2	2.26	0.70
1:B:163:LYS:HZ3	1:B:273:THR:HG22	1.54	0.70
1:B:401:THR:O	1:B:401:THR:HG22	1.90	0.70
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.27	0.69
2:A:793:NAG:H3	2:A:793:NAG:H83	1.75	0.68
1:A:357:PHE:CE1	3:A:900:B2Q:HGA	2.29	0.68
1:B:377:ASN:C	1:B:377:ASN:ND2	2.47	0.68
1:B:403:GLU:H	1:B:420:ASN:HD21	1.41	0.68
1:B:598:LEU:O	1:B:682:HIS:HE1	1.76	0.68
1:A:514:LEU:HD23	1:A:514:LEU:C	2.15	0.67
1:B:403:GLU:OE1	1:B:585:TYR:HA	1.95	0.67
1:A:160:VAL:CG1	1:A:160:VAL:O	2.40	0.67
1:B:345:HIS:CE1	4:B:28:HOH:O	2.46	0.67
1:A:657:SER:H	1:A:715:GLN:NE2	1.93	0.66
1:B:219:ASN:N	1:B:308:GLN:OE1	2.29	0.66
1:A:221:THR:O	1:A:273:THR:HB	1.95	0.66
1:B:620:ASP:OD1	1:B:622:LYS:N	2.29	0.66
1:A:482:LEU:HD13	1:A:491:LEU:HD12	1.79	0.65
1:B:518:ILE:O	1:B:519:LEU:HD12	1.96	0.65
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.31	0.65
1:A:735:TYR:OH	1:A:750:HIS:CD2	2.48	0.65
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:CG2	1:A:570:THR:OG1	2.46	0.64
1:A:377:ASN:ND2	1:A:377:ASN:C	2.44	0.64
1:B:680:LEU:CD2	1:B:684:ARG:HD3	2.26	0.63
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.81	0.63
1:B:63:ILE:HD13	1:B:69:LEU:HG	1.80	0.63
1:B:163:LYS:NZ	1:B:273:THR:HG22	2.14	0.62
1:B:267:LYS:HD2	1:B:286:GLN:HE22	1.62	0.62
1:B:42:THR:HG23	1:B:570:THR:OG1	2.00	0.62
1:B:621:ASN:C	1:B:621:ASN:HD22	2.02	0.61
1:B:267:LYS:HG3	4:B:772:HOH:O	1.99	0.61
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.36	0.61
1:B:660:GLU:OE2	4:B:778:HOH:O	2.16	0.61
1:A:273:THR:O	1:A:273:THR:HG23	2.00	0.60
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.83	0.60
1:A:736:THR:HG21	1:B:717:ALA:O	2.02	0.60
1:B:428:GLY:O	1:B:429:ARG:HG2	2.02	0.60
1:B:75:ASN:OD1	1:B:92:ASN:CB	2.49	0.60
1:B:137:LEU:C	1:B:139:LYS:H	2.04	0.60
1:B:327:ILE:HD13	1:B:389:ILE:HG12	1.84	0.59
1:B:543:LEU:HD23	1:B:544:LEU:N	2.17	0.59
1:A:453:ARG:O	1:A:475:PRO:HD2	2.03	0.59
1:B:594:ILE:HD11	1:B:602:GLU:N	2.17	0.59
1:B:435:GLN:NE2	1:B:441:LYS:HD3	2.18	0.58
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.38	0.58
1:B:611:ARG:O	1:B:614:SER:HB2	2.02	0.58
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.19	0.58
1:B:179:ASN:OD1	1:B:180:LEU:HD22	2.02	0.58
1:B:136:ASP:O	1:B:139:LYS:O	2.22	0.58
1:B:42:THR:CG2	1:B:570:THR:OG1	2.51	0.58
1:B:63:ILE:CD1	1:B:69:LEU:CD1	2.81	0.57
1:B:163:LYS:NZ	1:B:273:THR:CG2	2.67	0.57
1:A:305:TRP:CE3	1:A:311:ILE:HG12	2.39	0.57
1:A:340:LEU:O	1:A:342:ALA:N	2.37	0.57
1:B:242:SER:HG	1:B:246:LEU:HD12	1.68	0.57
1:B:257:PRO:CB	1:B:263:ASN:HD22	2.18	0.57
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.35	0.56
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.41	0.56
1:A:72:GLN:O	1:A:73:GLU:HB2	2.04	0.56
1:A:115:LEU:HD11	1:A:155:VAL:HG11	1.87	0.56
1:B:657:SER:H	1:B:715:GLN:HE21	1.52	0.56
1:B:598:LEU:O	1:B:682:HIS:CE1	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HB2	1:B:263:ASN:ND2	2.21	0.56
