Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:56 AM GMT

PDB ID	:	2OQI
Title	:	Human Dipeptidyl Peptidase IV (DPP4) with Piperidinone-constrained phenethylamine
Authors	:	Pei, Z.; Li, X.; von Geldern, T.W.; Longenecker, K.L.; Pireh, D.; Stewart, K.D.; Backes, B.J.; Lai, C.; Lubben, T.H.; Ballaron, S.J.; Beno, D.W.; Kempf-Grote, A.J.; Sham, H.L.; Trevillyan, J.M.
Deposited on	:	2007-01-31
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

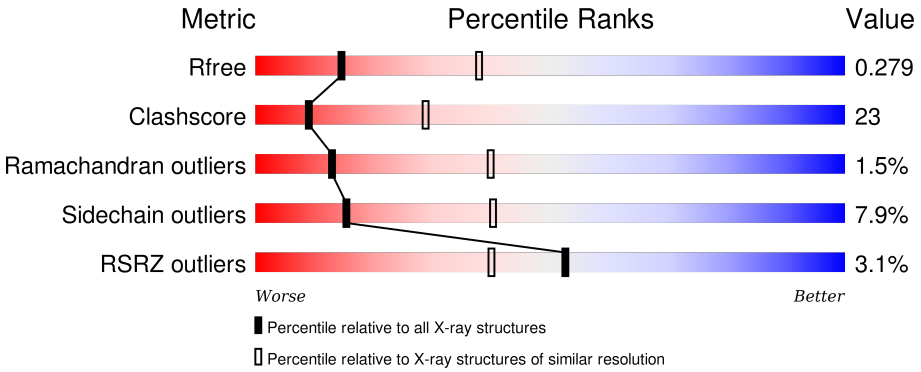
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	728	2% 60% 35% 5%
1	B	728	4% 61% 33% 5%
1	C	728	3% 55% 39% 5%
1	D	728	3% 56% 38% 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
2	GGO	B	901	-	-	-	X

2 Entry composition

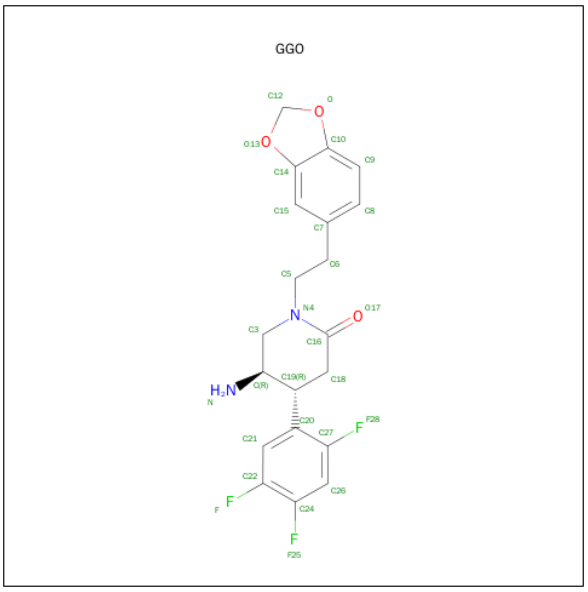
There are 2 unique types of molecules in this entry. The entry contains 23820 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	C	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	D	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			

- Molecule 2 is (4R,5R)-5-AMINO-1-[2-(1,3-BENZODIOXOL-5-YL)ETHYL]-4-(2,4,5-TRIFLUOROPHENYL)PIPERIDIN-2-ONE (three-letter code: GGO) (formula: $C_{20}H_{19}F_3N_2O_3$).



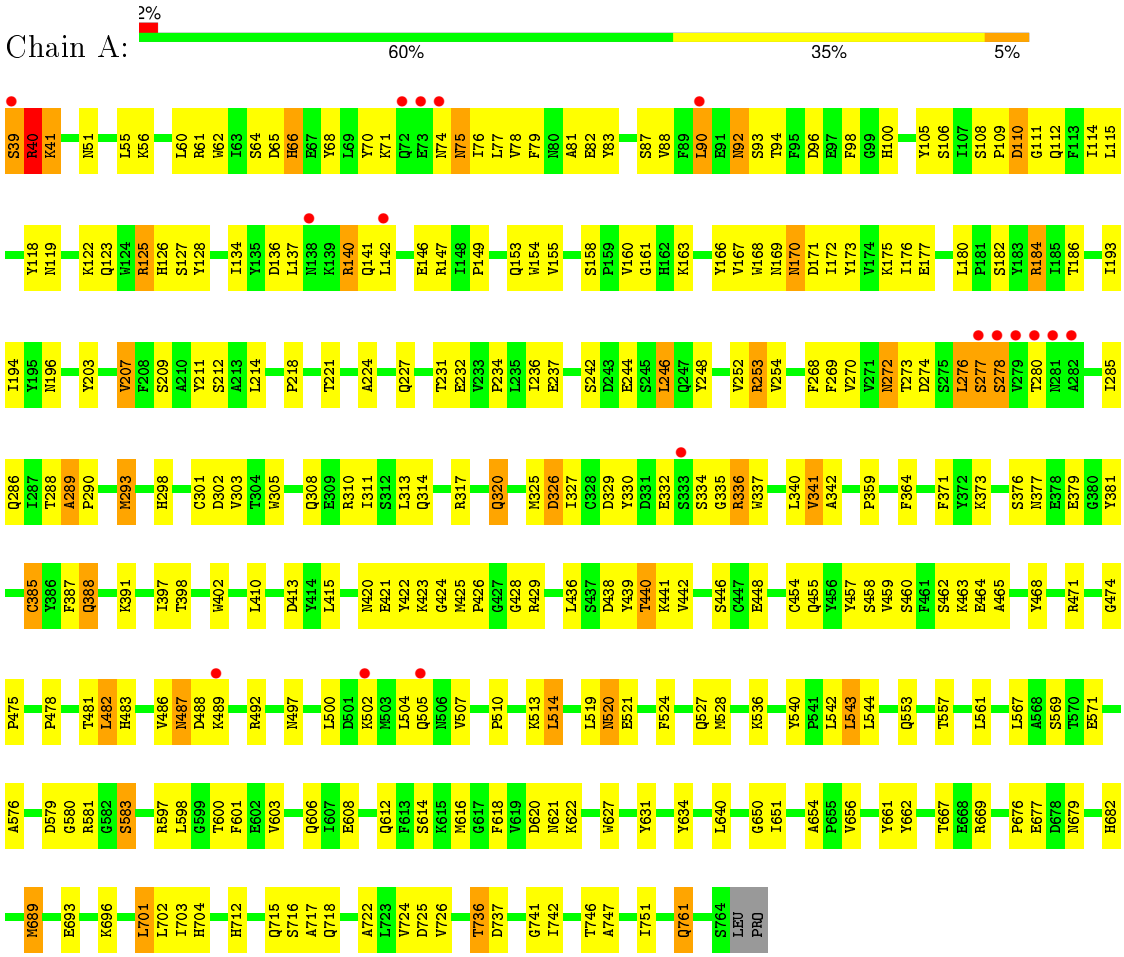
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

3 Residue-property plots (i)

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.

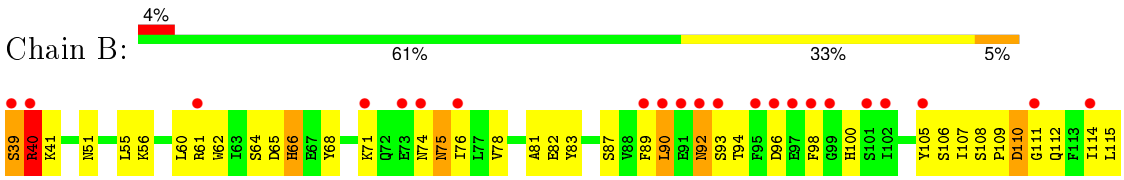
• Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)

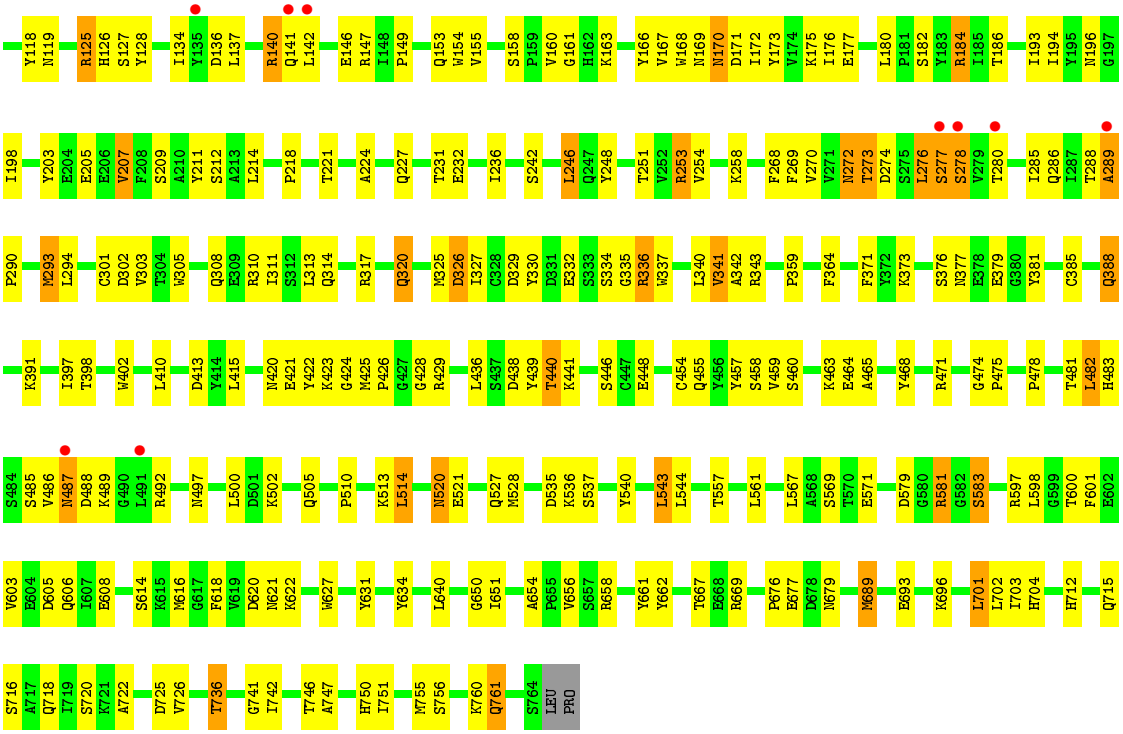
Chain A:



• Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)

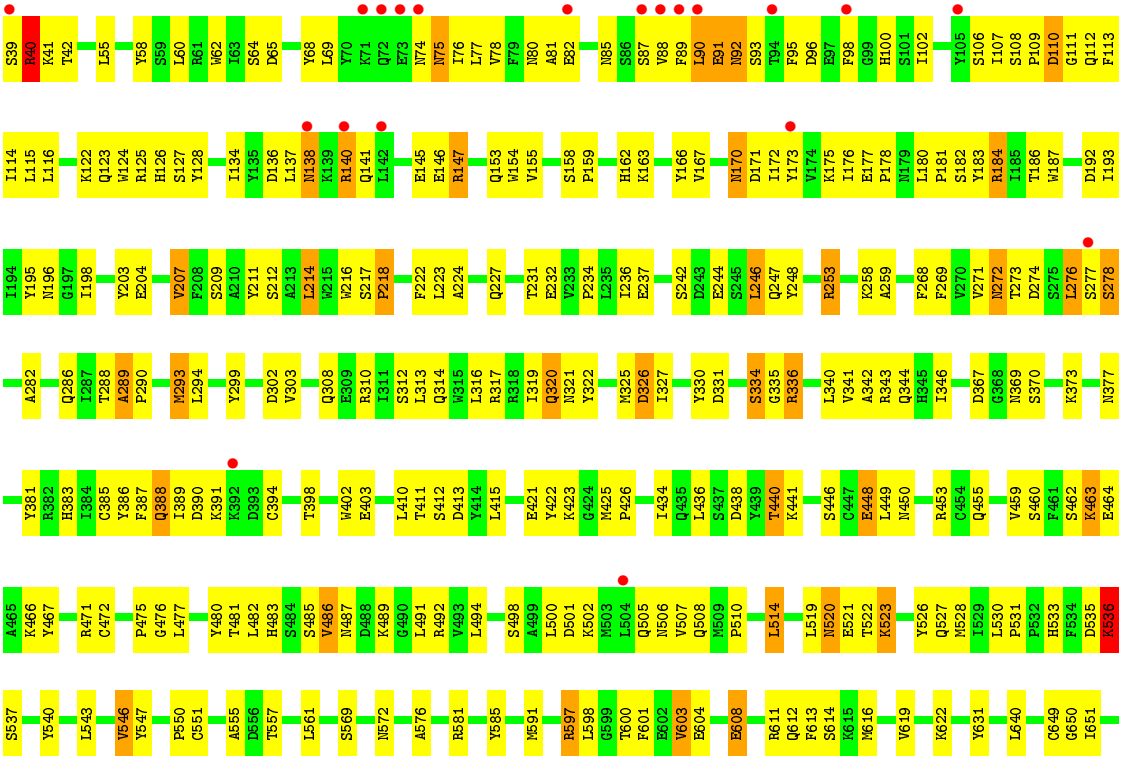
Chain B:

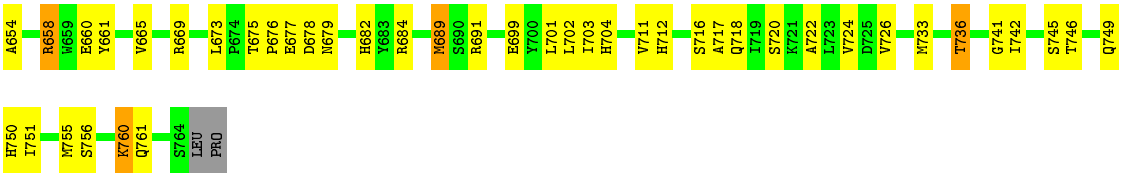




• Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)

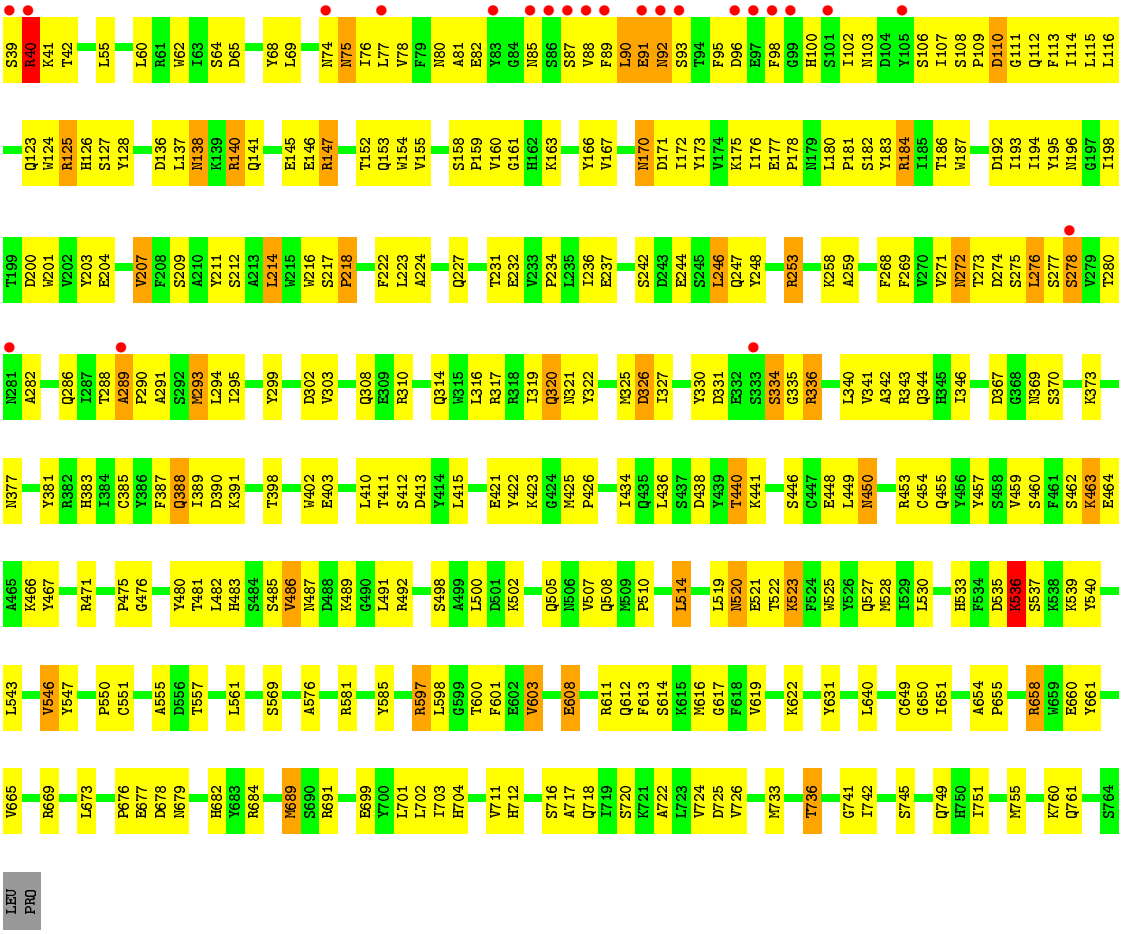
Chain C:





• Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.29Å 127.30Å 126.80Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 47.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (50.00-2.80) 90.0 (47.70-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.284 0.235 , 0.279	Depositor DCC
R_{free} test set	4148 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 83542 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23820	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GGO

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	0/6119	0.71	1/8321 (0.0%)
1	B	0.47	0/6119	0.70	1/8321 (0.0%)
1	C	0.45	0/6119	0.71	1/8321 (0.0%)
1	D	0.45	0/6119	0.71	1/8321 (0.0%)
All	All	0.46	0/24476	0.71	4/33284 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	341	VAL	N-CA-C	-6.23	94.18	111.00
1	B	341	VAL	N-CA-C	-5.78	95.39	111.00
1	D	214	LEU	CA-CB-CG	5.30	127.48	115.30
1	C	214	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5948	0	5667	261	0
1	B	5948	0	5667	251	0
1	C	5948	0	5667	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5948	0	5667	295	0
2	B	28	0	19	1	0
All	All	23820	0	22687	1074	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 23.

