WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:15 AM GMT

|		
PDB ID	:	2GBF
Title	:	rat dpp-IV with alkynyl cyanopyrrolidine #1
Authors	:	Longenecker, K.L.; Jakob, C.G.; Fry, E.H.; Wilk, S.
Deposited on	:	2006-03-10
Resolution	:	3.10 Å(reported)

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 3.10 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		25
Ramachandran outliers		3.7%
Sidechain outliers		7.9%
RSRZ outliers		1.0%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
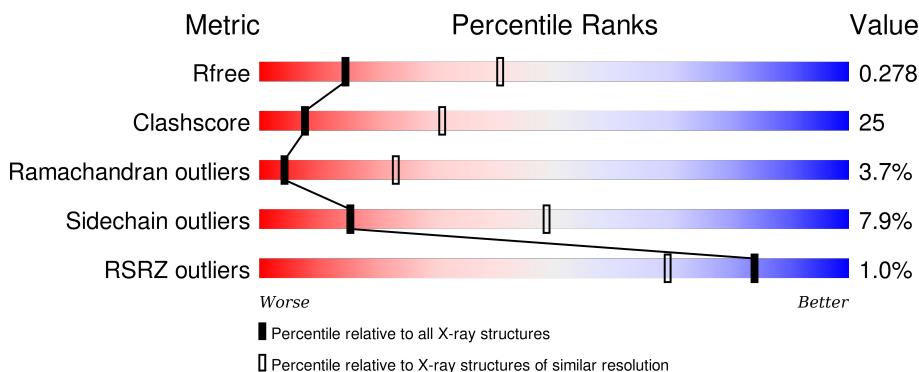
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	730	54%　　　40%　　　6% ·
1	B	730	54%　　　39%　　　6% ·
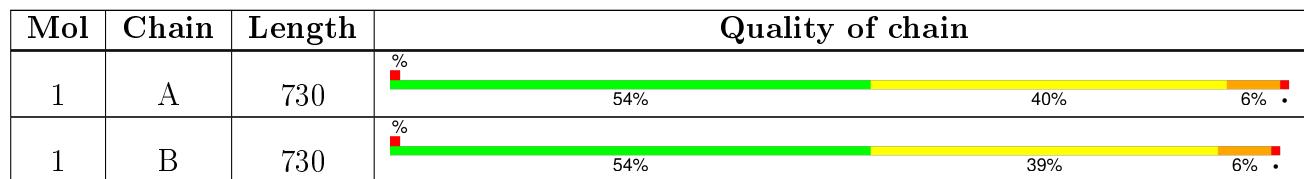
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AIA	A	768	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11858 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	730	Total 5920	C 3789	N 981	O 1124	S 26	0	0	0
1	B	730	Total 5920	C 3789	N 981	O 1124	S 26	0	0	0

- Molecule 2 is (1S)-2-[(2S,5R)-2-(AMINOMETHYL)-5-ETHYNYLPYRROLIDIN-1-YL]-1-CYCLOPENTYL-2-OXOETHANAMINE (three-letter code: AIA) (formula: $C_{14}H_{23}N_3O$).
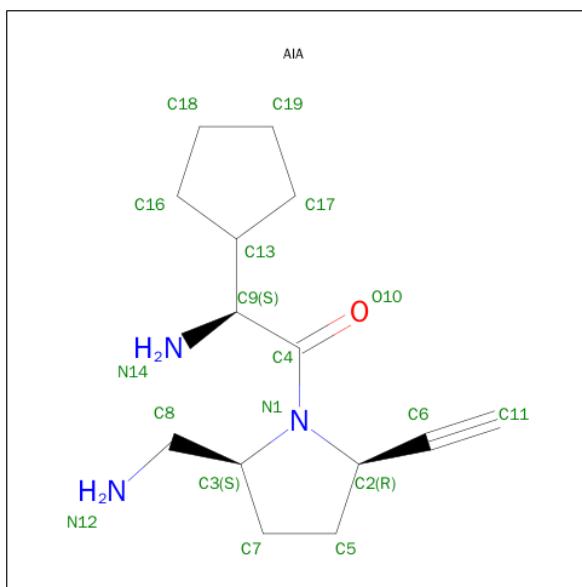
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 18	C 14	N 3	O 1	0	0

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 4
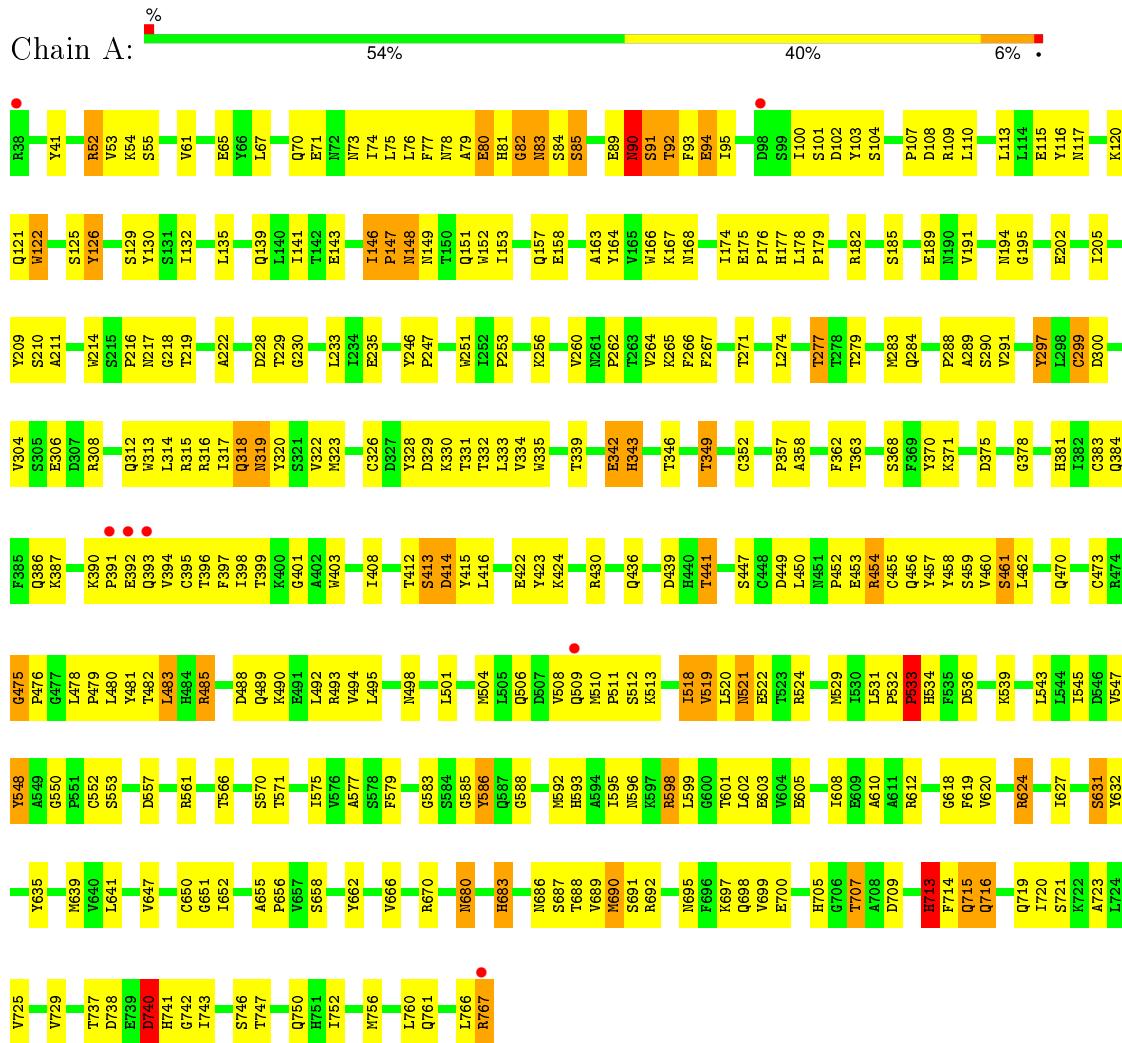
- Molecule 1: Dipeptidyl peptidase 4
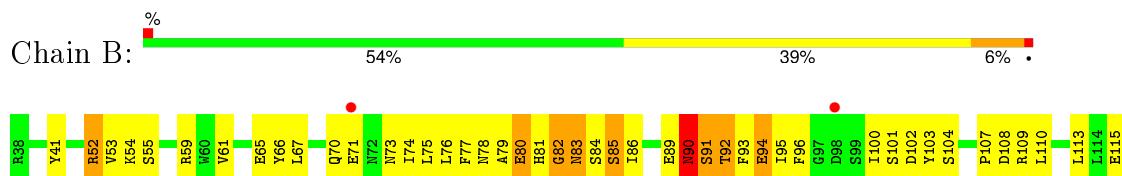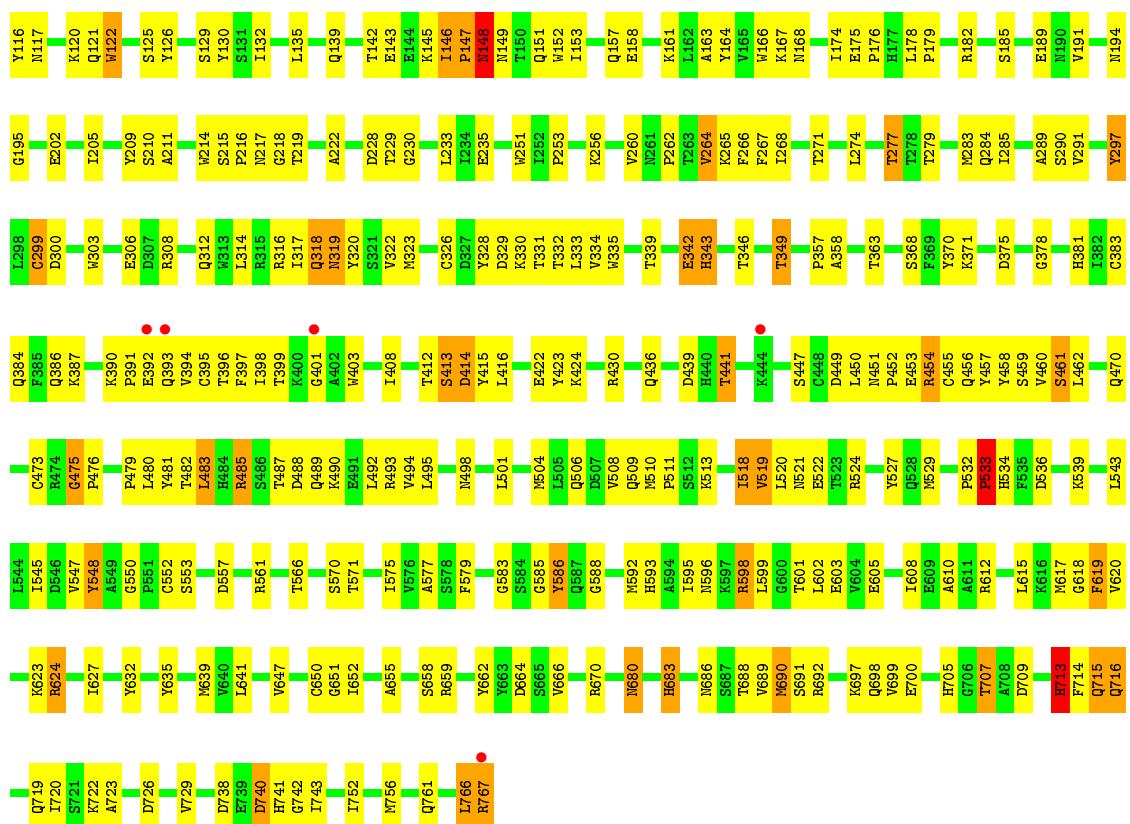
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	208.17Å 208.17Å 208.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.94 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.10) 99.3 (19.94-3.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.289 0.243 , 0.278	Depositor DCC
R_{free} test set	2743 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.3	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.54, < L^2 > = 0.38$	Xtriage
Outliers	1 of 53760 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11858	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	2/6088 (0.0%)	0.71	2/8278 (0.0%)
1	B	0.43	0/6088	0.70	2/8278 (0.0%)
All	All	0.45	2/12176 (0.0%)	0.71	4/16556 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	631	SER	C-O	8.88	1.40	1.23
1	A	352	CYS	CB-SG	-5.14	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	713	HIS	N-CA-C	7.29	130.67	111.00
1	A	713	HIS	N-CA-C	7.22	130.50	111.00
1	A	90	ASN	N-CA-C	-5.15	97.10	111.00
1	B	90	ASN	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5920	0	5631	294	0
1	B	5920	0	5632	292	0
2	A	18	0	21	0	0
All	All	11858	0	11284	584	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 25.