1:A:416:TYR:CE2	1:A:433:LYS:HG3	2.41	0.56
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.41	0.56
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.87	0.55
1:A:602:GLU:OE2	1:A:631:TYR:OH	2.17	0.55
1:A:614:SER:O	1:A:615:LYS:C	2.44	0.55
1:A:470:LEU:N	1:A:481:THR:O	2.38	0.55
1:A:326:ASP:OD2	1:A:339:CYS:HB3	2.06	0.55
1:A:760:LYS:HE2	4:A:38:HOH:O	2.06	0.55
1:B:710:ASN:C	1:B:710:ASN:HD22	2.09	0.55
1:B:397:ILE:HG13	1:B:439:TYR:CE2	2.42	0.54
3:B:900:B2Q:CH	4:B:11:HOH:O	2.49	0.54
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.90	0.54
1:B:105:TYR:CD1	1:B:105:TYR:C	2.80	0.54
1:B:703:ILE:HA	1:B:733:MET:O	2.07	0.54
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.43	0.54
1:B:588:ASP:O	1:B:589:LYS:C	2.44	0.54
1:A:721:LYS:NZ	1:B:242:SER:O	2.39	0.54
1:B:332:GLU:HG2	1:B:333:SER:N	2.23	0.53
1:B:520:ASN:O	1:B:521:GLU:HB2	2.08	0.53
1:B:257:PRO:CB	1:B:263:ASN:ND2	2.72	0.53
1:B:424:GLY:O	1:B:426:PRO:HD3	2.08	0.53
1:B:562:ASN:ND2	1:B:562:ASN:C	2.60	0.53
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.90	0.53
1:B:680:LEU:O	1:B:680:LEU:HD22	2.09	0.53
1:A:355:GLY:HA3	1:A:358:ARG:O	2.08	0.53
1:A:500:LEU:HA	1:A:503:MET:CE	2.39	0.53
1:B:620:ASP:O	1:B:620:ASP:OD1	2.25	0.53
1:A:641:GLY:O	1:A:694:ASN:ND2	2.36	0.53
1:A:82:GLU:OE1	1:A:82:GLU:HA	2.07	0.53
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.43	0.53
1:A:334:SER:OG	1:A:336:ARG:HG3	2.09	0.53
1:A:403:GLU:H	1:A:420:ASN:ND2	2.05	0.53
2:A:793:NAG:H3	2:A:793:NAG:C8	2.37	0.53
1:B:594:ILE:HG23	1:B:594:ILE:O	2.08	0.53
1:A:703:ILE:HA	1:A:733:MET:O	2.09	0.53
1:B:405:ILE:HD13	1:B:429:ARG:CD	2.38	0.53
1:A:273:THR:O	1:A:273:THR:CG2	2.57	0.52
1:A:41:LYS:HG2	1:A:42:THR:N	2.24	0.52
1:A:514:LEU:HD23	1:A:515:ASP:N	2.24	0.52
1:A:657:SER:H	1:A:715:GLN:HE21	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:ND2	1:B:379:GLU:H	2.07	0.52
1:B:386:TYR:HB2	1:B:397:ILE:CD1	2.40	0.52
1:B:267:LYS:NZ	1:B:286:GLN:HE22	2.07	0.52
1:B:594:ILE:HD11	1:B:602:GLU:H	1.73	0.52
1:A:105:TYR:HA	1:A:115:LEU:O	2.10	0.51
1:B:435:GLN:NE2	1:B:441:LYS:CD	2.73	0.51
1:B:377:ASN:ND2	1:B:379:GLU:N	2.57	0.51
1:A:514:LEU:CD2	1:A:514:LEU:C	2.78	0.51
1:A:377:ASN:ND2	1:A:379:GLU:H	2.08	0.51
1:A:463:LYS:O	1:A:464:GLU:HB2	2.09	0.51
1:A:654:ALA:N	1:A:655:PRO:HD3	2.27	0.50
1:A:73:GLU:N	4:A:774:HOH:O	2.39	0.50
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.10	0.50
1:A:528:MET:CE	1:A:530:LEU:HD21	2.42	0.50
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.46	0.50
1:B:397:ILE:HG13	1:B:439:TYR:CD2	2.47	0.50
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.41	0.50
1:A:720:SER:O	1:A:724:VAL:HG23	2.11	0.50
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.93	0.50
1:B:429:ARG:HG3	1:B:456:TYR:CZ	2.47	0.49
1:A:458:SER:OG	1:A:471:ARG:CG	2.60	0.49
1:B:666:TYR:CD2	3:B:900:B2Q:HR	2.47	0.49