All (1074) 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:D:334:SER:HB3	1:D:336:ARG:NE	1.65	1.12
1:C:334:SER:HB3	1:C:336:ARG:NE	1.66	1.10
1:B:172:ILE:H	1:B:186:THR:HG22	1.18	1.09
1:B:39:SER:HB2	1:B:40:ARG:HE	1.18	1.08
1:D:334:SER:HB3	1:D:336:ARG:HE	0.95	1.06
1:C:334:SER:HB3	1:C:336:ARG:HE	0.95	1.06
1:A:172:ILE:H	1:A:186:THR:HG22	1.16	1.05
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.39	1.04
1:A:39:SER:HB2	1:A:40:ARG:HE	1.20	1.02
1:A:92:ASN:HD22	1:A:93:SER:N	1.57	1.02
1:B:92:ASN:HD22	1:B:93:SER:N	1.56	1.01
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.41	1.01
1:D:289:ALA:HB1	1:D:290:PRO:HA	1.44	0.98
1:D:172:ILE:H	1:D:186:THR:HG22	1.27	0.97
1:C:172:ILE:H	1:C:186:THR:HG22	1.27	0.97
1:C:289:ALA:HB1	1:C:290:PRO:HA	1.48	0.95
1:A:172:ILE:H	1:A:186:THR:CG2	1.79	0.94
1:B:172:ILE:H	1:B:186:THR:CG2	1.80	0.94
1:A:253:ARG:HH22	1:B:253:ARG:HH22	0.98	0.92
1:D:114:ILE:HD11	1:D:137:LEU:HD21	1.52	0.91
1:C:172:ILE:H	1:C:186:THR:CG2	1.84	0.89
1:D:293:MET:HE2	1:D:317:ARG:HG3	1.53	0.89
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.54	0.89
1:C:253:ARG:HH22	1:D:253:ARG:NH2	1.71	0.88
1:C:253:ARG:NH2	1:D:253:ARG:HH22	1.71	0.88
1:C:334:SER:CB	1:C:336:ARG:HE	1.86	0.88
1:C:253:ARG:HH22	1:D:253:ARG:HH22	0.89	0.87
1:C:293:MET:HE2	1:C:317:ARG:HG3	1.54	0.87
1:D:289:ALA:HB1	1:D:290:PRO:CA	2.03	0.86
1:D:172:ILE:H	1:D:186:THR:CG2	1.86	0.86
1:C:114:ILE:HD11	1:C:137:LEU:HD21	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.05	0.86
1:B:39:SER:CB	1:B:40:ARG:HE	1.89	0.85
1:C:289:ALA:HB1	1:C:290:PRO:CA	2.06	0.84
1:C:651:ILE:HG21	1:C:755:MET:HE3	1.59	0.84
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.07	0.84
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.77	0.83
1:D:93:SER:HA	1:D:96:ASP:OD1	1.79	0.83
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.61	0.82
1:B:293:MET:HE2	1:B:317:ARG:HG3	1.61	0.82
1:D:334:SER:CB	1:D:336:ARG:HE	1.86	0.82
1:A:341:VAL:O	1:A:342:ALA:HB3	1.78	0.82
1:B:114:ILE:HD11	1:B:137:LEU:HD21	1.62	0.82
1:B:76:ILE:HD12	1:B:90:LEU:HD11	1.59	0.82
1:B:341:VAL:O	1:B:342:ALA:HB3	1.81	0.81
1:D:614:SER:HA	1:D:619:VAL:HB	1.63	0.81
1:D:276:LEU:H	1:D:276:LEU:CD2	1.94	0.81
1:D:651:ILE:HG21	1:D:755:MET:HE3	1.61	0.80
1:A:39:SER:CB	1:A:40:ARG:HE	1.93	0.80
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.79	0.80
1:A:334:SER:HB3	1:A:336:ARG:NE	1.97	0.80
1:B:334:SER:HB3	1:B:336:ARG:NE	1.96	0.80
1:C:614:SER:HA	1:C:619:VAL:HB	1.64	0.79
1:D:76:ILE:HD12	1:D:90:LEU:HD11	1.63	0.79
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.64	0.79
1:A:293:MET:HE2	1:A:317:ARG:HG3	1.62	0.78
1:C:276:LEU:H	1:C:276:LEU:CD2	1.96	0.78
1:A:293:MET:CE	1:A:317:ARG:HG3	2.12	0.78
1:C:93:SER:HA	1:C:96:ASP:OD1	1.82	0.78
1:D:114:ILE:CD1	1:D:137:LEU:HD21	2.12	0.78
1:A:334:SER:HB3	1:A:336:ARG:HE	1.49	0.77
1:C:114:ILE:CD1	1:C:137:LEU:HD21	2.15	0.77
1:B:487:ASN:HB3	1:B:489:LYS:HG3	1.66	0.77
1:D:293:MET:CE	1:D:317:ARG:HG3	2.15	0.76
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.50	0.76
1:C:110:ASP:HB3	1:C:112:GLN:HB2	1.64	0.76
1:B:293:MET:CE	1:B:317:ARG:HG3	2.16	0.76
1:A:114:ILE:HD11	1:A:137:LEU:HD21	1.66	0.76
1:C:147:ARG:HG2	1:C:147:ARG:HH11	1.50	0.76
1:C:486:VAL:HG13	1:C:487:ASN:N	2.01	0.76
1:A:76:ILE:HB	1:A:90:LEU:HD13	1.68	0.76
1:D:147:ARG:HG2	1:D:147:ARG:HH11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.68	0.75
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.21	0.75
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.69	0.75
1:B:76:ILE:HB	1:B:90:LEU:HD13	1.69	0.75
1:D:486:VAL:HG13	1:D:487:ASN:N	2.01	0.75
1:D:77:LEU:HD23	1:D:88:VAL:HA	1.69	0.75
1:A:487:ASN:HB3	1:A:489:LYS:HG3	1.68	0.75
1:C:486:VAL:HG13	1:C:487:ASN:H	1.51	0.75
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.67	0.75
1:B:114:ILE:CD1	1:B:137:LEU:HD21	2.17	0.74
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.68	0.74
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.71	0.74
1:B:334:SER:HB3	1:B:336:ARG:HE	1.50	0.73
1:D:486:VAL:HG13	1:D:487:ASN:H	1.53	0.73
1:A:597:ARG:HG3	1:A:600:THR:HG21	1.71	0.73
1:D:502:LYS:O	1:D:505:GLN:HG2	1.89	0.73
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.19	0.73
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.19	0.72
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.82	0.72
1:A:438:ASP:OD1	1:A:440:THR:HB	1.90	0.72
1:A:455:GLN:HG3	1:A:475:PRO:CD	2.19	0.72
1:C:293:MET:CE	1:C:317:ARG:HG3	2.18	0.72
1:C:502:LYS:O	1:C:505:GLN:HG2	1.90	0.72
1:D:272:ASN:HD22	1:D:274:ASP:H	1.38	0.72
1:C:528:MET:HG2	1:C:576:ALA:HB2	1.71	0.72
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.05	0.71
1:C:77:LEU:HD23	1:C:88:VAL:HA	1.70	0.71
1:D:110:ASP:HB3	1:D:112:GLN:HB2	1.70	0.71
1:B:597:ARG:HG3	1:B:600:THR:HG21	1.72	0.71
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.91	0.71
1:D:176:ILE:HD11	1:D:276:LEU:HD21	1.72	0.71
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.91	0.71
1:B:171:ASP:OD1	1:B:186:THR:HG23	1.90	0.71
1:B:455:GLN:HG3	1:B:475:PRO:CD	2.21	0.71
1:A:74:ASN:C	1:A:92:ASN:HB3	2.12	0.70
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.90	0.70
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.72	0.70
1:B:693:GLU:OE1	1:B:696:LYS:HE2	1.92	0.70
1:B:231:THR:HG22	1:B:232:GLU:HG3	1.72	0.70
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.73	0.70
1:A:693:GLU:OE1	1:A:696:LYS:HE2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:ARG:HG2	1:D:480:TYR:CD2	2.26	0.70
1:C:276:LEU:HD22	1:C:276:LEU:H	1.57	0.70
1:D:276:LEU:HD22	1:D:276:LEU:H	1.56	0.70
1:A:377:ASN:HB2	1:A:381:TYR:O	1.92	0.70
1:A:231:THR:HG22	1:A:232:GLU:HG3	1.74	0.70
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.71	0.70
1:B:438:ASP:OD1	1:B:440:THR:HB	1.90	0.70
1:C:331:ASP:HB3	1:C:334:SER:HB2	1.74	0.69
1:D:528:MET:HG2	1:D:576:ALA:HB2	1.72	0.69
1:B:76:ILE:HB	1:B:90:LEU:CD1	2.21	0.69
1:C:176:ILE:HD11	1:C:276:LEU:HD21	1.72	0.69
1:B:455:GLN:HG3	1:B:475:PRO:HD2	1.73	0.69
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.07	0.69
1:D:438:ASP:OD2	1:D:440:THR:HG22	1.91	0.69
1:A:455:GLN:HG3	1:A:475:PRO:HD2	1.72	0.69
1:C:183:TYR:HE1	1:C:277:SER:O	1.75	0.69
1:A:39:SER:HB2	1:A:40:ARG:NE	2.03	0.69
1:A:341:VAL:O	1:A:342:ALA:CB	2.41	0.69
1:A:108:SER:C	1:A:110:ASP:H	1.96	0.69
1:B:74:ASN:C	1:B:92:ASN:HB3	2.13	0.69
1:C:277:SER:O	1:C:278:SER:HB3	1.93	0.68
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.75	0.68