All (584) 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:761:GLN:HB3	1:A:767:ARG:HB3	1.39	1.03
1:B:349:THR:HB	1:B:593:HIS:HD2	1.26	0.99
1:A:460:VAL:HG22	1:A:461:SER:H	1.28	0.99
1:A:349:THR:HB	1:A:593:HIS:HD2	1.25	0.98
1:B:761:GLN:HB3	1:B:767:ARG:HB3	1.42	0.98
1:B:624:ARG:HB2	1:B:624:ARG:HH11	1.30	0.97
1:B:52:ARG:HB2	1:B:52:ARG:HH11	1.29	0.97
1:B:386:GLN:HG3	1:B:390:LYS:NZ	1.80	0.96
1:A:624:ARG:HB2	1:A:624:ARG:HH11	1.29	0.95
1:A:518:ILE:HD13	1:A:519:VAL:H	1.33	0.94
1:A:386:GLN:HG3	1:A:390:LYS:NZ	1.83	0.94
1:A:52:ARG:HH11	1:A:52:ARG:HB2	1.29	0.94
1:B:460:VAL:HG22	1:B:461:SER:H	1.29	0.94
1:A:54:LYS:H	1:A:498:ASN:HD21	1.17	0.92
1:A:383:CYS:HB3	1:A:397:PHE:HA	1.52	0.91
1:B:518:ILE:HD13	1:B:519:VAL:H	1.36	0.91
1:A:91:SER:HA	1:A:94:GLU:OE1	1.71	0.91
1:A:349:THR:HB	1:A:593:HIS:CD2	2.07	0.90
1:B:349:THR:HB	1:B:593:HIS:CD2	2.07	0.90
1:B:383:CYS:HB3	1:B:397:PHE:HA	1.54	0.89
1:A:151:GLN:HE22	1:A:168:ASN:H	1.17	0.89
1:B:151:GLN:HE22	1:B:168:ASN:H	1.20	0.89
1:B:91:SER:HA	1:B:94:GLU:OE1	1.73	0.87
1:A:412:THR:HG22	1:A:414:ASP:H	1.37	0.87
1:B:54:LYS:H	1:B:498:ASN:HD21	1.19	0.87
1:A:688:THR:HG22	1:A:691:SER:H	1.40	0.87
1:B:688:THR:HG22	1:B:691:SER:H	1.39	0.86
1:B:690:MET:CE	1:B:720:ILE:HA	2.08	0.84
1:B:412:THR:HG22	1:B:414:ASP:H	1.41	0.83
1:A:690:MET:CE	1:A:720:ILE:HA	2.09	0.82
1:A:79:ALA:O	1:A:80:GLU:HB2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:O	1:B:80:GLU:HB2	1.82	0.80
1:B:598:ARG:HB3	1:B:683:HIS:HD2	1.47	0.79
1:B:52:ARG:NH1	1:B:52:ARG:HB2	1.97	0.79
1:A:52:ARG:NH1	1:A:52:ARG:HB2	1.96	0.79
1:A:277:THR:HG21	1:A:279:THR:O	1.84	0.78
1:A:386:GLN:HG3	1:A:390:LYS:HZ1	1.48	0.78
1:A:235:GLU:OE2	1:A:251:TRP:HB3	1.84	0.78
1:A:598:ARG:HB3	1:A:683:HIS:HD2	1.48	0.78
1:B:235:GLU:OE2	1:B:251:TRP:HB3	1.83	0.77
1:A:460:VAL:HG22	1:A:461:SER:N	1.99	0.77
1:B:277:THR:HG21	1:B:279:THR:O	1.85	0.77
1:B:639:MET:CE	1:B:689:VAL:HA	2.16	0.76
1:B:384:GLN:HG3	1:B:398:ILE:HD11	1.66	0.76
1:A:384:GLN:HG3	1:A:398:ILE:HD11	1.66	0.76
1:B:483:LEU:HB3	1:B:495:LEU:HD11	1.68	0.75
1:B:235:GLU:HG2	1:B:251:TRP:HB3	1.67	0.75
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.66	0.75
1:A:639:MET:CE	1:A:689:VAL:HA	2.15	0.75
1:B:460:VAL:HG22	1:B:461:SER:N	2.01	0.75
1:A:518:ILE:HD13	1:A:519:VAL:N	2.02	0.74
1:A:121:GLN:O	1:A:125:SER:HB2	1.88	0.74
1:B:449:ASP:O	1:B:452:PRO:HD3	1.88	0.74
1:B:624:ARG:NH1	1:B:624:ARG:HB2	2.03	0.73
1:A:612:ARG:HG3	1:A:612:ARG:HH11	1.54	0.73
1:B:52:ARG:HH11	1:B:52:ARG:CB	2.02	0.73
1:A:624:ARG:HB2	1:A:624:ARG:NH1	2.04	0.72
1:B:612:ARG:HH11	1:B:612:ARG:HG3	1.54	0.72
1:A:52:ARG:HH11	1:A:52:ARG:CB	2.01	0.72
1:A:483:LEU:HB3	1:A:495:LEU:HD11	1.70	0.72
1:A:449:ASP:O	1:A:452:PRO:HD3	1.89	0.72
1:B:121:GLN:O	1:B:125:SER:HB2	1.90	0.72
1:B:485:ARG:HG3	1:B:485:ARG:O	1.89	0.72
1:B:151:GLN:HE21	1:B:167:LYS:H	1.38	0.72
1:B:688:THR:CG2	1:B:690:MET:HG2	2.19	0.72
1:B:386:GLN:HG3	1:B:390:LYS:HZ2	1.55	0.71
1:A:101:SER:HB3	1:A:115:GLU:HG2	1.72	0.71
1:A:586:TYR:CD1	1:A:586:TYR:N	2.57	0.71
1:A:80:GLU:H	1:A:493:ARG:HH22	1.38	0.71
1:A:151:GLN:HE21	1:A:167:LYS:H	1.39	0.71
1:A:485:ARG:HG3	1:A:485:ARG:O	1.90	0.70
1:A:54:LYS:H	1:A:498:ASN:ND2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TRP:CE3	1:B:422:GLU:HB2	2.27	0.69
1:A:688:THR:CG2	1:A:690:MET:HG2	2.21	0.69
1:B:386:GLN:HG3	1:B:390:LYS:HZ1	1.55	0.69
1:B:518:ILE:HD13	1:B:519:VAL:N	2.06	0.68
1:A:658:SER:H	1:A:716:GLN:NE2	1.91	0.68
1:A:108:ASP:OD2	1:A:110:LEU:HD12	1.93	0.68
1:A:439:ASP:OD1	1:A:441:THR:HB	1.93	0.68
1:B:54:LYS:H	1:B:498:ASN:ND2	1.90	0.68
1:B:108:ASP:OD2	1:B:110:LEU:HD12	1.93	0.68
1:B:80:GLU:H	1:B:493:ARG:HH22	1.41	0.68
1:A:107:PRO:HG2	1:A:158:GLU:O	1.94	0.68
1:B:101:SER:HB3	1:B:115:GLU:HG2	1.74	0.68
1:B:439:ASP:OD1	1:B:441:THR:HB	1.95	0.67
1:B:317:ILE:HG22	1:B:319:ASN:HB2	1.76	0.67
1:B:586:TYR:N	1:B:586:TYR:CD1	2.59	0.67
1:B:462:LEU:N	1:B:462:LEU:HD12	2.08	0.67
1:B:767:ARG:HH11	1:B:767:ARG:HG3	1.59	0.67
1:A:317:ILE:HG22	1:A:319:ASN:HB2	1.77	0.67
1:B:151:GLN:NE2	1:B:168:ASN:H	1.93	0.67
1:A:641:LEU:HD11	1:A:651:GLY:HA3	1.77	0.66
1:B:767:ARG:C	1:B:767:ARG:HD2	2.16	0.66
1:B:107:PRO:HG2	1:B:158:GLU:O	1.95	0.66
1:A:767:ARG:HG3	1:A:767:ARG:HH11	1.60	0.66
1:A:403:TRP:CE3	1:A:422:GLU:HB2	2.30	0.66
1:A:151:GLN:NE2	1:A:167:LYS:N	2.44	0.66
1:B:78:ASN:HB3	1:B:83:ASN:HB3	1.77	0.66
1:A:462:LEU:N	1:A:462:LEU:HD12	2.10	0.65
1:A:54:LYS:N	1:A:498:ASN:HD21	1.92	0.65
1:B:151:GLN:NE2	1:B:167:LYS:N	2.43	0.65
1:B:688:THR:HG23	1:B:690:MET:HG2	1.77	0.65
1:A:151:GLN:HE22	1:A:168:ASN:N	1.92	0.65
1:A:381:HIS:CD2	1:A:399:THR:HG22	2.30	0.65
1:B:151:GLN:HE22	1:B:168:ASN:N	1.94	0.65
1:B:598:ARG:HB3	1:B:683:HIS:CD2	2.31	0.65
1:B:454:ARG:NH1	1:B:480:LEU:HB2	2.12	0.65
1:A:235:GLU:CG	1:A:251:TRP:HB3	2.26	0.65
1:B:54:LYS:N	1:B:498:ASN:HD21	1.93	0.65
1:B:412:THR:HG22	1:B:413:SER:N	2.11	0.65
1:B:658:SER:H	1:B:716:GLN:NE2	1.94	0.65
1:A:598:ARG:HB3	1:A:683:HIS:CD2	2.33	0.64
1:A:130:TYR:HB2	1:A:146:ILE:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:CE2	1:A:284:GLN:HB2	2.33	0.64
1:B:235:GLU:CG	1:B:251:TRP:HB3	2.28	0.64
1:A:412:THR:HG22	1:A:413:SER:N	2.13	0.64
1:B:641:LEU:HD11	1:B:651:GLY:HA3	1.80	0.64
1:B:412:THR:CG2	1:B:413:SER:N	2.61	0.64
1:B:81:HIS:O	1:B:83:ASN:N	2.30	0.64
1:A:216:PRO:O	1:A:306:GLU:HG3	1.98	0.64
1:A:688:THR:HG23	1:A:690:MET:HG2	1.80	0.63
1:A:690:MET:HE1	1:A:720:ILE:HA	1.80	0.63
1:B:639:MET:HE3	1:B:689:VAL:HA	1.79	0.63
1:A:81:HIS:O	1:A:83:ASN:N	2.32	0.63
1:A:641:LEU:HD22	1:A:699:VAL:HG11	1.79	0.63
1:B:89:GLU:C	1:B:91:SER:N	2.51	0.62
1:A:151:GLN:NE2	1:A:168:ASN:H	1.93	0.62
1:B:267:PHE:CE2	1:B:284:GLN:HB2	2.33	0.62
1:A:89:GLU:C	1:A:91:SER:N	2.50	0.62
1:A:639:MET:HE3	1:A:689:VAL:HA	1.81	0.62
1:A:78:ASN:HB3	1:A:83:ASN:HB3	1.79	0.62
1:A:595:ILE:CG2	1:A:599:LEU:HD23	2.30	0.62
1:B:265:LYS:HG2	1:B:284:GLN:HE22	1.64	0.62
1:A:601:THR:HG22	1:A:602:LEU:N	2.15	0.62
1:B:601:THR:HG22	1:B:602:LEU:N	2.14	0.61
1:A:412:THR:CG2	1:A:413:SER:N	2.62	0.61
1:B:690:MET:HE1	1:B:720:ILE:HA	1.81	0.61
1:B:216:PRO:O	1:B:306:GLU:HG3	2.00	0.61
1:A:454:ARG:NH1	1:A:480:LEU:HB2	2.15	0.61
1:B:408:ILE:HG23	1:B:416:LEU:HD11	1.83	0.61
1:B:116:TYR:O	1:B:117:ASN:HB2	2.00	0.61
1:A:332:THR:O	1:A:334:VAL:HG23	2.01	0.61
1:B:151:GLN:HE21	1:B:167:LYS:N	1.99	0.61
1:B:146:ILE:HD12	1:B:153:ILE:HD12	1.83	0.61
1:A:460:VAL:CG2	1:A:461:SER:H	2.08	0.60
1:A:323:MET:O	1:A:342:GLU:O	2.20	0.60