1:B:513:LYS:O	1:B:527:GLN:HA	2.12	0.49
1:A:596:ARG:HA	1:A:670:TYR:O	2.13	0.49
1:A:499:ALA:O	1:A:502:LYS:HG3	2.13	0.49
1:B:110:ASP:CG	1:B:161:GLY:H	2.16	0.49
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.95	0.49
1:B:137:LEU:C	1:B:139:LYS:N	2.66	0.49
1:A:594:ILE:HD11	1:A:602:GLU:H	1.78	0.48
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.13	0.48
1:B:420:ASN:C	1:B:420:ASN:HD22	2.16	0.48
1:B:483:HIS:CD2	1:B:490:GLY:HA2	2.48	0.48
1:B:267:LYS:CG	4:B:772:HOH:O	2.59	0.48
1:B:459:VAL:HG22	1:B:460:SER:N	2.29	0.48
1:A:532:PRO:O	1:A:533:HIS:HB2	2.13	0.48
1:A:60:LEU:C	1:A:60:LEU:HD23	2.34	0.48
1:A:66:HIS:ND1	4:A:781:HOH:O	2.35	0.48
1:B:402:TRP:HB2	1:B:420:ASN:ND2	2.28	0.48
1:A:42:THR:HG21	1:A:570:THR:OG1	2.13	0.48
1:A:397:ILE:HG22	1:A:439:TYR:CD2	2.48	0.48
1:A:734:TRP:HE1	1:A:736:THR:HG22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.96	0.47
1:B:408:GLU:OE1	4:B:24:HOH:O	2.20	0.47
1:B:163:LYS:HZ3	1:B:273:THR:CG2	2.22	0.47
1:B:46:THR:CG2	1:B:50:LYS:HD3	2.41	0.47
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.50	0.47
2:B:793:NAG:H3	2:B:793:NAG:C8	2.44	0.47
1:A:741:GLY:O	1:A:742:ILE:C	2.53	0.47
1:B:689:MET:SD	1:B:689:MET:N	2.87	0.47
1:A:458:SER:OG	1:A:471:ARG:HG3	2.15	0.47
1:A:629:TRP:HA	1:A:653:VAL:O	2.15	0.47
1:A:654:ALA:N	1:A:655:PRO:CD	2.77	0.47
1:A:105:TYR:C	1:A:105:TYR:CD1	2.88	0.47
1:A:404:VAL:HG13	1:A:417:TYR:CD2	2.49	0.47
1:A:419:SER:OG	1:A:420:ASN:N	2.45	0.47
1:A:615:LYS:O	1:A:616:MET:C	2.53	0.47
1:B:88:VAL:O	1:B:88:VAL:HG22	2.14	0.47
1:A:656:VAL:HG21	3:A:900:B2Q:HP	1.96	0.47
1:B:562:ASN:ND2	1:B:565:THR:H	2.12	0.47
1:A:137:LEU:O	1:A:139:LYS:O	2.33	0.47
1:B:564:ALA:O	1:B:565:THR:C	2.52	0.47
1:B:92:ASN:OD1	1:B:93:SER:N	2.48	0.47
1:A:323:SER:OG	1:A:347:GLU:HB2	2.14	0.46
1:B:405:ILE:HD13	1:B:429:ARG:NE	2.30	0.46
1:A:340:LEU:HB3	1:A:343:ARG:HD2	1.97	0.46
1:A:596:ARG:N	1:A:670:TYR:O	2.48	0.46
1:B:435:GLN:HE22	1:B:441:LYS:HD3	1.79	0.46
1:B:543:LEU:HD23	1:B:543:LEU:C	2.35	0.46
1:B:677:GLU:H	1:B:677:GLU:HG3	1.45	0.46
1:A:316:LEU:HD22	1:A:320:GLN:HA	1.98	0.46
1:B:164:LEU:HB2	1:B:175:LYS:HB2	1.96	0.46
1:B:343:ARG:O	1:B:343:ARG:HG2	2.16	0.46
1:B:648:LYS:HE3	1:B:762:CYS:O	2.15	0.46
1:B:48:TYR:CD2	1:B:49:LEU:HD13	2.51	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.51	0.46
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.80	0.46
1:B:598:LEU:HD22	1:B:631:TYR:OH	2.16	0.46
1:B:741:GLY:O	1:B:742:ILE:C	2.53	0.46
1:B:584:GLY:O	1:B:585:TYR:HB2	2.15	0.46
1:A:300:LEU:HD23	1:A:300:LEU:C	2.36	0.46
1:B:435:GLN:HE21	1:B:441:LYS:HB3	1.81	0.46
1:A:305:TRP:CZ3	1:A:311:ILE:CG1	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:VAL:HG22	1:A:606:GLN:OE1	2.16	0.46
1:B:405:ILE:HD13	1:B:429:ARG:HD3	1.97	0.46
1:B:42:THR:OG1	1:B:569:SER:O	2.34	0.45
1:A:588:ASP:O	1:A:589:LYS:C	2.53	0.45
1:A:726:VAL:O	1:A:726:VAL:CG1	2.64	0.45