1:B:377:ASN:HB2	1:B:381:TYR:O	1.93	0.68
1:D:289:ALA:CB	1:D:290:PRO:HA	2.22	0.68
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.24	0.68
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.92	0.68
1:B:108:SER:C	1:B:110:ASP:H	1.96	0.68
1:D:415:LEU:HB3	1:D:434:ILE:HG22	1.76	0.68
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.74	0.67
1:D:277:SER:O	1:D:278:SER:HB3	1.95	0.67
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.74	0.67
1:B:273:THR:HA	1:B:276:LEU:HD13	1.75	0.67
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.91	0.67
1:D:272:ASN:ND2	1:D:274:ASP:H	1.92	0.67
1:D:334:SER:HB3	1:D:336:ARG:CD	2.25	0.67
1:B:140:ARG:HG2	1:B:140:ARG:HH11	1.59	0.67
1:C:528:MET:HE2	1:C:530:LEU:HD21	1.76	0.67
1:B:173:TYR:CE2	1:B:184:ARG:HG2	2.30	0.67
1:A:74:ASN:HB3	1:A:92:ASN:OD1	1.96	0.66
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.95	0.66
1:D:612:GLN:O	1:D:616:MET:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:GLN:O	1:C:616:MET:HG3	1.95	0.66
1:C:272:ASN:ND2	1:C:274:ASP:H	1.94	0.66
1:B:172:ILE:N	1:B:186:THR:HG22	2.01	0.66
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.77	0.66
1:C:415:LEU:HB3	1:C:434:ILE:HG22	1.78	0.66
1:D:341:VAL:C	1:D:343:ARG:H	1.99	0.66
1:D:76:ILE:HB	1:D:90:LEU:CD1	2.25	0.66
1:C:272:ASN:HD22	1:C:274:ASP:H	1.41	0.66
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.78	0.66
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.94	0.66
1:B:39:SER:HB2	1:B:40:ARG:NE	2.02	0.65
1:C:341:VAL:C	1:C:343:ARG:H	1.99	0.65
1:A:273:THR:HA	1:A:276:LEU:HD13	1.77	0.65
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.31	0.65
1:B:170:ASN:O	1:B:196:ASN:HB2	1.97	0.65
1:A:172:ILE:N	1:A:186:THR:HG22	2.01	0.65
1:A:289:ALA:CB	1:A:290:PRO:HA	2.22	0.65
1:C:334:SER:HB3	1:C:336:ARG:CD	2.26	0.65
1:C:289:ALA:CB	1:C:290:PRO:HA	2.25	0.65
1:D:183:TYR:HE1	1:D:277:SER:O	1.80	0.65
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.96	0.65
1:D:704:HIS:HD2	1:D:716:SER:OG	1.80	0.64
1:D:170:ASN:N	1:D:170:ASN:HD22	1.95	0.64
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.78	0.64
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.80	0.64
1:B:92:ASN:ND2	1:B:93:SER:N	2.39	0.64
1:B:334:SER:HB3	1:B:336:ARG:CD	2.28	0.64
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.33	0.63
1:B:676:PRO:HG2	1:B:677:GLU:OE2	1.98	0.63
1:D:410:LEU:HD13	1:D:415:LEU:HD23	1.80	0.63
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.83	0.63
1:D:613:PHE:O	1:D:616:MET:HB2	1.98	0.63
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.29	0.63
1:D:115:LEU:HD21	1:D:155:VAL:HG11	1.80	0.63
1:A:334:SER:HB3	1:A:336:ARG:CD	2.29	0.63
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.14	0.63
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.81	0.63
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.80	0.63
1:A:290:PRO:HG3	1:A:326:ASP:OD2	1.98	0.63
1:D:289:ALA:CB	1:D:290:PRO:CA	2.76	0.63
1:A:170:ASN:O	1:A:196:ASN:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.14	0.63
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.29	0.62
1:C:341:VAL:HG22	1:C:342:ALA:N	2.13	0.62
1:C:438:ASP:OD2	1:C:440:THR:HG22	1.99	0.62
1:A:170:ASN:N	1:A:170:ASN:HD22	1.95	0.62
1:B:90:LEU:O	1:B:90:LEU:HD22	2.00	0.62
1:D:676:PRO:HG2	1:D:677:GLU:OE2	2.00	0.62
1:D:276:LEU:N	1:D:276:LEU:CD2	2.63	0.61
1:B:170:ASN:N	1:B:170:ASN:HD22	1.96	0.61
1:B:160:VAL:HG23	1:B:161:GLY:N	2.14	0.61
1:C:276:LEU:N	1:C:276:LEU:CD2	2.63	0.61
1:C:455:GLN:HG3	1:C:475:PRO:HD2	1.82	0.61
1:B:289:ALA:CB	1:B:290:PRO:HA	2.24	0.61
1:D:74:ASN:O	1:D:92:ASN:HB3	2.00	0.61
1:D:388:GLN:CB	1:D:391:LYS:HB2	2.31	0.61
1:D:341:VAL:HG22	1:D:342:ALA:N	2.14	0.61
1:D:455:GLN:HG3	1:D:475:PRO:HD2	1.83	0.61
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.00	0.61
1:D:528:MET:HE2	1:D:530:LEU:HD21	1.83	0.61
1:C:246:LEU:HD22	1:C:248:TYR:O	2.01	0.61
1:D:528:MET:CE	1:D:530:LEU:HD21	2.30	0.61
1:C:108:SER:C	1:C:110:ASP:H	2.04	0.61
1:B:92:ASN:HD22	1:B:93:SER:H	1.47	0.61
1:C:115:LEU:HD21	1:C:155:VAL:HG11	1.83	0.61
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.31	0.60
1:C:289:ALA:CB	1:C:290:PRO:CA	2.79	0.60
1:B:341:VAL:O	1:B:342:ALA:CB	2.46	0.60
1:C:613:PHE:O	1:C:616:MET:HB2	2.01	0.60
1:D:192:ASP:O	1:D:193:ILE:HD13	2.00	0.60
1:B:290:PRO:HG3	1:B:326:ASP:OD2	2.00	0.60
1:A:111:GLY:O	1:A:137:LEU:HD12	2.02	0.60
1:A:272:ASN:C	1:A:272:ASN:HD22	2.05	0.60
1:B:81:ALA:O	1:B:492:ARG:NH2	2.33	0.60
1:C:340:LEU:O	1:C:343:ARG:HB3	2.01	0.60
1:B:272:ASN:C	1:B:272:ASN:HD22	2.05	0.60
1:C:388:GLN:CB	1:C:391:LYS:HB2	2.32	0.60
1:D:325:MET:O	1:D:344:GLN:HB2	2.02	0.60
1:D:146:GLU:OE1	1:D:181:PRO:HA	2.02	0.60
1:C:39:SER:O	1:C:40:ARG:HD2	2.02	0.60
1:C:528:MET:CE	1:C:530:LEU:HD21	2.32	0.60
1:D:39:SER:O	1:D:40:ARG:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ASN:O	1:B:521:GLU:HB2	2.01	0.60
1:B:92:ASN:C	1:B:92:ASN:HD22	2.05	0.60
1:C:203:TYR:HA	1:C:207:VAL:HG13	1.83	0.60
1:B:325:MET:CE	1:B:327:ILE:HD11	2.32	0.60
1:C:411:THR:C	1:C:413:ASP:H	2.06	0.60
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.32	0.60
1:B:334:SER:CB	1:B:336:ARG:HD2	2.32	0.59
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.17	0.59
1:A:579:ASP:HB3	1:A:583:SER:OG	2.01	0.59
1:C:704:HIS:HD2	1:C:716:SER:OG	1.85	0.59
1:D:340:LEU:O	1:D:343:ARG:HB3	2.02	0.59
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.84	0.59
1:A:334:SER:CB	1:A:336:ARG:HD2	2.32	0.59
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.84	0.59
1:C:377:ASN:HB2	1:C:381:TYR:O	2.01	0.59
1:B:111:GLY:O	1:B:137:LEU:HD12	2.03	0.59
1:C:192:ASP:O	1:C:193:ILE:HD13	2.02	0.59
1:A:325:MET:CE	1:A:327:ILE:HD11	2.31	0.59
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.84	0.59
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.84	0.59
1:A:90:LEU:O	1:A:90:LEU:HD22	2.02	0.58
1:A:520:ASN:O	1:A:521:GLU:HB2	2.03	0.58
1:C:325:MET:O	1:C:344:GLN:HB2	2.03	0.58
1:A:78:VAL:HG12	1:A:87:SER:O	2.03	0.58
1:B:115:LEU:HD12	1:B:134:ILE:HG12	1.84	0.58
1:D:109:PRO:HG3	1:D:158:SER:O	2.03	0.58
1:C:471:ARG:HG2	1:C:480:TYR:HD2	1.68	0.58
1:A:160:VAL:HG23	1:A:161:GLY:N	2.19	0.58
1:D:39:SER:O	1:D:40:ARG:O	2.20	0.58
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.85	0.58
1:C:183:TYR:CE1	1:C:277:SER:O	2.56	0.58
1:A:301:CYS:SG	1:A:359:PRO:HG2	2.44	0.58
1:C:411:THR:O	1:C:413:ASP:N	2.36	0.58
1:A:459:VAL:HG22	1:A:460:SER:N	2.18	0.58
1:C:720:SER:O	1:C:724:VAL:HG23	2.04	0.58
1:A:81:ALA:O	1:A:492:ARG:NH2	2.37	0.58