1:B:460:VAL:CG2	1:B:461:SER:H	2.09	0.60
1:A:662:TYR:OH	1:A:719:GLN:HG2	2.01	0.60
1:B:401:GLY:HA3	1:B:403:TRP:NE1	2.16	0.60
1:A:235:GLU:HG2	1:A:251:TRP:CB	2.32	0.60
1:A:151:GLN:NE2	1:A:167:LYS:H	2.00	0.59
1:B:67:LEU:HD22	1:B:74:ILE:HG22	1.83	0.59
1:A:713:HIS:O	1:A:714:PHE:HB3	2.01	0.59
1:A:277:THR:CG2	1:A:279:THR:O	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ILE:CG2	1:B:599:LEU:HD23	2.31	0.59
1:A:447:SER:HB2	1:A:458:TYR:CE1	2.36	0.59
1:A:265:LYS:HG2	1:A:284:GLN:HE22	1.67	0.59
1:B:447:SER:HB2	1:B:458:TYR:CE1	2.38	0.59
1:A:767:ARG:HD2	1:A:767:ARG:C	2.22	0.59
1:A:91:SER:O	1:A:93:PHE:N	2.35	0.59
1:B:235:GLU:HG2	1:B:251:TRP:CB	2.33	0.59
1:A:125:SER:O	1:A:126:TYR:HB3	2.02	0.59
1:B:332:THR:O	1:B:334:VAL:HG23	2.03	0.59
1:B:91:SER:O	1:B:93:PHE:N	2.35	0.59
1:A:690:MET:HE1	1:A:720:ILE:CA	2.33	0.59
1:A:408:ILE:HG23	1:A:416:LEU:HD11	1.85	0.59
1:A:151:GLN:HE21	1:A:167:LYS:N	2.00	0.58
1:B:690:MET:HE1	1:B:720:ILE:CA	2.32	0.58
1:B:697:LYS:HG2	1:B:729:VAL:HG22	1.85	0.58
1:B:612:ARG:HG3	1:B:612:ARG:NH1	2.19	0.58
1:A:297:TYR:CE2	1:A:666:VAL:HG22	2.39	0.58
1:B:151:GLN:NE2	1:B:167:LYS:H	1.99	0.58
1:A:529:MET:HE2	1:A:575:ILE:HG21	1.86	0.58
1:B:381:HIS:CD2	1:B:399:THR:HG22	2.38	0.58
1:B:256:LYS:NZ	1:B:713:HIS:HD2	2.02	0.57
1:A:547:VAL:HG12	1:A:548:TYR:N	2.19	0.57
1:A:612:ARG:NH1	1:A:612:ARG:HG3	2.19	0.57
1:A:146:ILE:HD12	1:A:153:ILE:HD12	1.86	0.57
1:A:547:VAL:HG21	1:A:627:ILE:HD11	1.86	0.57
1:B:392:GLU:C	1:B:393:GLN:HG3	2.24	0.57
1:B:545:ILE:HG22	1:B:547:VAL:HG22	1.86	0.57
1:A:392:GLU:C	1:A:393:GLN:HG3	2.23	0.57
1:B:55:SER:HA	1:B:481:TYR:CE1	2.38	0.57
1:B:529:MET:HE2	1:B:575:ILE:HG21	1.87	0.57
1:B:297:TYR:CE2	1:B:666:VAL:HG22	2.40	0.57
1:B:488:ASP:O	1:B:489:GLN:HB2	2.05	0.57
1:B:511:PRO:HD3	1:B:570:SER:HB2	1.87	0.57
1:B:713:HIS:O	1:B:714:PHE:HB3	2.04	0.56
1:A:116:TYR:O	1:A:117:ASN:HB2	2.05	0.56
1:B:146:ILE:CD1	1:B:153:ILE:HD12	2.36	0.56
1:A:67:LEU:HD22	1:A:74:ILE:HG22	1.86	0.56
1:A:235:GLU:CD	1:A:251:TRP:HB3	2.26	0.56
1:B:641:LEU:HD22	1:B:699:VAL:HG11	1.85	0.56
1:B:323:MET:O	1:B:342:GLU:O	2.24	0.56
1:B:662:TYR:OH	1:B:719:GLN:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:SER:O	1:B:126:TYR:HB3	2.05	0.56
1:B:158:GLU:HG2	1:B:217:ASN:HA	1.87	0.56
1:A:697:LYS:HG2	1:A:729:VAL:HG22	1.87	0.56
1:A:158:GLU:HG2	1:A:217:ASN:HA	1.88	0.56
1:A:401:GLY:HA3	1:A:403:TRP:NE1	2.21	0.56
1:A:690:MET:HE2	1:A:719:GLN:O	2.06	0.56
1:A:386:GLN:HG3	1:A:390:LYS:HZ2	1.68	0.56
1:A:89:GLU:HB2	1:A:91:SER:HB3	1.88	0.56
1:A:256:LYS:NZ	1:A:713:HIS:HD2	2.03	0.56
1:A:381:HIS:CD2	1:A:399:THR:CG2	2.89	0.56
1:B:547:VAL:HG21	1:B:627:ILE:HD11	1.88	0.55
1:B:339:THR:O	1:B:342:GLU:HB2	2.06	0.55
1:A:256:LYS:HZ3	1:A:713:HIS:HD2	1.54	0.55
1:A:55:SER:HA	1:A:481:TYR:CE1	2.42	0.55
1:A:761:GLN:HB3	1:A:767:ARG:CB	2.26	0.55
1:B:256:LYS:HZ3	1:B:713:HIS:HD2	1.52	0.55
1:B:767:ARG:HG3	1:B:767:ARG:NH1	2.21	0.55
1:A:370:TYR:CE2	1:A:384:GLN:HG2	2.41	0.55
1:B:401:GLY:HA3	1:B:403:TRP:HE1	1.72	0.55
1:B:277:THR:CG2	1:B:279:THR:O	2.53	0.55
1:B:595:ILE:HD11	1:B:603:GLU:HB3	1.87	0.55
1:B:547:VAL:HG12	1:B:548:TYR:N	2.21	0.55
1:A:70:GLN:HG2	1:A:71:GLU:HG3	1.87	0.55
1:B:235:GLU:CD	1:B:251:TRP:HB3	2.27	0.55
1:A:339:THR:O	1:A:342:GLU:HB2	2.05	0.55
1:A:548:TYR:CD2	1:A:553:SER:HB2	2.42	0.55
1:B:707:THR:CG2	1:B:738:ASP:H	2.19	0.55
1:A:473:CYS:O	1:A:479:PRO:HA	2.07	0.55
1:B:548:TYR:CD2	1:B:553:SER:HB2	2.42	0.55
1:B:498:ASN:HB3	1:B:501:LEU:HB3	1.89	0.54
1:A:235:GLU:HG2	1:A:251:TRP:HA	1.89	0.54
1:B:235:GLU:HG2	1:B:251:TRP:HA	1.89	0.54
1:A:707:THR:CG2	1:A:738:ASP:H	2.19	0.54
1:B:79:ALA:O	1:B:80:GLU:CB	2.55	0.54
1:A:511:PRO:HD3	1:A:570:SER:HB2	1.88	0.54
1:B:473:CYS:O	1:B:479:PRO:HA	2.07	0.54
1:B:130:TYR:HB2	1:B:146:ILE:HD13	1.89	0.54
1:A:299:CYS:SG	1:A:314:LEU:HD22	2.48	0.54
1:A:652:ILE:HG21	1:A:756:MET:HE2	1.89	0.54
1:B:383:CYS:CB	1:B:397:PHE:HA	2.34	0.54
1:B:91:SER:CA	1:B:94:GLU:OE1	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:HG12	1:B:265:LYS:H	1.72	0.54
1:A:488:ASP:O	1:A:489:GLN:HB2	2.08	0.54
1:B:766:LEU:O	1:B:767:ARG:O	2.26	0.54
1:A:498:ASN:HB3	1:A:501:LEU:HB3	1.90	0.54
1:A:767:ARG:HG3	1:A:767:ARG:NH1	2.23	0.54
1:A:383:CYS:CB	1:A:397:PHE:HA	2.33	0.54
1:B:205:ILE:CD1	1:B:666:VAL:HG11	2.38	0.54
1:A:690:MET:HB3	1:A:723:ALA:HB2	1.90	0.54
1:A:264:VAL:HG12	1:A:265:LYS:H	1.73	0.53
1:B:690:MET:HE1	1:B:720:ILE:N	2.24	0.53
1:B:358:ALA:O	1:B:371:LYS:HE3	2.08	0.53
1:B:89:GLU:HB2	1:B:91:SER:HB3	1.89	0.53
1:A:485:ARG:NH2	1:A:490:LYS:HD3	2.23	0.53
1:A:545:ILE:HG22	1:A:547:VAL:HG22	1.89	0.53
1:B:482:THR:HG22	1:B:494:VAL:HG22	1.89	0.53
1:A:595:ILE:HD11	1:A:603:GLU:HB3	1.90	0.53
1:A:299:CYS:SG	1:A:357:PRO:HD2	2.48	0.53
1:A:205:ILE:CD1	1:A:666:VAL:HG11	2.39	0.53
1:A:415:TYR:HD2	1:A:436:GLN:HA	1.73	0.53
1:A:328:TYR:HB2	1:A:335:TRP:CH2	2.44	0.53
1:A:147:PRO:HG3	1:A:164:TYR:CE1	2.44	0.53
1:A:761:GLN:CB	1:A:767:ARG:HB3	2.24	0.53
1:B:147:PRO:HG3	1:B:164:TYR:CE1	2.45	0.53
1:B:81:HIS:C	1:B:83:ASN:H	2.13	0.53
1:A:219:THR:O	1:A:271:THR:HB	2.08	0.53
1:B:70:GLN:O	1:B:73:ASN:HB2	2.09	0.53
1:B:65:GLU:HB3	1:B:76:LEU:HD11	1.90	0.52
1:A:455:CYS:HA	1:A:475:GLY:HA3	1.91	0.52
1:B:454:ARG:HH11	1:B:480:LEU:HB2	1.75	0.52
1:B:415:TYR:HD2	1:B:436:GLN:HA	1.74	0.52
1:B:189:GLU:O	1:B:191:VAL:HG23	2.10	0.52
1:B:70:GLN:HG2	1:B:71:GLU:HG3	1.90	0.52
1:B:742:GLY:O	1:B:743:ILE:C	2.46	0.52
1:B:485:ARG:NH2	1:B:490:LYS:HD3	2.24	0.52
1:A:583:GLY:HA2	1:A:592:MET:O	2.09	0.52
1:A:65:GLU:HB3	1:A:76:LEU:HD11	1.91	0.52
1:A:79:ALA:O	1:A:80:GLU:CB	2.55	0.52
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.74	0.52
1:B:299:CYS:SG	1:B:314:LEU:HD22	2.50	0.52
1:B:752:ILE:O	1:B:756:MET:HG3	2.10	0.52
1:B:524:ARG:HH11	1:B:524:ARG:HG2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:ASN:HD21	1:B:683:HIS:CG	2.28	0.51
1:A:766:LEU:O	1:A:767:ARG:O	2.28	0.51
1:B:761:GLN:CB	1:B:767:ARG:HB3	2.27	0.51
1:B:398:ILE:HG22	1:B:398:ILE:O	2.10	0.51
1:A:752:ILE:O	1:A:756:MET:HG3	2.10	0.51
1:A:358:ALA:O	1:A:371:LYS:HE3	2.11	0.51
1:B:219:THR:O	1:B:271:THR:HB	2.09	0.51
1:B:229:THR:HG22	1:B:230:GLY:N	2.25	0.51
1:A:403:TRP:CD2	1:A:422:GLU:HB2	2.46	0.51
1:B:548:TYR:CE2	1:B:553:SER:HB2	2.45	0.51
1:B:205:ILE:HD13	1:B:666:VAL:HG11	1.92	0.51
1:A:320:TYR:CE2	1:A:322:VAL:HG23	2.45	0.51
1:B:328:TYR:HB2	1:B:335:TRP:CH2	2.45	0.51
1:B:652:ILE:HG21	1:B:756:MET:HE2	1.92	0.51
1:A:91:SER:CA	1:A:94:GLU:OE1	2.51	0.51