1:B:345:HIS:HE1	4:B:28:HOH:O	1.91	0.45
1:A:154:TRP:O	1:A:166:TYR:HA	2.16	0.45
1:A:219:ASN:N	1:A:308:GLN:OE1	2.49	0.45
1:B:734:TRP:C	1:B:734:TRP:CD1	2.90	0.45
1:A:420:ASN:C	1:A:420:ASN:HD22	2.18	0.44
1:B:206:GLU:O	3:B:900:B2Q:CA	2.65	0.44
1:A:500:LEU:HD11	1:A:504:LEU:HD11	1.99	0.44
1:A:514:LEU:CD1	1:A:557:THR:HG22	2.47	0.44
1:A:710:ASN:C	1:A:710:ASN:HD22	2.21	0.44
1:B:403:GLU:H	1:B:420:ASN:ND2	2.13	0.44
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.99	0.44
1:A:600:THR:O	1:A:603:VAL:N	2.49	0.44
1:B:133:ASP:OD1	1:B:147:ARG:NH1	2.50	0.44
1:B:137:LEU:O	1:B:139:LYS:N	2.50	0.44
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.52	0.44
1:A:482:LEU:CD1	1:A:491:LEU:HD12	2.46	0.44
1:A:562:ASN:O	1:A:565:THR:HB	2.18	0.44
1:B:117:GLU:HG3	1:B:132:TYR:CZ	2.52	0.44
1:B:293:MET:O	1:B:298:HIS:HD2	2.01	0.44
1:B:556:ASP:OD1	1:B:558:VAL:HG13	2.18	0.44
1:B:63:ILE:CD1	1:B:69:LEU:HG	2.46	0.44
1:A:487:ASN:O	1:A:488:ASP:C	2.55	0.44
1:B:169:ASN:O	1:B:170:ASN:HB2	2.17	0.44
1:A:626:ILE:O	1:A:650:GLY:HA2	2.18	0.44
1:A:669:ARG:HG3	1:A:669:ARG:HH11	1.82	0.44
1:A:760:LYS:CE	4:A:38:HOH:O	2.65	0.44
1:B:383:HIS:HD2	1:B:398:THR:HB	1.83	0.44
1:A:556:ASP:OD1	1:A:556:ASP:C	2.57	0.43
1:A:603:VAL:O	1:A:604:GLU:C	2.56	0.43
1:B:236:ILE:HD12	1:B:712:HIS:NE2	2.33	0.43
1:B:267:LYS:CD	1:B:286:GLN:HE22	2.29	0.43
1:A:658:ARG:HB3	1:A:661:TYR:CD2	2.53	0.43
1:B:177:GLU:HB2	1:B:180:LEU:HD23	2.00	0.43
1:B:355:GLY:HA3	1:B:358:ARG:O	2.18	0.43
1:B:543:LEU:CD2	1:B:543:LEU:C	2.86	0.43
1:B:562:ASN:O	1:B:563:TRP:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:SER:OG	1:B:740:HIS:NE2	2.42	0.43
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.74	0.43
1:B:738:GLU:OE2	1:B:744:SER:OG	2.24	0.43
1:A:477:LEU:HD22	1:A:500:LEU:HD12	1.99	0.43
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.49	0.43
1:B:405:ILE:CD1	1:B:429:ARG:HD3	2.48	0.43
1:A:519:LEU:HA	1:A:519:LEU:HD23	1.64	0.43
1:A:594:ILE:HG23	1:A:594:ILE:O	2.19	0.43
1:B:158:SER:OG	1:B:163:LYS:HB2	2.18	0.43
1:B:253:ARG:CD	4:B:767:HOH:O	2.50	0.43
1:A:370:SER:HB2	1:A:387:PHE:O	2.18	0.43
1:A:729:ASP:OD2	1:B:757:HIS:HD2	2.00	0.43
1:B:551:CYS:HB2	1:B:591:MET:SD	2.59	0.43
1:B:742:ILE:HG22	1:B:742:ILE:O	2.18	0.43
1:B:597:ARG:O	1:B:600:THR:HB	2.19	0.43
1:B:256:TYR:CZ	1:B:663:ASP:HB3	2.54	0.43
1:B:312:SER:OG	1:B:325:MET:HE3	2.19	0.43
1:A:327:ILE:HB	1:A:343:ARG:HG3	2.01	0.42
1:B:63:ILE:HD13	1:B:69:LEU:CG	2.46	0.42
1:B:726:VAL:HG12	1:B:728:VAL:HG23	2.01	0.42
1:A:327:ILE:HD13	1:A:389:ILE:HG12	2.00	0.42
1:A:377:ASN:ND2	1:A:381:TYR:H	2.16	0.42
1:B:428:GLY:C	1:B:429:ARG:HG2	2.39	0.42
1:B:522:THR:HG22	1:B:523:LYS:N	2.33	0.42
1:B:567:LEU:O	1:B:571:GLU:HB2	2.20	0.42
1:B:305:TRP:CE3	1:B:311:ILE:HG12	2.55	0.42
1:A:110:ASP:OD1	1:A:110:ASP:C	2.58	0.42
1:B:320:GLN:OE1	1:B:669:ARG:CD	2.62	0.42
1:A:367:ASP:OD1	1:A:368:GLY:N	2.52	0.42