1:D:108:SER:C	1:D:110:ASP:H	2.07	0.58
1:C:146:GLU:OE1	1:C:181:PRO:HA	2.03	0.58
1:B:78:VAL:HG12	1:B:87:SER:O	2.03	0.58
1:B:74:ASN:HB3	1:B:92:ASN:OD1	2.03	0.58
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASN:CB	1:A:489:LYS:HG3	2.34	0.58
1:C:146:GLU:O	1:C:175:LYS:HE2	2.03	0.58
1:D:377:ASN:HB2	1:D:381:TYR:O	2.03	0.58
1:C:170:ASN:HD22	1:C:170:ASN:N	2.00	0.58
1:C:81:ALA:O	1:C:492:ARG:NH2	2.23	0.58
1:D:177:GLU:CG	1:D:180:LEU:HD22	2.34	0.58
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.03	0.57
1:A:289:ALA:CB	1:A:290:PRO:CA	2.79	0.57
1:B:314:GLN:HE22	1:B:373:LYS:NZ	2.01	0.57
1:C:411:THR:C	1:C:413:ASP:N	2.58	0.57
1:D:177:GLU:HB2	1:D:180:LEU:HD22	1.87	0.57
1:A:82:GLU:HG2	1:A:83:TYR:CZ	2.39	0.57
1:C:93:SER:HB2	1:C:96:ASP:OD2	2.05	0.57
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.39	0.57
1:A:172:ILE:N	1:A:186:THR:CG2	2.61	0.57
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.05	0.57
1:D:82:GLU:HB2	1:D:467:TYR:OH	2.03	0.57
1:B:579:ASP:HB3	1:B:583:SER:OG	2.04	0.57
1:A:237:GLU:OE1	1:B:251:THR:OG1	2.19	0.57
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.04	0.57
1:C:88:VAL:HG11	1:C:91:GLU:OE2	2.05	0.57
1:D:136:ASP:OD1	1:D:138:ASN:HB2	2.05	0.57
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.40	0.57
1:A:92:ASN:HD22	1:A:92:ASN:C	2.08	0.57
1:A:92:ASN:HD22	1:A:93:SER:H	1.44	0.57
1:C:74:ASN:O	1:C:92:ASN:HB3	2.05	0.57
1:D:242:SER:HB3	1:D:246:LEU:HD12	1.86	0.57
1:D:246:LEU:HD22	1:D:248:TYR:O	2.04	0.57
1:C:600:THR:O	1:C:603:VAL:HG13	2.06	0.56
1:D:93:SER:HB2	1:D:96:ASP:OD2	2.06	0.56
1:C:377:ASN:HB2	1:C:381:TYR:H	1.70	0.56
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.40	0.56
1:D:411:THR:C	1:D:413:ASP:H	2.09	0.56
1:D:93:SER:HA	1:D:96:ASP:CG	2.25	0.56
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.40	0.56
1:D:370:SER:HB3	1:D:388:GLN:NE2	2.20	0.56
1:B:193:ILE:HG22	1:B:194:ILE:HG13	1.86	0.56
1:D:146:GLU:O	1:D:175:LYS:HE2	2.05	0.56
1:C:341:VAL:HG22	1:C:342:ALA:H	1.70	0.56
1:A:65:ASP:HB3	1:A:66:HIS:CE1	2.40	0.56
1:C:736:THR:HG21	1:D:717:ALA:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLN:HB3	1:C:211:TYR:CE2	2.41	0.56
1:C:272:ASN:HD22	1:C:272:ASN:C	2.08	0.56
1:B:272:ASN:HD22	1:B:274:ASP:H	1.53	0.56
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.56
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.88	0.56
1:B:172:ILE:N	1:B:186:THR:CG2	2.62	0.56
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.40	0.56
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.88	0.56
1:A:334:SER:HB3	1:A:336:ARG:HD2	1.88	0.55
1:C:93:SER:HA	1:C:96:ASP:CG	2.26	0.55
1:D:88:VAL:HG11	1:D:91:GLU:OE2	2.06	0.55
1:C:370:SER:HB3	1:C:388:GLN:NE2	2.21	0.55
1:D:377:ASN:HB2	1:D:381:TYR:H	1.71	0.55
1:D:377:ASN:HB2	1:D:381:TYR:N	2.21	0.55
1:A:115:LEU:HD12	1:A:134:ILE:HG12	1.87	0.55
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.07	0.55
1:D:341:VAL:O	1:D:342:ALA:HB3	2.06	0.55
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.89	0.55
1:D:489:LYS:HB3	1:D:489:LYS:NZ	2.21	0.55
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.40	0.55
1:D:183:TYR:CE1	1:D:277:SER:O	2.59	0.55
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.41	0.55
1:C:290:PRO:HG3	1:C:326:ASP:OD2	2.07	0.55
1:B:487:ASN:CB	1:B:489:LYS:HG3	2.35	0.55
1:C:377:ASN:HB2	1:C:381:TYR:N	2.21	0.55
1:C:110:ASP:HB3	1:C:112:GLN:H	1.71	0.55
1:D:272:ASN:C	1:D:272:ASN:HD22	2.08	0.55
1:B:693:GLU:HA	1:B:726:VAL:HG11	1.87	0.55
1:C:109:PRO:HG3	1:C:158:SER:O	2.06	0.55
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.41	0.55
1:C:102:ILE:HD13	1:C:116:LEU:HD22	1.89	0.55
1:B:305:TRP:CE3	1:B:311:ILE:HB	2.42	0.55
1:C:598:LEU:HD22	1:C:631:TYR:OH	2.06	0.55
1:D:598:LEU:HD22	1:D:631:TYR:OH	2.07	0.55
1:D:383:HIS:HB3	1:D:398:THR:OG1	2.07	0.55
1:D:486:VAL:CG1	1:D:487:ASN:N	2.70	0.55
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.89	0.55
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.88	0.55
1:C:383:HIS:HB3	1:C:398:THR:OG1	2.06	0.55
1:D:81:ALA:O	1:D:492:ARG:NH2	2.28	0.54
1:C:536:LYS:NZ	1:C:536:LYS:CB	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:HB3	1:B:112:GLN:HB2	1.90	0.54
1:D:102:ILE:HD13	1:D:116:LEU:HD22	1.88	0.54
1:C:80:ASN:HB3	1:C:85:ASN:OD1	2.06	0.54
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.42	0.54
1:D:80:ASN:HB3	1:D:85:ASN:OD1	2.07	0.54
1:A:60:LEU:C	1:A:60:LEU:HD12	2.27	0.54
1:C:486:VAL:CG1	1:C:487:ASN:H	2.19	0.54
1:A:177:GLU:CG	1:A:180:LEU:HD22	2.36	0.54
1:D:341:VAL:HG22	1:D:342:ALA:H	1.71	0.54
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.72	0.54
1:D:720:SER:O	1:D:724:VAL:HG23	2.06	0.54
1:B:622:LYS:NZ	1:B:622:LYS:HB2	2.23	0.54
1:C:65:ASP:OD2	1:C:466:LYS:HB2	2.07	0.54
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.42	0.54
1:B:56:LYS:HB2	1:B:497:ASN:OD1	2.07	0.54
1:C:60:LEU:HD12	1:C:60:LEU:C	2.27	0.54
1:A:489:LYS:HB3	1:A:489:LYS:NZ	2.22	0.54
1:D:704:HIS:HE1	1:D:711:VAL:O	1.91	0.54
1:D:388:GLN:HB2	1:D:391:LYS:HB2	1.90	0.54
1:A:168:TRP:O	1:A:169:ASN:HB2	2.07	0.54
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.28	0.54
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.23	0.54
1:D:273:THR:O	1:D:276:LEU:HD21	2.07	0.54
1:B:459:VAL:HG22	1:B:460:SER:N	2.22	0.54
1:B:177:GLU:CG	1:B:180:LEU:HD22	2.38	0.54
1:B:272:ASN:ND2	1:B:274:ASP:H	2.06	0.54
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.42	0.54
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.89	0.54
1:C:69:LEU:HD22	1:C:76:ILE:HG22	1.90	0.54
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.43	0.54
1:B:205:GLU:OE2	2:B:901:GGO:N	2.41	0.54
1:A:455:GLN:HG3	1:A:475:PRO:HD3	1.90	0.54
1:C:39:SER:O	1:C:40:ARG:O	2.26	0.54
1:B:301:CYS:SG	1:B:359:PRO:HG2	2.48	0.54
1:A:528:MET:HE3	1:A:618:PHE:HE1	1.72	0.54
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.08	0.53
1:B:149:PRO:HB2	1:B:168:TRP:CD1	2.43	0.53
1:D:388:GLN:HB3	1:D:391:LYS:HB2	1.90	0.53
1:D:411:THR:O	1:D:413:ASP:N	2.41	0.53
1:A:39:SER:O	1:A:40:ARG:O	2.26	0.53
1:A:92:ASN:ND2	1:A:93:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:PHE:CE2	1:C:286:GLN:HB2	2.44	0.53
1:A:726:VAL:HG12	1:A:726:VAL:O	2.08	0.53
1:C:177:GLU:CG	1:C:180:LEU:HD22	2.38	0.53
1:B:167:VAL:HA	1:B:171:ASP:O	2.07	0.53
1:B:39:SER:O	1:B:40:ARG:O	2.26	0.53
1:C:286:GLN:NE2	1:C:288:THR:HG22	2.24	0.53
1:D:153:GLN:HB3	1:D:211:TYR:CE2	2.44	0.53
1:B:176:ILE:HD11	1:B:276:LEU:HD21	1.91	0.53