1:A:229:THR:HG22	1:A:230:GLY:N	2.24	0.51
1:B:370:TYR:CE2	1:B:384:GLN:HG2	2.46	0.51
1:B:320:TYR:CE2	1:B:322:VAL:HG23	2.46	0.51
1:B:767:ARG:C	1:B:767:ARG:CD	2.79	0.50
1:B:84:SER:O	1:B:85:SER:HB2	2.11	0.50
1:B:299:CYS:SG	1:B:357:PRO:HD2	2.51	0.50
1:B:690:MET:HE2	1:B:719:GLN:O	2.12	0.50
1:B:639:MET:O	1:B:692:ARG:NH1	2.44	0.50
1:B:403:TRP:CD2	1:B:422:GLU:HB2	2.46	0.50
1:A:680:ASN:HD21	1:A:683:HIS:CG	2.30	0.50
1:A:548:TYR:CE2	1:A:553:SER:HB2	2.46	0.50
1:B:543:LEU:HD12	1:B:575:ILE:O	2.12	0.50
1:B:75:LEU:HB2	1:B:77:PHE:HE1	1.76	0.50
1:B:147:PRO:HG3	1:B:164:TYR:HE1	1.76	0.50
1:A:456:GLN:OE1	1:A:476:PRO:HG2	2.12	0.50
1:A:129:SER:HB3	1:A:148:ASN:ND2	2.26	0.50
1:B:381:HIS:CD2	1:B:399:THR:CG2	2.95	0.49
1:B:690:MET:HB3	1:B:723:ALA:HB2	1.92	0.49
1:A:713:HIS:O	1:A:714:PHE:CB	2.61	0.49
1:B:412:THR:CG2	1:B:413:SER:H	2.25	0.49
1:B:583:GLY:HA2	1:B:592:MET:O	2.12	0.49
1:A:81:HIS:C	1:A:83:ASN:H	2.16	0.49
1:B:601:THR:HG22	1:B:602:LEU:H	1.77	0.49
1:A:205:ILE:HD13	1:A:666:VAL:HG11	1.93	0.49
1:A:398:ILE:O	1:A:398:ILE:HG22	2.12	0.49
1:A:401:GLY:HA3	1:A:403:TRP:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASP:HA	1:A:397:PHE:CZ	2.47	0.49
1:A:109:ARG:O	1:A:135:LEU:HD12	2.13	0.49
1:B:41:TYR:CD2	1:B:566:THR:HG22	2.47	0.49
1:B:455:CYS:HA	1:B:475:GLY:HA3	1.93	0.49
1:B:456:GLN:OE1	1:B:476:PRO:HG2	2.12	0.49
1:B:571:THR:O	1:B:571:THR:HG22	2.12	0.49
1:A:147:PRO:HG3	1:A:164:TYR:HE1	1.76	0.49
1:A:412:THR:CG2	1:A:413:SER:H	2.25	0.49
1:A:381:HIS:CG	1:A:399:THR:HG22	2.48	0.49
1:A:473:CYS:HB3	1:A:480:LEU:O	2.12	0.49
1:A:70:GLN:O	1:A:73:ASN:HB2	2.12	0.49
1:B:761:GLN:HB3	1:B:767:ARG:CB	2.28	0.48
1:A:624:ARG:HH11	1:A:624:ARG:CB	2.14	0.48
1:A:146:ILE:CD1	1:A:153:ILE:HD12	2.43	0.48
1:A:482:THR:HG22	1:A:494:VAL:HG22	1.94	0.48
1:B:174:ILE:N	1:B:174:ILE:HD12	2.28	0.48
1:A:690:MET:HB3	1:A:723:ALA:CB	2.44	0.48
1:A:334:VAL:HG12	1:A:335:TRP:N	2.28	0.48
1:A:41:TYR:CD2	1:A:566:THR:HG22	2.48	0.48
1:A:84:SER:O	1:A:85:SER:HB2	2.12	0.48
1:A:174:ILE:N	1:A:174:ILE:HD12	2.28	0.48
1:B:75:LEU:HB2	1:B:77:PHE:CE1	2.49	0.48
1:A:631:SER:HA	1:A:655:ALA:O	2.14	0.48
1:A:318:GLN:OE1	1:A:670:ARG:HD3	2.13	0.48
1:A:690:MET:HE1	1:A:720:ILE:N	2.29	0.48
1:A:485:ARG:HG2	1:A:490:LYS:HB3	1.96	0.48
1:A:102:ASP:OD1	1:A:103:TYR:N	2.40	0.48
1:B:113:LEU:HD23	1:B:132:ILE:HD13	1.95	0.48
1:B:109:ARG:O	1:B:135:LEU:HD12	2.13	0.48
1:A:228:ASP:OD1	1:A:262:PRO:HB3	2.14	0.48
1:A:233:LEU:HD23	1:A:253:PRO:HA	1.96	0.48
1:A:595:ILE:HG21	1:A:599:LEU:HD23	1.95	0.48
1:A:331:THR:HG22	1:A:332:THR:N	2.28	0.47
1:B:331:THR:HG22	1:B:332:THR:N	2.27	0.47
1:A:189:GLU:O	1:A:191:VAL:HG23	2.14	0.47
1:B:363:THR:HG23	1:B:368:SER:O	2.14	0.47
1:B:289:ALA:C	1:B:291:VAL:H	2.17	0.47
1:B:329:ASP:OD1	1:B:332:THR:N	2.47	0.47
1:A:543:LEU:HD12	1:A:575:ILE:O	2.14	0.47
1:A:742:GLY:O	1:A:743:ILE:C	2.51	0.47
1:A:639:MET:O	1:A:692:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:VAL:HG12	1:B:335:TRP:N	2.29	0.47
1:A:658:SER:H	1:A:716:GLN:HE21	1.60	0.47
1:B:473:CYS:HB3	1:B:480:LEU:O	2.15	0.47
1:A:601:THR:HG22	1:A:602:LEU:H	1.78	0.47
1:B:102:ASP:OD1	1:B:103:TYR:N	2.43	0.47
1:A:297:TYR:CE1	1:A:316:ARG:HA	2.50	0.47
1:B:462:LEU:CD1	1:B:462:LEU:N	2.76	0.47
1:B:328:TYR:HB2	1:B:335:TRP:CZ3	2.50	0.47
1:B:297:TYR:CE1	1:B:316:ARG:HA	2.50	0.47
1:A:289:ALA:C	1:A:291:VAL:H	2.18	0.47
1:A:163:ALA:HB2	1:A:214:TRP:CZ2	2.49	0.47
1:B:81:HIS:C	1:B:83:ASN:N	2.68	0.47
1:A:328:TYR:HB2	1:A:335:TRP:CZ3	2.50	0.47
1:A:299:CYS:SG	1:A:314:LEU:HB2	2.55	0.47
1:B:163:ALA:HB2	1:B:214:TRP:CZ2	2.50	0.46
1:A:195:GLY:C	1:A:211:ALA:HB3	2.35	0.46
1:A:363:THR:HG23	1:A:368:SER:O	2.14	0.46
1:A:647:VAL:HG12	1:A:647:VAL:O	2.14	0.46
1:B:233:LEU:HD23	1:B:253:PRO:HA	1.97	0.46
1:B:216:PRO:O	1:B:306:GLU:OE2	2.33	0.46
1:B:264:VAL:HG12	1:B:265:LYS:N	2.30	0.46
1:A:342:GLU:O	1:A:343:HIS:HB2	2.15	0.46
1:A:75:LEU:HB2	1:A:77:PHE:HE1	1.80	0.46
1:B:129:SER:HB3	1:B:148:ASN:ND2	2.29	0.46
1:B:680:ASN:ND2	1:B:683:HIS:HB2	2.31	0.46
1:B:378:GLY:O	1:B:588:GLY:HA2	2.15	0.46
1:B:195:GLY:C	1:B:211:ALA:HB3	2.35	0.46
1:A:168:ASN:O	1:A:194:ASN:HB2	2.15	0.46
1:B:713:HIS:O	1:B:714:PHE:CB	2.63	0.46
1:B:267:PHE:CD2	1:B:284:GLN:HB2	2.51	0.46
1:B:529:MET:HE2	1:B:575:ILE:CG2	2.46	0.46
1:B:386:GLN:HG3	1:B:390:LYS:CE	2.46	0.46
1:A:624:ARG:NH1	1:A:624:ARG:CB	2.76	0.46
1:B:639:MET:HE3	1:B:689:VAL:CA	2.45	0.46
1:A:709:ASP:OD2	1:A:741:HIS:HA	2.15	0.46
1:A:462:LEU:CD1	1:A:462:LEU:N	2.77	0.46
1:A:82:GLY:O	1:A:83:ASN:C	2.53	0.46
1:B:375:ASP:HA	1:B:397:PHE:CZ	2.50	0.46
1:A:264:VAL:HG12	1:A:265:LYS:N	2.30	0.46
1:B:299:CYS:SG	1:B:314:LEU:HB2	2.55	0.46
1:A:518:ILE:CD1	1:A:519:VAL:N	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASN:O	1:B:194:ASN:HB2	2.16	0.45
1:A:430:ARG:HG2	1:A:457:TYR:CE1	2.51	0.45
1:A:658:SER:HB2	1:A:690:MET:SD	2.57	0.45
1:A:267:PHE:CD2	1:A:284:GLN:HB2	2.50	0.45
1:B:595:ILE:HG22	1:B:599:LEU:HD23	1.96	0.45
1:B:92:THR:O	1:B:95:ILE:HG13	2.17	0.45
1:A:120:LYS:CG	1:A:121:GLN:N	2.79	0.45
1:B:601:THR:CG2	1:B:602:LEU:H	2.30	0.45
1:A:721:SER:O	1:A:725:VAL:HG23	2.17	0.45
1:A:182:ARG:HH21	1:A:185:SER:HA	1.81	0.45
1:A:737:THR:HB	1:B:722:LYS:HB2	1.98	0.45
1:B:709:ASP:OD2	1:B:741:HIS:HA	2.16	0.45
1:A:216:PRO:O	1:A:306:GLU:OE2	2.35	0.45
1:B:222:ALA:HB1	1:B:266:PHE:CZ	2.51	0.45
1:A:378:GLY:O	1:A:588:GLY:HA2	2.17	0.45
1:B:557:ASP:OD1	1:B:561:ARG:NH2	2.50	0.45
1:A:579:PHE:CD2	1:A:610:ALA:HB2	2.51	0.45
1:A:639:MET:HE3	1:A:689:VAL:CA	2.45	0.45
1:A:529:MET:HE2	1:A:575:ILE:CG2	2.46	0.45
1:A:415:TYR:CD2	1:A:436:GLN:HA	2.52	0.45
1:A:655:ALA:HA	1:A:705:HIS:CE1	2.51	0.45
1:B:82:GLY:O	1:B:83:ASN:C	2.54	0.45
1:B:690:MET:HB3	1:B:723:ALA:CB	2.46	0.45
1:A:370:TYR:OH	1:A:384:GLN:NE2	2.50	0.45
1:A:81:HIS:C	1:A:83:ASN:N	2.70	0.45
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.56	0.45
1:B:120:LYS:CG	1:B:121:GLN:N	2.79	0.45
1:B:312:GLN:HG2	1:B:323:MET:HG3	1.98	0.45
1:B:658:SER:HB2	1:B:690:MET:SD	2.57	0.45
1:A:680:ASN:ND2	1:A:683:HIS:HB2	2.32	0.45
1:A:595:ILE:HG22	1:A:599:LEU:HD23	1.98	0.45
1:B:91:SER:OG	1:B:92:THR:N	2.49	0.44
1:A:492:LEU:HB3	1:A:493:ARG:NH1	2.32	0.44
1:B:485:ARG:HG2	1:B:490:LYS:HB3	1.99	0.44
1:A:312:GLN:HG2	1:A:323:MET:HG3	1.98	0.44
1:B:579:PHE:CD2	1:B:610:ALA:HB2	2.52	0.44
1:B:618:GLY:O	1:B:620:VAL:N	2.47	0.44
1:B:228:ASP:OD1	1:B:262:PRO:HB3	2.17	0.44
1:A:557:ASP:OD1	1:A:561:ARG:NH2	2.49	0.44
1:A:509:GLN:O	1:A:533:PRO:HG3	2.17	0.44