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.87	0.42
1:B:562:ASN:HD22	1:B:565:THR:H	1.66	0.42
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.49	0.42
1:B:143:ILE:HG13	1:B:143:ILE:O	2.13	0.41
1:A:45:LEU:HG	1:A:49:LEU:HD22	2.02	0.41
1:A:669:ARG:HG3	1:A:669:ARG:NH1	2.35	0.41
1:A:662:TYR:HE1	1:A:710:ASN:HD22	1.68	0.41
1:B:69:LEU:HD11	1:B:107:ILE:HD12	2.02	0.41
1:B:146:GLU:O	1:B:175:LYS:NZ	2.50	0.41
1:A:358:ARG:HB2	1:A:359:PRO:HD2	2.02	0.41
1:B:594:ILE:HD12	1:B:601:PHE:HB2	2.01	0.41
1:A:340:LEU:C	1:A:342:ALA:N	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:HG23	1:A:43:TYR:N	2.35	0.41
1:A:500:LEU:HD22	1:A:504:LEU:HG	2.02	0.41
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.02	0.41
1:A:65:ASP:N	1:A:65:ASP:OD1	2.52	0.41
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.21	0.41
1:B:310:ARG:NH2	1:B:389:ILE:HD13	2.35	0.41
1:B:543:LEU:CD2	1:B:627:TRP:HD1	2.11	0.41
1:B:69:LEU:HD23	1:B:78:VAL:HG22	2.03	0.41
1:B:154:TRP:NE1	1:B:156:THR:OG1	2.53	0.41
1:B:630:SER:O	1:B:631:TYR:C	2.59	0.41
2:B:793:NAG:H82	2:B:793:NAG:C1	2.51	0.41
1:A:431:LEU:HD13	1:A:445:LEU:HD12	2.01	0.41
1:A:48:TYR:CD2	1:A:49:LEU:HD13	2.55	0.41
1:B:113:PHE:CE1	1:B:178:PRO:HG2	2.56	0.41
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.85	0.41
1:B:236:ILE:HD13	1:B:238:TYR:HD1	1.86	0.41
1:A:248:TYR:CZ	1:B:258:LYS:HD2	2.55	0.41
1:A:340:LEU:C	1:A:342:ALA:H	2.24	0.41
1:B:397:ILE:CG1	1:B:439:TYR:CE2	3.03	0.41
1:B:580:GLY:O	1:B:583:SER:OG	2.26	0.41
1:A:500:LEU:HA	1:A:503:MET:HE2	2.01	0.41
1:A:208:PHE:O	1:A:209:SER:C	2.56	0.41
1:A:662:TYR:HE1	1:A:710:ASN:ND2	2.19	0.41
1:B:120:TYR:CD1	1:B:120:TYR:C	2.94	0.41
1:B:60:LEU:C	1:B:60:LEU:CD2	2.89	0.41
1:A:420:ASN:C	1:A:420:ASN:ND2	2.75	0.41
1:A:263:ASN:HD21	1:A:664:SER:CB	2.34	0.41
1:B:109:PRO:HD2	1:B:161:GLY:O	2.21	0.40
1:B:545:ASP:N	1:B:576:ALA:O	2.54	0.40
1:B:637:SER:HG	1:B:700:TYR:HH	1.69	0.40
1:A:175:LYS:NZ	1:A:178:PRO:O	2.54	0.40
1:B:397:ILE:HG12	1:B:439:TYR:CE1	2.56	0.40
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.53	0.40
1:B:267:LYS:CE	1:B:286:GLN:HE22	2.34	0.40
1:B:418:ILE:HA	1:B:430:ASN:O	2.20	0.40
1:A:169:ASN:O	1:A:170:ASN:HB2	2.22	0.40
1:A:73:GLU:CA	4:A:774:HOH:O	2.68	0.40
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.04	0.40
1:B:114:ILE:O	1:B:114:ILE:HG23	2.21	0.40
1:B:500:LEU:HD22	1:B:504:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	726/728 (100%)	676 (93%)	44 (6%)	6 (1%)	19 43
1	B	726/728 (100%)	674 (93%)	50 (7%)	2 (0%)	41 66
All	All	1452/1456 (100%)	1350 (93%)	94 (6%)	8 (1%)	25 50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	ASP
1	A	488	ASP
1	B	111	GLY
1	A	393	ASP
1	B	630	SER
1	A	742	ILE
1	A	341	VAL
1	A	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	653/653 (100%)	599 (92%)	54 (8%)	11 25
1	B	653/653 (100%)	592 (91%)	61 (9%)	9 21
All	All	1306/1306 (100%)	1191 (91%)	115 (9%)	10 23