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.90	0.53
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.89	0.53
1:D:60:LEU:C	1:D:60:LEU:HD12	2.29	0.53
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.74	0.53
1:B:489:LYS:NZ	1:B:489:LYS:HB3	2.22	0.53
1:D:110:ASP:HB3	1:D:112:GLN:H	1.74	0.53
1:B:108:SER:C	1:B:110:ASP:N	2.62	0.53
1:C:388:GLN:HB3	1:C:391:LYS:HB2	1.91	0.53
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.44	0.53
1:A:167:VAL:HA	1:A:171:ASP:O	2.09	0.53
1:B:314:GLN:HE22	1:B:373:LYS:HZ3	1.57	0.53
1:D:411:THR:C	1:D:413:ASP:N	2.62	0.53
1:C:64:SER:O	1:C:463:LYS:HG2	2.09	0.53
1:A:193:ILE:HG22	1:A:194:ILE:HG13	1.90	0.53
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.06	0.53
1:C:704:HIS:HE1	1:C:711:VAL:O	1.92	0.53
1:D:60:LEU:HD12	1:D:60:LEU:O	2.09	0.53
1:D:216:TRP:CZ3	1:D:273:THR:HG21	2.44	0.52
1:C:341:VAL:O	1:C:342:ALA:HB3	2.10	0.52
1:A:106:SER:HB3	1:A:115:LEU:HB3	1.91	0.52
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.91	0.52
1:B:622:LYS:HZ2	1:B:622:LYS:HB2	1.73	0.52
1:B:544:LEU:HD21	1:B:606:GLN:HG3	1.89	0.52
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.90	0.52
1:D:69:LEU:HD22	1:D:76:ILE:HG22	1.92	0.52
1:B:55:LEU:HD23	1:B:500:LEU:HD22	1.91	0.52
1:C:62:TRP:CE3	1:C:68:TYR:HB3	2.44	0.52
1:A:177:GLU:CB	1:A:180:LEU:HD22	2.40	0.52
1:C:60:LEU:HD12	1:C:60:LEU:O	2.09	0.52
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.45	0.52
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.45	0.52
1:D:600:THR:O	1:D:603:VAL:HG13	2.10	0.52
1:A:62:TRP:CE3	1:A:68:TYR:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:LYS:HB3	1:C:489:LYS:NZ	2.25	0.52
1:C:717:ALA:O	1:D:736:THR:HG21	2.10	0.52
1:B:168:TRP:O	1:B:169:ASN:HB2	2.09	0.52
1:D:745:SER:O	1:D:749:GLN:HG3	2.09	0.52
1:B:60:LEU:C	1:B:60:LEU:HD12	2.29	0.52
1:B:334:SER:HB3	1:B:336:ARG:HD2	1.89	0.52
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.29	0.52
1:B:71:LYS:NZ	1:B:105:TYR:HB2	2.25	0.52
1:D:486:VAL:CG1	1:D:487:ASN:H	2.21	0.52
1:D:341:VAL:O	1:D:343:ARG:N	2.43	0.52
1:D:726:VAL:HG12	1:D:726:VAL:O	2.08	0.51
1:C:273:THR:O	1:C:276:LEU:HD21	2.10	0.51
1:C:486:VAL:CG1	1:C:487:ASN:N	2.70	0.51
1:D:471:ARG:HG2	1:D:480:TYR:HD2	1.75	0.51
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.45	0.51
1:C:536:LYS:HB3	1:C:536:LYS:HZ3	1.76	0.51
1:B:110:ASP:C	1:B:112:GLN:H	2.12	0.51
1:B:71:LYS:HZ3	1:B:105:TYR:HB2	1.76	0.51
1:C:673:LEU:O	1:C:678:ASP:HB3	2.11	0.51
1:D:62:TRP:CE3	1:D:68:TYR:HB3	2.46	0.51
1:A:125:ARG:HG2	1:A:126:HIS:CD2	2.45	0.51
1:A:305:TRP:CE3	1:A:311:ILE:HB	2.46	0.51
1:D:600:THR:OG1	1:D:601:PHE:N	2.43	0.51
1:B:115:LEU:HD21	1:B:155:VAL:HG11	1.93	0.51
1:C:388:GLN:HB2	1:C:391:LYS:HB2	1.91	0.51
1:D:177:GLU:HG3	1:D:180:LEU:HD22	1.92	0.51
1:B:616:MET:HE1	1:B:618:PHE:HZ	1.76	0.51
1:A:110:ASP:C	1:A:112:GLN:H	2.14	0.51
1:B:65:ASP:HB3	1:B:66:HIS:CE1	2.46	0.51
1:B:528:MET:HE3	1:B:618:PHE:HE1	1.75	0.51
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.46	0.51
1:B:726:VAL:O	1:B:726:VAL:HG12	2.11	0.51
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.93	0.51
1:C:64:SER:C	1:C:463:LYS:HG2	2.32	0.51
1:D:65:ASP:OD2	1:D:466:LYS:HB2	2.10	0.51
1:D:170:ASN:O	1:D:196:ASN:HB2	2.10	0.51
1:B:330:TYR:HE1	1:B:335:GLY:HA2	1.76	0.51
1:C:341:VAL:O	1:C:343:ARG:N	2.42	0.50
1:C:154:TRP:O	1:C:166:TYR:HA	2.11	0.50
1:B:468:TYR:O	1:B:482:LEU:HD23	2.11	0.50
1:A:137:LEU:O	1:A:140:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:LEU:O	1:D:492:ARG:HB3	2.12	0.50
1:A:248:TYR:CE1	1:B:258:LYS:HD2	2.47	0.50
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.75	0.50
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.26	0.50
1:D:64:SER:C	1:D:463:LYS:HG2	2.31	0.50
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.47	0.50
1:D:173:TYR:CE2	1:D:184:ARG:HG2	2.46	0.50
1:A:231:THR:HG22	1:A:232:GLU:CG	2.41	0.50
1:C:277:SER:O	1:C:278:SER:CB	2.60	0.50
1:A:272:ASN:HD22	1:A:274:ASP:H	1.60	0.50
1:A:622:LYS:NZ	1:A:622:LYS:HB2	2.26	0.50
1:A:724:VAL:HG13	1:B:750:HIS:HB2	1.93	0.50
1:C:446:SER:HA	1:C:449:LEU:HG	1.93	0.50
1:A:110:ASP:HB3	1:A:112:GLN:HB2	1.93	0.50
1:C:597:ARG:NH1	1:C:682:HIS:HB2	2.27	0.50
1:C:111:GLY:O	1:C:137:LEU:HD12	2.11	0.50
1:B:377:ASN:CB	1:B:381:TYR:H	2.24	0.50
1:B:704:HIS:HD2	1:B:716:SER:OG	1.95	0.50
1:D:449:LEU:O	1:D:450:ASN:HB2	2.12	0.50
1:B:147:ARG:HG2	1:B:147:ARG:HH11	1.77	0.50
1:C:184:ARG:HD3	1:C:186:THR:O	2.11	0.50
1:C:276:LEU:N	1:C:276:LEU:HD23	2.27	0.50
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.47	0.50
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.46	0.50
1:D:154:TRP:O	1:D:166:TYR:HA	2.12	0.50
1:D:536:LYS:CB	1:D:536:LYS:NZ	2.75	0.50
1:D:550:PRO:O	1:D:551:CYS:HB3	2.12	0.50
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.93	0.49
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.47	0.49
1:D:111:GLY:O	1:D:137:LEU:HD12	2.12	0.49
1:B:455:GLN:HG3	1:B:475:PRO:HD3	1.93	0.49
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.47	0.49
1:A:64:SER:O	1:A:463:LYS:HG2	2.12	0.49
1:D:269:PHE:CE2	1:D:286:GLN:HB2	2.47	0.49
1:B:377:ASN:HB2	1:B:381:TYR:H	1.76	0.49
1:C:741:GLY:O	1:C:742:ILE:C	2.50	0.49
1:C:415:LEU:HD13	1:C:415:LEU:C	2.33	0.49
1:A:272:ASN:ND2	1:A:274:ASP:H	2.09	0.49
1:D:446:SER:HA	1:D:449:LEU:HG	1.93	0.49
1:A:689:MET:HB3	1:A:722:ALA:HB2	1.95	0.49
1:C:113:PHE:CE2	1:C:178:PRO:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:CD1	1:B:128:TYR:C	2.85	0.49
1:D:113:PHE:CE2	1:D:178:PRO:HG2	2.48	0.49
1:A:93:SER:HA	1:A:96:ASP:OD1	2.12	0.49
1:D:276:LEU:N	1:D:276:LEU:HD23	2.26	0.49
1:A:428:GLY:O	1:A:429:ARG:HD3	2.12	0.49
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.94	0.49
1:D:127:SER:O	1:D:128:TYR:HB3	2.11	0.49
1:A:454:CYS:HA	1:A:474:GLY:O	2.12	0.49
1:C:608:GLU:O	1:C:611:ARG:HB3	2.13	0.49
1:D:140:ARG:HH11	1:D:140:ARG:HG2	1.76	0.49
1:C:173:TYR:HB3	1:C:182:SER:OG	2.13	0.49
1:D:272:ASN:HD21	1:D:274:ASP:HB2	1.78	0.49
1:B:153:GLN:HB3	1:B:211:TYR:CE2	2.47	0.49
1:D:597:ARG:NH1	1:D:682:HIS:HB2	2.26	0.49
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.93	0.49
1:A:277:SER:OG	1:A:280:THR:HB	2.13	0.49
1:B:171:ASP:HA	1:B:186:THR:CG2	2.43	0.49
1:A:39:SER:CB	1:A:40:ARG:NE	2.70	0.49
1:C:171:ASP:OD1	1:C:186:THR:HG23	2.12	0.49
1:A:487:ASN:O	1:A:488:ASP:HB2	2.13	0.49
1:D:654:ALA:HA	1:D:704:HIS:CD2	2.48	0.49
1:B:125:ARG:HG2	1:B:126:HIS:CD2	2.47	0.49
1:B:614:SER:HB2	1:B:621:ASN:HB3	1.95	0.49
1:C:745:SER:O	1:C:749:GLN:HG3	2.13	0.49
1:D:608:GLU:O	1:D:611:ARG:HB3	2.12	0.48