1:B:506:GLN:HA	1:B:506:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.16	0.44
1:B:147:PRO:HB2	1:B:166:TRP:CD1	2.52	0.44
1:A:383:CYS:HB2	1:A:396:THR:O	2.17	0.44
1:A:84:SER:O	1:A:85:SER:CB	2.65	0.44
1:B:509:GLN:O	1:B:533:PRO:HG3	2.18	0.44
1:B:647:VAL:O	1:B:647:VAL:HG12	2.16	0.44
1:A:618:GLY:O	1:A:620:VAL:N	2.46	0.44
1:A:235:GLU:HG2	1:A:251:TRP:CA	2.48	0.44
1:B:84:SER:O	1:B:85:SER:CB	2.65	0.44
1:A:61:VAL:HG11	1:A:109:ARG:CD	2.48	0.44
1:A:113:LEU:HD23	1:A:132:ILE:HD13	2.00	0.44
1:A:386:GLN:HG3	1:A:390:LYS:CE	2.46	0.44
1:B:93:PHE:O	1:B:100:ILE:HG13	2.18	0.44
1:B:713:HIS:C	1:B:715:GLN:H	2.21	0.44
1:B:235:GLU:HG2	1:B:251:TRP:CA	2.48	0.44
1:A:75:LEU:HB2	1:A:77:PHE:CE1	2.52	0.44
1:A:93:PHE:O	1:A:100:ILE:HG13	2.18	0.44
1:A:147:PRO:HB2	1:A:166:TRP:CD1	2.53	0.44
1:A:524:ARG:CG	1:A:524:ARG:HH11	2.30	0.44
1:B:53:VAL:HG22	1:B:501:LEU:HD22	1.99	0.43
1:B:122:TRP:N	1:B:122:TRP:CE3	2.86	0.43
1:A:767:ARG:CD	1:A:767:ARG:C	2.87	0.43
1:B:125:SER:OG	1:B:202:GLU:OE1	2.35	0.43
1:B:423:TYR:CZ	1:B:424:LYS:HE3	2.52	0.43
1:A:506:GLN:OE1	1:A:506:GLN:HA	2.18	0.43
1:B:714:PHE:C	1:B:716:GLN:N	2.69	0.43
1:A:601:THR:CG2	1:A:602:LEU:H	2.31	0.43
1:A:529:MET:CE	1:A:575:ILE:HG21	2.47	0.43
1:B:659:ARG:HG2	1:B:662:TYR:CE2	2.53	0.43
1:B:492:LEU:HB3	1:B:493:ARG:NH1	2.32	0.43
1:A:552:CYS:HB2	1:A:592:MET:SD	2.59	0.43
1:A:329:ASP:OD1	1:A:332:THR:N	2.50	0.43
1:B:370:TYR:OH	1:B:384:GLN:NE2	2.50	0.43
1:A:125:SER:OG	1:A:202:GLU:OE1	2.35	0.43
1:A:550:GLY:HA2	1:A:632:TYR:CE2	2.53	0.43
1:A:122:TRP:CE3	1:A:122:TRP:N	2.86	0.43
1:A:120:LYS:HE3	1:A:740:ASP:OD2	2.19	0.43
1:B:157:GLN:HB2	1:B:158:GLU:OE2	2.19	0.43
1:A:605:GLU:O	1:A:608:ILE:N	2.49	0.43
1:B:386:GLN:O	1:B:387:LYS:C	2.57	0.43
1:A:690:MET:CE	1:A:720:ILE:CA	2.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLU:O	1:B:343:HIS:HB2	2.18	0.43
1:B:415:TYR:CD2	1:B:436:GLN:HA	2.53	0.43
1:A:747:THR:HG21	1:B:726:ASP:HA	2.01	0.43
1:A:386:GLN:O	1:A:387:LYS:C	2.57	0.43
1:A:92:THR:O	1:A:95:ILE:HG13	2.18	0.43
1:A:157:GLN:HB2	1:A:158:GLU:OE2	2.19	0.43
1:B:161:LYS:NZ	1:B:271:THR:HG21	2.34	0.43
1:A:520:LEU:O	1:A:522:GLU:N	2.51	0.43
1:A:714:PHE:C	1:A:716:GLN:N	2.72	0.43
1:A:317:ILE:C	1:A:319:ASN:H	2.21	0.43
1:A:529:MET:HG2	1:A:577:ALA:HB2	2.00	0.43
1:B:330:LYS:O	1:B:333:LEU:HD23	2.19	0.43
1:A:650:CYS:HB3	1:A:700:GLU:HB2	2.00	0.43
1:A:308:ARG:HA	1:A:326:CYS:O	2.19	0.43
1:B:715:GLN:HB3	1:B:715:GLN:HE21	1.58	0.43
1:B:217:ASN:HB2	1:B:306:GLU:OE2	2.19	0.43
1:B:182:ARG:HH21	1:B:185:SER:HA	1.84	0.43
1:A:508:VAL:HG12	1:A:510:MET:HE2	2.01	0.43
1:A:536:ASP:HB3	1:A:539:LYS:NZ	2.34	0.42
1:A:635:TYR:OH	1:A:687:SER:HB2	2.18	0.42
1:B:178:LEU:HB3	1:B:179:PRO:HD2	2.01	0.42
1:A:423:TYR:CZ	1:A:424:LYS:HE3	2.53	0.42
1:B:605:GLU:O	1:B:608:ILE:N	2.52	0.42
1:A:53:VAL:HG22	1:A:501:LEU:HD22	2.01	0.42
1:A:713:HIS:C	1:A:715:GLN:H	2.22	0.42
1:A:601:THR:CG2	1:A:602:LEU:N	2.77	0.42
1:B:583:GLY:HA3	1:B:595:ILE:HG13	2.02	0.42
1:A:222:ALA:HB1	1:A:266:PHE:CZ	2.55	0.42
1:A:412:THR:HG22	1:A:414:ASP:N	2.19	0.42
1:A:454:ARG:HH11	1:A:480:LEU:HB2	1.81	0.42
1:B:529:MET:CE	1:B:575:ILE:HG21	2.48	0.42
1:A:141:ILE:HG12	1:A:177:HIS:CE1	2.55	0.42
1:B:53:VAL:HG22	1:B:501:LEU:CD2	2.50	0.42
1:B:399:THR:HG23	1:B:403:TRP:CH2	2.55	0.42
1:A:61:VAL:HG11	1:A:109:ARG:HD3	2.02	0.42
1:A:583:GLY:HA3	1:A:595:ILE:HG13	2.00	0.42
1:B:650:CYS:HB3	1:B:700:GLU:HB2	2.02	0.42
1:B:308:ARG:HA	1:B:326:CYS:O	2.19	0.42
1:A:330:LYS:O	1:A:333:LEU:HD23	2.19	0.42
1:B:89:GLU:O	1:B:90:ASN:C	2.58	0.42
1:A:601:THR:HG22	1:A:602:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HB2	1:B:67:LEU:HB2	2.02	0.42
1:B:524:ARG:CG	1:B:524:ARG:HH11	2.31	0.42
1:B:66:TYR:CE1	1:B:77:PHE:HB2	2.55	0.42
1:B:132:ILE:HG21	1:B:176:PRO:HB3	2.00	0.42
1:A:521:ASN:O	1:A:522:GLU:HB2	2.20	0.42
1:B:142:THR:O	1:B:145:LYS:HE3	2.19	0.42
1:A:89:GLU:O	1:A:90:ASN:C	2.58	0.42
1:B:383:CYS:HB2	1:B:396:THR:O	2.20	0.42
1:B:536:ASP:HB3	1:B:539:LYS:NZ	2.34	0.42
1:B:655:ALA:HA	1:B:705:HIS:CE1	2.55	0.42
1:A:655:ALA:N	1:A:656:PRO:CD	2.83	0.42
1:B:688:THR:HG22	1:B:691:SER:N	2.21	0.42
1:B:152:TRP:CE2	1:B:210:SER:HB2	2.54	0.42
1:B:75:LEU:HD23	1:B:86:ILE:HA	2.02	0.41
1:B:527:TYR:HB3	1:B:579:PHE:HD1	1.85	0.41
1:A:571:THR:HG22	1:A:571:THR:O	2.20	0.41
1:A:152:TRP:CE2	1:A:210:SER:HB2	2.55	0.41
1:B:595:ILE:HG21	1:B:599:LEU:HD23	1.99	0.41
1:B:61:VAL:O	1:B:61:VAL:HG12	2.19	0.41
1:B:632:TYR:O	1:B:635:TYR:HB3	2.19	0.41
1:B:61:VAL:HG11	1:B:109:ARG:CD	2.50	0.41
1:A:532:PRO:O	1:A:533:PRO:O	2.38	0.41
1:B:430:ARG:HG2	1:B:457:TYR:CE1	2.54	0.41
1:A:454:ARG:NH1	1:A:478:LEU:O	2.53	0.41
1:B:552:CYS:HB2	1:B:592:MET:SD	2.61	0.41
1:A:61:VAL:HG12	1:A:61:VAL:O	2.20	0.41
1:A:132:ILE:HG21	1:A:176:PRO:HB3	2.02	0.41
1:B:166:TRP:O	1:B:167:LYS:HB2	2.21	0.41
1:B:449:ASP:O	1:B:451:ASN:N	2.54	0.41
1:B:529:MET:HG2	1:B:577:ALA:HB2	2.03	0.41
1:B:624:ARG:NH1	1:B:624:ARG:CB	2.78	0.41
1:B:707:THR:HG21	1:B:738:ASP:H	1.86	0.41
1:B:550:GLY:HA2	1:B:632:TYR:CE2	2.56	0.41
1:B:104:SER:HB3	1:B:113:LEU:HB2	2.02	0.41
1:B:532:PRO:O	1:B:533:PRO:O	2.39	0.41
1:A:178:LEU:HB3	1:A:179:PRO:HD2	2.02	0.41
1:B:520:LEU:O	1:B:522:GLU:N	2.54	0.41
1:A:304:VAL:HG22	1:A:362:PHE:CD1	2.55	0.41
1:B:623:LYS:HD3	1:B:623:LYS:HA	1.86	0.41
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.88	0.41
1:A:512:SER:OG	1:A:531:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:SER:O	1:A:750:GLN:HG3	2.21	0.41
1:A:53:VAL:HG22	1:A:501:LEU:CD2	2.50	0.40
1:B:508:VAL:HG12	1:B:510:MET:HE2	2.02	0.40
1:A:91:SER:OG	1:A:92:THR:N	2.51	0.40
1:A:513:LYS:HA	1:A:529:MET:O	2.21	0.40
1:A:104:SER:HB3	1:A:113:LEU:HB2	2.03	0.40
1:B:624:ARG:CB	1:B:624:ARG:HH11	2.16	0.40
1:B:518:ILE:CD1	1:B:519:VAL:N	2.80	0.40
1:B:473:CYS:HB3	1:B:480:LEU:H	1.87	0.40
1:B:41:TYR:HB2	1:B:510:MET:HE1	2.04	0.40
1:A:760:LEU:HA	1:A:760:LEU:HD23	1.97	0.40
1:B:215:SER:HB3	1:B:303:TRP:CZ2	2.56	0.40
1:B:268:ILE:HD11	1:B:285:ILE:HD11	2.03	0.40
1:A:288:PRO:HD2	1:A:313:TRP:CD1	2.56	0.40
1:A:246:TYR:HA	1:A:247:PRO:HD2	1.97	0.40
1:B:96:PHE:CB	1:B:100:ILE:HD11	2.52	0.40
1:B:513:LYS:HA	1:B:529:MET:O	2.22	0.40
1:A:315:ARG:HD2	1:A:320:TYR:HB3	2.02	0.40
1:B:615:LEU:HD23	1:B:620:VAL:CG1	2.51	0.40
1:B:617:MET:HE1	1:B:619:PHE:HZ	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	728/730 (100%)	614 (84%)	87 (12%)	27 (4%)	4	23
1	B	728/730 (100%)	615 (84%)	86 (12%)	27 (4%)	4	23
All	All	1456/1460 (100%)	1229 (84%)	173 (12%)	54 (4%)	4	23