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	42	THR
1	A	49	LEU
1	A	60	LEU
1	A	82	GLU
1	A	87	SER
1	A	88	VAL
1	A	107	ILE
1	A	120	TYR
1	A	180	LEU
1	A	202	VAL
1	A	211	TYR
1	A	223	LEU
1	A	230	ASP
1	A	246	LEU
1	A	273	THR
1	A	277	SER
1	A	278	SER
1	A	294	LEU
1	A	316	LEU
1	A	326	ASP
1	A	343	ARG
1	A	350	THR
1	A	377	ASN
1	A	385	CYS
1	A	399	LYS
1	A	410	LEU
1	A	419	SER
1	A	420	ASN
1	A	431	LEU
1	A	435	GLN
1	A	452	GLU
1	A	460	SER
1	A	471	ARG
1	A	472	CYS
1	A	473	SER
1	A	479	LEU
1	A	482	LEU
1	A	500	LEU
1	A	502	LYS
1	A	513	LYS
1	A	543	LEU

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Mol	Chain	Res	Type
1	A	544	LEU
1	A	621	ASN
1	A	630	SER
1	A	663	ASP
1	A	669	ARG
1	A	679	ASN
1	A	684	ARG
1	A	710	ASN
1	A	715	GLN
1	A	736	THR
1	A	745	SER
1	B	41	LYS
1	B	42	THR
1	B	49	LEU
1	B	60	LEU
1	B	63	ILE
1	B	71	LYS
1	B	88	VAL
1	B	90	LEU
1	B	91	GLU
1	B	94	THR
1	B	129	THR
1	B	143	ILE
1	B	156	THR
1	B	202	VAL
1	B	214	LEU
1	B	217	SER
1	B	223	LEU
1	B	230	ASP
1	B	236	ILE
1	B	246	LEU
1	B	263	ASN
1	B	273	THR
1	B	288	THR
1	B	295	ILE
1	B	300	LEU
1	B	302	ASP
1	B	314	GLN
1	B	326	ASP
1	B	332	GLU
1	B	334	SER
1	B	350	THR

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Mol	Chain	Res	Type
1	B	377	ASN
1	B	385	CYS
1	B	389	ILE
1	B	392	LYS
1	B	397	ILE
1	B	420	ASN
1	B	452	GLU
1	B	479	LEU
1	B	486	VAL
1	B	500	LEU
1	B	507	VAL
1	B	514	LEU
1	B	558	VAL
1	B	562	ASN
1	B	566	TYR
1	B	594	ILE
1	B	600	THR
1	B	619	VAL
1	B	620	ASP
1	B	621	ASN
1	B	630	SER
1	B	644	SER
1	B	677	GLU
1	B	679	ASN
1	B	680	LEU
1	B	684	ARG
1	B	710	ASN
1	B	715	GLN
1	B	726	VAL
1	B	733	MET

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	123	GLN
1	A	169	ASN
1	A	247	GLN
1	A	263	ASN
1	A	377	ASN
1	A	420	ASN
1	A	483	HIS
1	A	508	GLN

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Mol	Chain	Res	Type
1	A	533	HIS
1	A	592	HIS
1	A	621	ASN
1	A	679	ASN
1	A	710	ASN
1	A	715	GLN
1	A	750	HIS
1	B	126	HIS
1	B	169	ASN
1	B	263	ASN
1	B	286	GLN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	483	HIS
1	B	562	ASN
1	B	621	ASN
1	B	679	ASN
1	B	682	HIS
1	B	710	ASN
1	B	715	GLN
1	B	750	HIS
1	B	757	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	793	1	14,14,15	0.76	1 (7%)	17,19,21	1.77	3 (17%)
2	NAG	B	793	1	14,14,15	0.69	0	17,19,21	2.21	6 (35%)
2	NAG	B	797	1	14,14,15	0.46	0	17,19,21	2.85	6 (35%)
2	NAG	A	796	1	14,14,15	0.88	1 (7%)	17,19,21	1.82	5 (29%)
2	NAG	B	794	1	14,14,15	0.74	0	17,19,21	1.22	1 (5%)
3	B2Q	B	900	-	25,25,25	0.93	2 (8%)	32,35,35	2.79	11 (34%)
2	NAG	A	795	1	14,14,15	0.61	0	17,19,21	2.00	3 (17%)
3	B2Q	A	900	-	25,25,25	0.61	0	32,35,35	2.17	10 (31%)
2	NAG	B	796	1	14,14,15	0.88	1 (7%)	17,19,21	1.56	2 (11%)
2	NAG	A	794	1	14,14,15	0.78	0	17,19,21	1.80	6 (35%)

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	793	1	-	5/6/23/26	0/1/1/1
2	NAG	B	793	1	-	5/6/23/26	0/1/1/1