1:D:459:VAL:HG22	1:D:460:SER:N	2.28	0.48
1:B:231:THR:HG22	1:B:232:GLU:CG	2.40	0.48
1:A:277:SER:O	1:A:278:SER:HB3	2.13	0.48
1:B:747:ALA:O	1:B:751:ILE:HG22	2.13	0.48
1:A:364:PHE:CD2	1:A:371:PHE:HB3	2.48	0.48
1:B:64:SER:O	1:B:463:LYS:HG2	2.14	0.48
1:D:171:ASP:OD1	1:D:186:THR:HG23	2.13	0.48
1:B:137:LEU:O	1:B:140:ARG:NH1	2.47	0.48
1:C:223:LEU:O	1:C:271:VAL:HG12	2.14	0.48
1:D:308:GLN:HA	1:D:308:GLN:OE1	2.13	0.48
1:A:149:PRO:HB2	1:A:168:TRP:CD1	2.48	0.48
1:A:704:HIS:HD2	1:A:716:SER:OG	1.96	0.48
1:B:701:LEU:HD22	1:B:703:ILE:HG13	1.94	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.48
1:A:310:ARG:NH1	1:A:329:ASP:OD2	2.47	0.48
1:C:147:ARG:CG	1:C:147:ARG:HH11	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.42	0.48
1:D:341:VAL:C	1:D:343:ARG:N	2.67	0.48
1:B:109:PRO:HG2	1:B:161:GLY:O	2.12	0.48
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.44	0.48
1:C:522:THR:HG22	1:C:523:LYS:N	2.29	0.48
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.28	0.48
1:A:171:ASP:HA	1:A:186:THR:CG2	2.44	0.48
1:C:170:ASN:O	1:C:196:ASN:HB2	2.14	0.48
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.48	0.48
1:D:673:LEU:O	1:D:678:ASP:HB3	2.13	0.48
1:B:428:GLY:O	1:B:429:ARG:HD3	2.14	0.48
1:A:747:ALA:O	1:A:751:ILE:HG22	2.14	0.48
1:C:535:ASP:OD1	1:C:537:SER:HB3	2.14	0.48
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.96	0.48
1:A:276:LEU:H	1:A:276:LEU:CD2	2.26	0.48
1:A:330:TYR:HE1	1:A:335:GLY:HA2	1.79	0.48
1:A:614:SER:HB2	1:A:621:ASN:HB3	1.96	0.48
1:D:316:LEU:HD21	1:D:320:GLN:CG	2.44	0.48
1:D:415:LEU:HD13	1:D:415:LEU:C	2.34	0.48
1:C:491:LEU:O	1:C:492:ARG:HB3	2.13	0.48
1:C:122:LYS:HE2	1:C:124:TRP:O	2.14	0.48
1:A:108:SER:C	1:A:110:ASP:N	2.63	0.48
1:D:177:GLU:HB2	1:D:180:LEU:HB2	1.96	0.48
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.96	0.48
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.49	0.48
1:C:453:ARG:HG3	1:C:476:GLY:HA3	1.96	0.48
1:D:691:ARG:HH11	1:D:691:ARG:HG3	1.79	0.48
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.49	0.47
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.94	0.47
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.49	0.47
1:D:114:ILE:CG1	1:D:137:LEU:HD21	2.44	0.47
1:A:377:ASN:CB	1:A:381:TYR:H	2.26	0.47
1:B:689:MET:HB3	1:B:722:ALA:HB2	1.95	0.47
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.49	0.47
1:D:289:ALA:HB1	1:D:290:PRO:C	2.35	0.47
1:A:513:LYS:O	1:A:527:GLN:HA	2.15	0.47
1:B:277:SER:O	1:B:278:SER:HB3	2.14	0.47
1:D:64:SER:O	1:D:463:LYS:HG2	2.15	0.47
1:D:217:SER:HB3	1:D:222:PHE:HB2	1.97	0.47
1:B:146:GLU:O	1:B:175:LYS:HE2	2.15	0.47
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:CYS:HA	1:B:474:GLY:O	2.15	0.47
1:A:425:MET:HA	1:A:426:PRO:HD2	1.77	0.47
1:A:701:LEU:HD22	1:A:703:ILE:HG13	1.96	0.47
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.96	0.47
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.97	0.47
1:D:172:ILE:N	1:D:186:THR:HG22	2.11	0.47
1:C:172:ILE:N	1:C:186:THR:CG2	2.67	0.47
1:C:75:ASN:ND2	1:C:92:ASN:OD1	2.48	0.47
1:A:726:VAL:O	1:A:726:VAL:CG1	2.62	0.47
1:D:159:PRO:HB2	1:D:218:PRO:O	2.14	0.47
1:D:453:ARG:HG3	1:D:476:GLY:HA3	1.96	0.47
1:D:522:THR:HG22	1:D:523:LYS:N	2.30	0.47
1:D:319:ILE:O	1:D:321:ASN:N	2.43	0.47
1:D:527:GLN:HG2	1:D:555:ALA:HA	1.97	0.47
1:D:331:ASP:CB	1:D:334:SER:HB2	2.44	0.47
1:A:438:ASP:OD2	1:A:441:LYS:HG3	2.14	0.47
1:A:314:GLN:NE2	1:A:373:LYS:HZ1	2.13	0.47
1:C:600:THR:OG1	1:C:601:PHE:N	2.47	0.47
1:C:159:PRO:HB2	1:C:218:PRO:O	2.15	0.47
1:C:127:SER:O	1:C:128:TYR:HB3	2.15	0.47
1:D:539:LYS:NZ	1:D:617:GLY:O	2.47	0.47
1:C:622:LYS:HB2	1:C:622:LYS:NZ	2.30	0.47
1:D:184:ARG:HD3	1:D:186:THR:O	2.15	0.47
1:A:377:ASN:HB2	1:A:381:TYR:H	1.80	0.47
1:C:341:VAL:C	1:C:343:ARG:N	2.67	0.47
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.97	0.47
1:C:422:TYR:CE2	1:C:423:LYS:HD3	2.50	0.47
1:A:761:GLN:HE21	1:A:761:GLN:HB3	1.60	0.47
1:B:293:MET:HE2	1:B:317:ARG:CG	2.39	0.47
1:D:177:GLU:CB	1:D:180:LEU:HD22	2.45	0.47
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.35	0.47
1:D:689:MET:HE3	1:D:718:GLN:HB3	1.97	0.47
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.50	0.47
1:C:236:ILE:HG12	1:C:712:HIS:CE1	2.49	0.47
1:D:303:VAL:O	1:D:303:VAL:HG22	2.14	0.47
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.50	0.46
1:C:114:ILE:CG1	1:C:137:LEU:HD21	2.44	0.46
1:B:513:LYS:O	1:B:527:GLN:HA	2.15	0.46
1:D:520:ASN:O	1:D:521:GLU:HB2	2.15	0.46
1:D:286:GLN:NE2	1:D:288:THR:HG22	2.31	0.46
1:C:425:MET:HA	1:C:426:PRO:HD2	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:GLN:OE1	1:D:533:HIS:HE1	1.98	0.46
1:C:308:GLN:OE1	1:C:308:GLN:HA	2.16	0.46
1:C:289:ALA:HB1	1:C:290:PRO:C	2.35	0.46
1:D:614:SER:HA	1:D:619:VAL:CB	2.41	0.46
1:D:551:CYS:O	1:D:551:CYS:SG	2.73	0.46
1:B:420:ASN:HB2	1:B:426:PRO:HA	1.97	0.46
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.50	0.46
1:C:153:GLN:HE22	1:C:170:ASN:HD21	1.60	0.46
1:A:136:ASP:O	1:A:140:ARG:HA	2.16	0.46
1:C:536:LYS:HB3	1:C:536:LYS:NZ	2.30	0.46
1:B:125:ARG:O	1:B:125:ARG:HG3	2.15	0.46
1:C:299:TYR:CE1	1:C:665:VAL:HG22	2.50	0.46
1:C:597:ARG:HD3	1:C:597:ARG:HA	1.74	0.46
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.50	0.46
1:C:247:GLN:HG2	1:D:258:LYS:HD2	1.98	0.46
1:D:74:ASN:C	1:D:92:ASN:HB3	2.36	0.46
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.96	0.46
1:C:310:ARG:HD3	1:C:327:ILE:HG23	1.97	0.46
1:A:60:LEU:O	1:A:60:LEU:HD12	2.16	0.46
1:A:125:ARG:HG2	1:A:126:HIS:NE2	2.31	0.46
1:A:468:TYR:O	1:A:482:LEU:HD23	2.15	0.46
1:B:364:PHE:CD2	1:B:371:PHE:HB3	2.50	0.46
1:B:761:GLN:HB3	1:B:761:GLN:HE21	1.60	0.46
1:C:173:TYR:CE2	1:C:184:ARG:HG2	2.51	0.46
1:B:170:ASN:ND2	1:B:170:ASN:N	2.64	0.46
1:D:310:ARG:HD3	1:D:327:ILE:HG23	1.97	0.46
1:A:276:LEU:HD23	1:A:276:LEU:O	2.16	0.46
1:D:55:LEU:HD23	1:D:500:LEU:HD22	1.98	0.46
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.31	0.46
1:A:269:PHE:CE2	1:A:286:GLN:HB2	2.50	0.46
1:B:285:ILE:HD12	1:B:285:ILE:N	2.31	0.46
1:A:502:LYS:O	1:A:505:GLN:HG2	2.16	0.46
1:B:93:SER:HA	1:B:96:ASP:OD1	2.15	0.46
1:D:153:GLN:HE22	1:D:170:ASN:HD21	1.56	0.46
1:A:236:ILE:O	1:A:253:ARG:HA	2.16	0.46
1:D:75:ASN:ND2	1:D:92:ASN:OD1	2.49	0.46
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.98	0.46
1:B:446:SER:HB2	1:B:457:TYR:CD1	2.51	0.46
1:A:746:THR:HG21	1:B:725:ASP:HA	1.98	0.46
1:D:173:TYR:HB3	1:D:182:SER:OG	2.15	0.45
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:HD21	1:C:274:ASP:HB2	1.81	0.45