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	143	GLU
1	A	450	LEU
1	A	521	ASN
1	A	533	PRO
1	A	585	GLY
1	A	619	PHE
1	A	713	HIS
1	B	80	GLU
1	B	143	GLU
1	B	450	LEU
1	B	533	PRO
1	B	585	GLY
1	B	619	PHE
1	B	713	HIS
1	A	82	GLY
1	A	85	SER
1	A	91	SER
1	A	92	THR
1	A	318	GLN
1	A	475	GLY
1	A	534	HIS
1	B	82	GLY
1	B	85	SER
1	B	91	SER
1	B	92	THR
1	B	218	GLY
1	B	318	GLN
1	B	461	SER
1	B	475	GLY
1	B	521	ASN
1	A	147	PRO
1	A	218	GLY
1	A	391	PRO
1	A	461	SER
1	B	147	PRO
1	B	391	PRO
1	B	534	HIS
1	B	596	ASN
1	A	83	ASN
1	A	290	SER
1	A	596	ASN
1	B	290	SER

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Mol	Chain	Res	Type
1	B	740	ASP
1	A	126	TYR
1	A	274	LEU
1	A	343	HIS
1	B	83	ASN
1	B	274	LEU
1	B	343	HIS
1	A	695	ASN
1	A	740	ASP
1	B	148	ASN
1	B	766	LEU