2	NAG	B	797	1	-	4/6/23/26	0/1/1/1
2	NAG	A	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	794	1	-	0/6/23/26	0/1/1/1
3	B2Q	B	900	-	2/2/4/4	1/8/33/33	0/3/3/3
2	NAG	A	795	1	-	6/6/23/26	0/1/1/1
3	B2Q	A	900	-	2/2/4/4	2/8/33/33	0/3/3/3
2	NAG	B	796	1	-	2/6/23/26	0/1/1/1
2	NAG	A	794	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	900	B2Q	CL-CR	-3.12	1.47	1.53
2	B	796	NAG	O5-C1	-2.66	1.39	1.43
2	A	796	NAG	O5-C1	-2.50	1.39	1.43
2	A	793	NAG	O5-C1	-2.09	1.40	1.43
3	B	900	B2Q	CM-CL	-2.09	1.46	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	900	B2Q	CN-CM-CL	7.51	140.61	115.17
2	B	797	NAG	C1-O5-C5	-7.36	102.22	112.19
3	B	900	B2Q	CK-CL-CR	6.96	119.06	110.44
3	B	900	B2Q	CL-CK-NJ	-6.88	103.22	112.23
2	B	793	NAG	C1-O5-C5	6.41	120.88	112.19
2	B	797	NAG	C1-C2-N2	-5.37	101.31	110.49
2	A	795	NAG	C1-O5-C5	5.20	119.24	112.19
3	A	900	B2Q	CM-CL-CR	-5.07	107.01	113.03
2	B	797	NAG	O5-C1-C2	5.05	119.27	111.29
2	B	796	NAG	O5-C1-C2	-4.53	104.13	111.29
3	B	900	B2Q	CT-CR-NS	-4.35	95.39	110.84
3	A	900	B2Q	CT-CR-NS	-4.34	95.42	110.84
2	A	795	NAG	C4-C3-C2	-4.19	104.88	111.02
3	A	900	B2Q	CL-CK-NJ	-4.15	106.80	112.23
2	A	796	NAG	C3-C4-C5	-4.00	103.11	110.24
3	A	900	B2Q	CN-CM-CL	3.92	128.44	115.17
2	A	794	NAG	C4-C3-C2	-3.71	105.58	111.02
3	B	900	B2Q	CH-NJ-CE	3.65	118.55	111.27
2	A	795	NAG	C1-C2-N2	3.65	116.72	110.49
3	A	900	B2Q	CH-NJ-CE	3.65	118.54	111.27
2	B	793	NAG	C4-C3-C2	-3.57	105.79	111.02
2	A	793	NAG	C1-O5-C5	3.30	116.66	112.19
2	A	793	NAG	O5-C5-C6	-3.15	102.26	107.20
3	A	900	B2Q	CL-CR-NS	-3.12	100.59	111.44
3	B	900	B2Q	CF-CD-CE	-3.09	118.01	121.57
3	A	900	B2Q	CF-CD-CE	-3.08	118.01	121.57
2	B	797	NAG	C3-C4-C5	-3.00	104.90	110.24
2	B	793	NAG	O5-C1-C2	2.94	115.92	111.29
2	A	796	NAG	O3-C3-C2	-2.90	103.46	109.47
3	B	900	B2Q	CL-CR-NS	-2.81	101.65	111.44
3	B	900	B2Q	CT-CR-CL	-2.72	106.77	111.69
2	A	794	NAG	C6-C5-C4	-2.65	106.79	113.00
3	B	900	B2Q	OB-CB-CV	2.55	118.96	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	794	NAG	C3-C4-C5	-2.55	105.70	110.24
2	A	796	NAG	O7-C7-N2	2.54	126.62	121.95
3	A	900	B2Q	OB-CB-CV	2.53	118.93	115.41
3	A	900	B2Q	OW-CV-CB	2.51	118.91	115.41
2	A	794	NAG	O5-C5-C6	2.48	111.10	107.20
3	B	900	B2Q	OW-CV-CB	2.47	118.84	115.41
2	B	794	NAG	C1-O5-C5	2.39	115.43	112.19
2	A	793	NAG	C3-C4-C5	2.39	114.50	110.24
2	B	797	NAG	C2-N2-C7	-2.38	119.51	122.90
2	A	796	NAG	O4-C4-C5	2.38	115.20	109.30
2	B	793	NAG	C8-C7-N2	2.32	120.03	116.10
2	B	797	NAG	O5-C5-C6	2.24	110.72	107.20
2	B	793	NAG	C6-C5-C4	-2.20	107.86	113.00
2	B	793	NAG	O3-C3-C2	2.17	113.95	109.47
3	A	900	B2Q	CK-CL-CR	2.14	113.09	110.44
2	B	796	NAG	O5-C5-C6	-2.14	103.85	107.20
2	A	794	NAG	O7-C7-C8	-2.14	118.08	122.06
2	A	794	NAG	C2-N2-C7	-2.12	119.89	122.90
3	B	900	B2Q	CM-CL-CR	2.12	115.54	113.03
2	A	796	NAG	O5-C1-C2	-2.07	108.01	111.29

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	900	B2Q	CE