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	643/651 (99%)	594 (92%)	49 (8%)	16	51
1	B	643/651 (99%)	591 (92%)	52 (8%)	15	47
All	All	1286/1302 (99%)	1185 (92%)	101 (8%)	15	49

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	90	ASN
1	A	94	GLU
1	A	122	TRP
1	A	139	GLN
1	A	146	ILE
1	A	148	ASN
1	A	149	ASN
1	A	175	GLU
1	A	209	TYR
1	A	260	VAL
1	A	277	THR

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Mol	Chain	Res	Type
1	A	283	MET
1	A	297	TYR
1	A	299	CYS
1	A	300	ASP
1	A	319	ASN
1	A	342	GLU
1	A	346	THR
1	A	349	THR
1	A	394	VAL
1	A	395	CYS
1	A	413	SER
1	A	414	ASP
1	A	441	THR
1	A	453	GLU
1	A	454	ARG
1	A	459	SER
1	A	470	GLN
1	A	483	LEU
1	A	485	ARG
1	A	504	MET
1	A	518	ILE
1	A	519	VAL
1	A	533	PRO
1	A	548	TYR
1	A	586	TYR
1	A	598	ARG
1	A	624	ARG
1	A	680	ASN
1	A	683	HIS
1	A	686	ASN
1	A	690	MET
1	A	698	GLN
1	A	707	THR
1	A	715	GLN
1	A	716	GLN
1	A	740	ASP
1	A	767	ARG
1	B	52	ARG
1	B	90	ASN
1	B	94	GLU
1	B	122	TRP
1	B	139	GLN