3	B	900	B2Q	CL
3	A	900	B2Q	CE
3	A	900	B2Q	CL

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	793	NAG	C8-C7-N2-C2
2	B	793	NAG	O7-C7-N2-C2
3	A	900	B2Q	CK-CL-CM-CN
2	B	797	NAG	C4-C5-C6-O6
2	B	793	NAG	O5-C5-C6-O6
2	B	797	NAG	O5-C5-C6-O6
2	B	797	NAG	C8-C7-N2-C2
2	B	797	NAG	O7-C7-N2-C2
2	A	795	NAG	C8-C7-N2-C2
2	B	793	NAG	C4-C5-C6-O6

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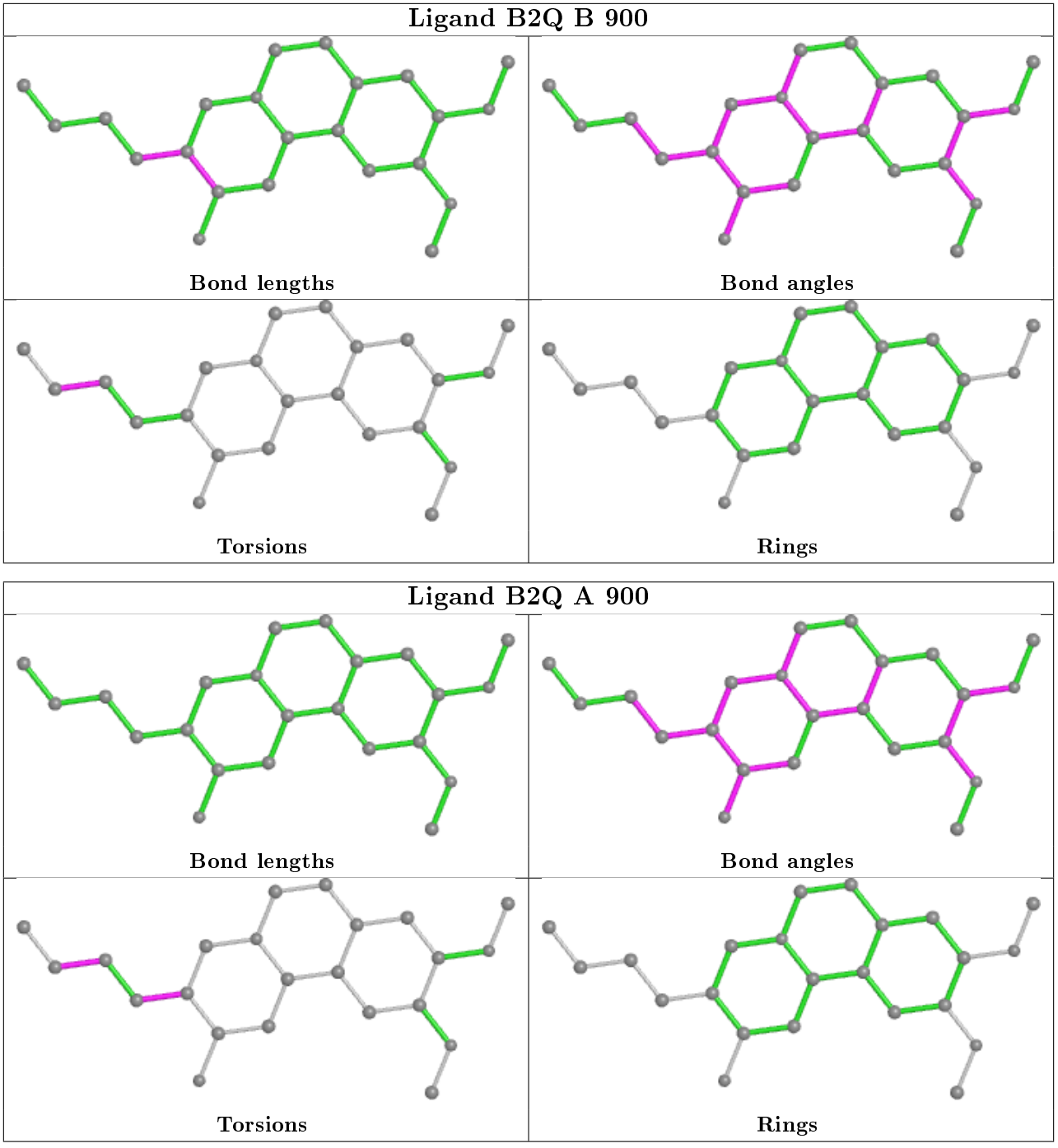
Mol	Chain	Res	Type	Atoms
2	A	795	NAG	O5-C5-C6-O6
2	A	795	NAG	O7-C7-N2-C2
2	A	793	NAG	C8-C7-N2-C2
2	A	793	NAG	O7-C7-N2-C2
2	A	795	NAG	C4-C5-C6-O6
2	B	793	NAG	C1-C2-N2-C7
2	B	796	NAG	C4-C5-C6-O6
2	A	793	NAG	O5-C5-C6-O6
2	A	793	NAG	C4-C5-C6-O6
3	A	900	B2Q	CM-CN-CO-CP
2	B	796	NAG	O5-C5-C6-O6
2	A	795	NAG	C1-C2-N2-C7
2	A	793	NAG	C3-C2-N2-C7
2	A	795	NAG	C3-C2-N2-C7
3	B	900	B2Q	CM-CN-CO-CP

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	793	NAG	2	0
2	B	793	NAG	2	0
2	B	794	NAG	1	0
3	B	900	B2Q	4	0
3	A	900	B2Q	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	728/728 (100%)	-0.24	20 (2%) 54 55	27, 44, 68, 93	0
1	B	728/728 (100%)	-0.20	21 (2%) 51 52	27, 44, 65, 84	0
All	All	1456/1456 (100%)	-0.22	41 (2%) 53 54	27, 44, 67, 93	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	ARG	5.2
1	A	140	ARG	5.1
1	B	97	GLU	5.0
1	B	279	VAL	4.7
1	A	74	ASN	4.5
1	B	278	SER	4.1
1	B	332	GLU	3.9
1	A	141	GLN	3.6
1	A	275	SER	3.3
1	A	99	GLY	3.2
1	B	39	SER	3.0
1	B	138	ASN	3.0
1	B	144	THR	2.9
1	B	487	ASN	2.9
1	A	487	ASN	2.9
1	A	615	LYS	2.8
1	B	96	ASP	2.7
1	B	617	GLY	2.6
1	B	145	GLU	2.6
1	A	378	GLU	2.6
1	B	536	LYS	2.5
1	A	145	GLU	2.5
1	A	677	GLU	2.5
1	B	392	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	97	GLU	2.4
1	B	110	ASP	2.4
1	A	521	GLU	2.4
1	A	333	SER	2.3
1	B	350	THR	2.3
1	A	336	ARG	2.2
1	B	597	ARG	2.2
1	B	91	GLU	2.2
1	A	73	GLU	2.2
1	A	277	SER	2.2
1	A	348	MET	2.1
1	A	138	ASN	2.1
1	B	761	GLN	2.1
1	B	766	PRO	2.1
1	A	471	ARG	2.0
1	A	278	SER	2.0
1	B	615	LYS	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	NAG	A	795	14/15	0.68	0.35	83,85,87,87	0
2	NAG	B	797	14/15	0.77	0.37	81,83,85,85	0
2	NAG	B	793	14/15	0.84	0.35	72,79,81,82	0
2	NAG	B	796	14/15	0.84	0.26	57,62,63,65	0
2	NAG	A	796	14/15	0.89	0.20	49,52,54,56	0
2	NAG	A	793	14/15	0.92	0.20	71,73,76,76	0

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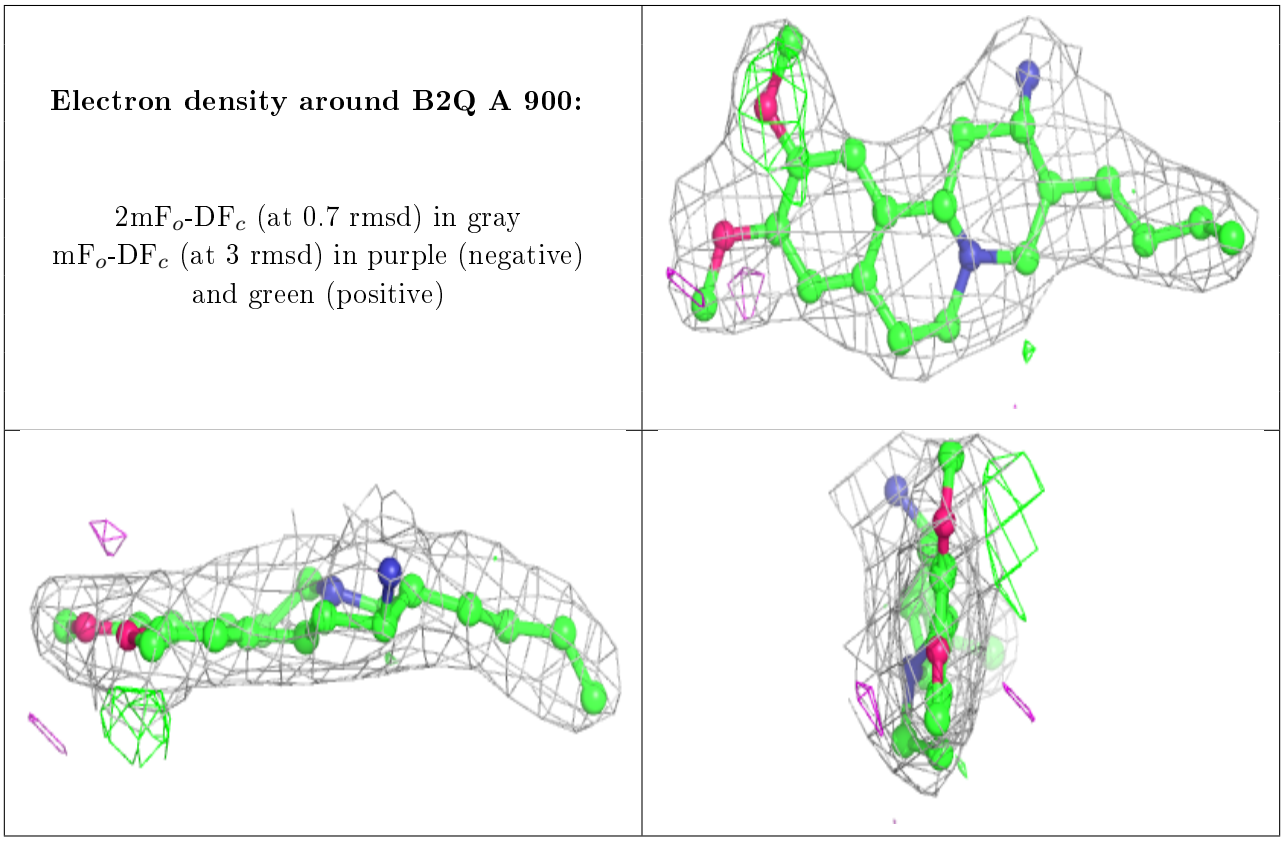
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	B2Q	A	900	23/23	0.93	0.15	42,45,46,47	0
3	B2Q	B	900	23/23	0.93	0.15	41,48,49,49	0
2	NAG	A	794	14/15	0.93	0.18	46,48,53,54	0
2	NAG	B	794	14/15	0.94	0.20	53,55,56,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

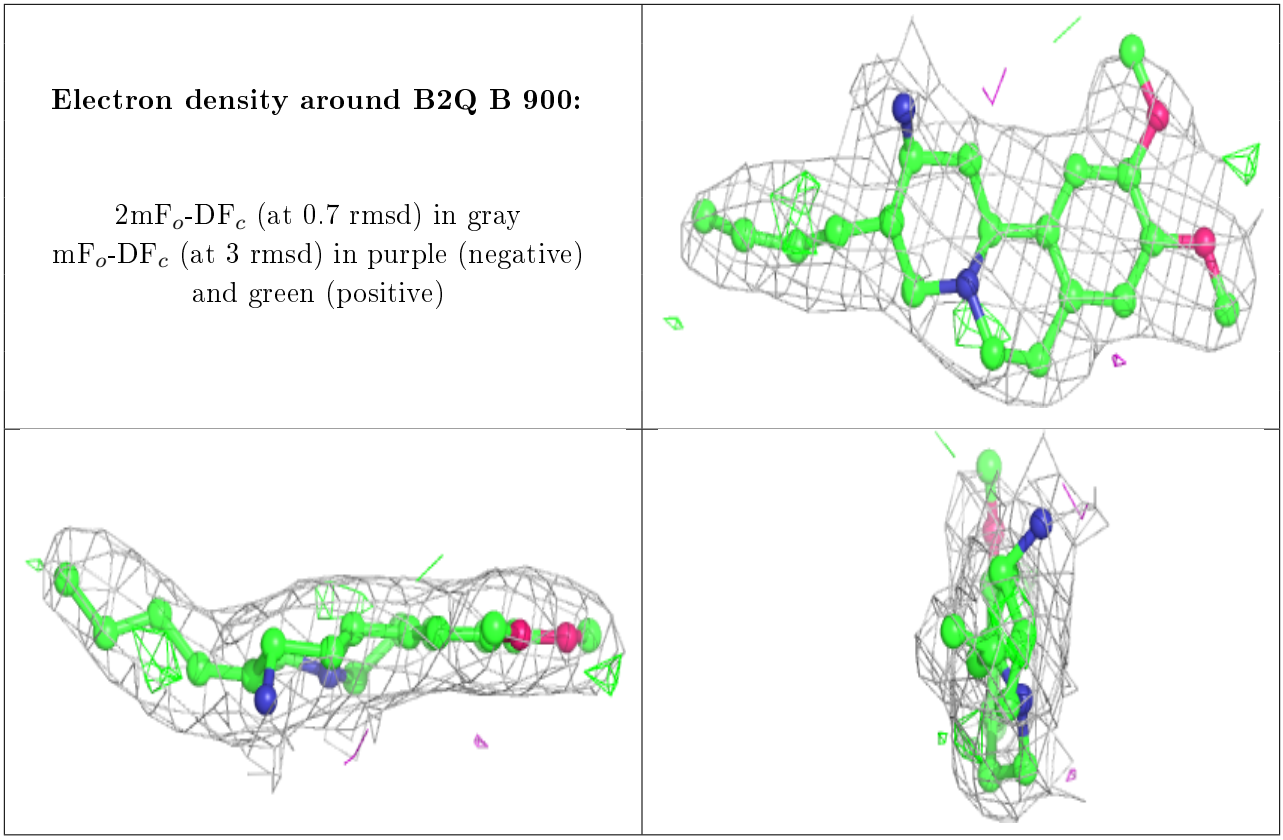
Electron density around B2Q A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around B2Q B 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.