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Mol	Chain	Res	Type
1	B	146	ILE
1	B	148	ASN
1	B	149	ASN
1	B	175	GLU
1	B	209	TYR
1	B	260	VAL
1	B	264	VAL
1	B	277	THR
1	B	283	MET
1	B	297	TYR
1	B	299	CYS
1	B	300	ASP
1	B	319	ASN
1	B	342	GLU
1	B	346	THR
1	B	349	THR
1	B	394	VAL
1	B	395	CYS
1	B	413	SER
1	B	414	ASP
1	B	441	THR
1	B	453	GLU
1	B	454	ARG
1	B	459	SER
1	B	470	GLN
1	B	483	LEU
1	B	485	ARG
1	B	487	THR
1	B	504	MET
1	B	518	ILE
1	B	519	VAL
1	B	533	PRO
1	B	548	TYR
1	B	586	TYR
1	B	598	ARG
1	B	624	ARG
1	B	664	ASP
1	B	680	ASN
1	B	683	HIS
1	B	686	ASN
1	B	690	MET
1	B	698	GLN

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Mol	Chain	Res	Type
1	B	707	THR
1	B	715	GLN
1	B	716	GLN
1	B	740	ASP
1	B	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	151	GLN
1	A	284	GLN
1	A	319	ASN
1	A	381	HIS
1	A	384	GLN
1	A	386	GLN
1	A	470	GLN
1	A	484	HIS
1	A	498	ASN
1	A	593	HIS
1	A	607	GLN
1	A	680	ASN
1	A	683	HIS
1	A	698	GLN
1	A	713	HIS
1	A	715	GLN
1	A	716	GLN
1	A	719	GLN
1	A	749	HIS
1	B	148	ASN
1	B	151	GLN
1	B	284	GLN
1	B	319	ASN
1	B	341	GLN
1	B	381	HIS
1	B	384	GLN
1	B	386	GLN
1	B	470	GLN
1	B	484	HIS
1	B	498	ASN
1	B	593	HIS
1	B	607	GLN

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Mol	Chain	Res	Type
1	B	680	ASN
1	B	683	HIS
1	B	698	GLN
1	B	713	HIS
1	B	715	GLN
1	B	716	GLN
1	B	719	GLN
1	B	749	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	AIA	A	768	1	17,19,19	1.40	2 (11%)	15,26,26	1.36	2 (13%)

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	AIA	A	768	1	-	0/14/36/36	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	768	AIA	C8-N12	-4.70	1.35	1.47
2	A	768	AIA	C4-N1	2.01	1.39	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	768	AIA	C7-C3-N1	2.27	104.32	101.93
2	A	768	AIA	C13-C9-C4	2.66	116.56	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	730/730 (100%)	-0.35	7 (0%)	84	69	32, 58, 91, 165	0
1	B	730/730 (100%)	-0.23	7 (0%)	84	69	35, 65, 104, 161	0
All	All	1460/1460 (100%)	-0.29	14 (0%)	84	69	32, 61, 99, 165	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	ARG	7.1
1	A	393	GLN	3.1
1	B	392	GLU	3.0
1	B	393	GLN	2.8
1	A	98	ASP	2.6
1	B	98	ASP	2.5
1	A	391	PRO	2.4
1	A	509	GLN	2.4
1	A	38	ARG	2.3
1	B	444	LYS	2.3
1	B	401	GLY	2.2
1	A	392	GLU	2.2
1	B	767	ARG	2.2
1	B	71	GLU	2.1

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	AIA	A	768	18/18	0.92	0.29	3.15	65,65,65,65	0

6.5　Other polymers (i)

There are no such residues in this entry.