1:D:370:SER:HB2	1:D:387:PHE:O	2.16	0.45
1:C:314:GLN:HE22	1:C:373:LYS:NZ	2.13	0.45
1:C:65:ASP:HB2	1:C:463:LYS:HB2	1.98	0.45
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.96	0.45
1:C:172:ILE:N	1:C:186:THR:HG22	2.11	0.45
1:A:244:GLU:CD	1:B:689:MET:HG3	2.37	0.45
1:D:741:GLY:O	1:D:742:ILE:C	2.54	0.45
1:C:258:LYS:HD2	1:D:247:GLN:HG2	1.97	0.45
1:C:167:VAL:HG21	1:C:198:ILE:HG23	1.98	0.45
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.99	0.45
1:D:195:TYR:O	1:D:227:GLN:HA	2.16	0.45
1:D:39:SER:HB2	1:D:40:ARG:NE	2.30	0.45
1:C:217:SER:HB3	1:C:222:PHE:HB2	1.98	0.45
1:C:527:GLN:HG2	1:C:555:ALA:HA	1.98	0.45
1:D:369:ASN:C	1:D:389:ILE:HG23	2.36	0.45
1:A:110:ASP:HB3	1:A:112:GLN:H	1.81	0.45
1:B:276:LEU:HD23	1:B:276:LEU:O	2.16	0.45
1:C:449:LEU:O	1:C:450:ASN:HB2	2.16	0.45
1:C:195:TYR:O	1:C:227:GLN:HA	2.15	0.45
1:C:508:GLN:OE1	1:C:533:HIS:HE1	2.00	0.45
1:D:425:MET:HA	1:D:426:PRO:HD2	1.73	0.45
1:C:459:VAL:HG22	1:C:460:SER:N	2.32	0.45
1:D:74:ASN:O	1:D:92:ASN:HA	2.16	0.45
1:C:597:ARG:HG3	1:C:600:THR:HG21	1.99	0.45
1:A:724:VAL:HG13	1:B:750:HIS:CB	2.47	0.45
1:A:286:GLN:NE2	1:A:288:THR:HG22	2.31	0.45
1:D:658:ARG:HD2	1:D:661:TYR:CE1	2.51	0.45
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.98	0.45
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.51	0.45
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.60	0.45
1:D:170:ASN:N	1:D:170:ASN:ND2	2.64	0.45
1:C:108:SER:C	1:C:110:ASP:N	2.69	0.45
1:D:519:LEU:O	1:D:520:ASN:C	2.55	0.45
1:C:78:VAL:HG12	1:C:87:SER:O	2.16	0.45
1:A:717:ALA:O	1:B:736:THR:HG21	2.16	0.45
1:C:289:ALA:HA	1:C:294:LEU:HG	1.99	0.45
1:C:237:GLU:HG2	1:C:253:ARG:HB3	1.98	0.45
1:C:614:SER:HA	1:C:619:VAL:CB	2.42	0.45
1:C:136:ASP:OD1	1:C:138:ASN:HB2	2.17	0.45
1:C:123:GLN:HG2	1:C:124:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:CD2	1:A:715:GLN:HG2	2.52	0.45
1:D:39:SER:HB2	1:D:40:ARG:HE	1.82	0.45
1:A:170:ASN:N	1:A:170:ASN:ND2	2.64	0.45
1:D:65:ASP:CG	1:D:464:GLU:HB2	2.36	0.45
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.17	0.45
1:D:299:TYR:CE1	1:D:665:VAL:HG22	2.52	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.99	0.45
1:D:223:LEU:O	1:D:271:VAL:HG12	2.17	0.45
1:C:726:VAL:O	1:C:726:VAL:HG12	2.16	0.45
1:A:620:ASP:C	1:A:622:LYS:H	2.20	0.45
1:D:322:TYR:OH	1:D:346:ILE:HD13	2.15	0.45
1:B:377:ASN:HB3	1:B:379:GLU:H	1.82	0.45
1:B:110:ASP:HB3	1:B:112:GLN:H	1.82	0.45
1:A:128:TYR:C	1:A:128:TYR:CD1	2.90	0.45
1:B:92:ASN:ND2	1:B:93:SER:H	2.11	0.44
1:D:316:LEU:HD21	1:D:320:GLN:HG2	1.98	0.44
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.63	0.44
1:C:370:SER:HB2	1:C:387:PHE:O	2.16	0.44
1:B:478:PRO:HB2	1:B:497:ASN:ND2	2.32	0.44
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.15	0.44
1:A:661:TYR:HD2	1:A:715:GLN:HG2	1.82	0.44
1:C:550:PRO:O	1:C:551:CYS:HB3	2.17	0.44
1:C:746:THR:HG21	1:D:725:ASP:HA	1.98	0.44
1:D:485:SER:O	1:D:486:VAL:C	2.56	0.44
1:A:620:ASP:OD1	1:A:622:LYS:HB2	2.17	0.44
1:A:154:TRP:O	1:A:166:TYR:HA	2.17	0.44
1:D:481:THR:OG1	1:D:483:HIS:HE1	2.00	0.44
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.46	0.44
1:A:41:LYS:O	1:A:507:VAL:HG23	2.16	0.44
1:A:293:MET:HE2	1:A:317:ARG:CG	2.39	0.44
1:C:327:ILE:HB	1:C:343:ARG:HG2	1.98	0.44
1:B:154:TRP:O	1:B:166:TYR:HA	2.17	0.44
1:B:425:MET:HA	1:B:426:PRO:HD2	1.80	0.44
1:B:310:ARG:NH1	1:B:329:ASP:OD2	2.51	0.44
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.99	0.44
1:A:285:ILE:N	1:A:285:ILE:HD12	2.31	0.44
1:B:39:SER:CB	1:B:40:ARG:NE	2.68	0.44
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.37	0.44
1:D:377:ASN:N	1:D:381:TYR:O	2.51	0.44
1:D:65:ASP:HB2	1:D:463:LYS:HB2	1.99	0.44
1:A:446:SER:HB2	1:A:457:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLN:HG2	1:D:124:TRP:CD2	2.53	0.44
1:D:171:ASP:HA	1:D:186:THR:CG2	2.48	0.44
1:D:90:LEU:C	1:D:90:LEU:HD22	2.38	0.44
1:D:327:ILE:HB	1:D:343:ARG:HG2	1.98	0.44
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.48	0.44
1:D:124:TRP:HB2	1:D:204:GLU:OE2	2.18	0.44
1:D:535:ASP:OD1	1:D:537:SER:HB3	2.17	0.44
1:C:367:ASP:OD2	1:C:369:ASN:OD1	2.35	0.44
1:B:634:TYR:HD1	1:B:656:VAL:O	2.00	0.44
1:B:289:ALA:HA	1:B:294:LEU:HD11	1.99	0.44
1:C:485:SER:O	1:C:486:VAL:C	2.56	0.44
1:B:726:VAL:O	1:B:726:VAL:CG1	2.65	0.44
1:B:286:GLN:NE2	1:B:288:THR:HG22	2.32	0.44
1:A:458:SER:OG	1:A:471:ARG:HB2	2.17	0.44
1:D:259:ALA:HB3	1:D:660:GLU:HA	1.98	0.44
1:C:90:LEU:C	1:C:90:LEU:HD22	2.37	0.44
1:A:66:HIS:ND1	1:A:66:HIS:N	2.65	0.44
1:A:420:ASN:HB2	1:A:426:PRO:HA	1.98	0.44
1:C:519:LEU:O	1:C:520:ASN:C	2.55	0.44
1:D:514:LEU:HD12	1:D:557:THR:CG2	2.47	0.44
1:D:703:ILE:HG12	1:D:733:MET:HB3	2.00	0.44
1:B:458:SER:OG	1:B:471:ARG:HB2	2.17	0.44
1:C:691:ARG:HG3	1:C:691:ARG:HH11	1.81	0.44
1:B:127:SER:HB3	1:B:211:TYR:CG	2.53	0.44
1:C:177:GLU:HG3	1:C:180:LEU:HD22	1.98	0.44
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.53	0.44
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.99	0.44
1:A:146:GLU:O	1:A:175:LYS:HE2	2.18	0.44
1:A:332:GLU:OE1	1:A:332:GLU:HA	2.18	0.44
1:C:90:LEU:HD22	1:C:90:LEU:O	2.18	0.44
1:B:314:GLN:NE2	1:B:373:LYS:HZ1	2.16	0.44
1:A:616:MET:HE1	1:A:618:PHE:HZ	1.82	0.44
1:B:276:LEU:CD2	1:B:276:LEU:H	2.30	0.43
1:D:310:ARG:HD3	1:D:327:ILE:CG2	2.48	0.43
1:A:464:GLU:O	1:A:465:ALA:HB3	2.17	0.43
1:C:42:THR:HB	1:C:569:SER:OG	2.18	0.43
1:C:303:VAL:HG22	1:C:303:VAL:O	2.18	0.43
1:B:136:ASP:O	1:B:140:ARG:HA	2.18	0.43
1:A:293:MET:HE1	1:A:317:ARG:HG3	1.95	0.43
1:D:40:ARG:NH1	1:D:505:GLN:O	2.51	0.43
1:C:40:ARG:NH1	1:C:505:GLN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ARG:HD3	1:D:597:ARG:HA	1.74	0.43
1:C:481:THR:OG1	1:C:483:HIS:HE1	2.01	0.43
1:D:614:SER:C	1:D:616:MET:H	2.22	0.43
1:D:277:SER:O	1:D:278:SER:CB	2.60	0.43
1:B:314:GLN:NE2	1:B:373:LYS:NZ	2.65	0.43
1:A:234:PRO:HB2	1:B:248:TYR:CE2	2.54	0.43
1:B:464:GLU:O	1:B:465:ALA:HB3	2.18	0.43
1:A:528:MET:HG2	1:A:576:ALA:HB2	2.00	0.43
1:A:175:LYS:NZ	1:A:182:SER:HB2	2.33	0.43
1:A:612:GLN:HB3	1:A:612:GLN:HE21	1.66	0.43
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.99	0.43
1:C:39:SER:HB2	1:C:40:ARG:NE	2.33	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.83	0.43
1:D:381:TYR:N	1:D:381:TYR:CD1	2.86	0.43
1:C:535:ASP:O	1:C:537:SER:N	2.51	0.43
1:B:446:SER:HB2	1:B:457:TYR:CE1	2.52	0.43
1:C:58:TYR:CD2	1:C:494:LEU:HB3	2.53	0.43
1:D:622:LYS:HB2	1:D:622:LYS:NZ	2.32	0.43
1:D:334:SER:HB3	1:D:336:ARG:HD2	1.99	0.43
1:A:76:ILE:CD1	1:A:90:LEU:HD11	2.37	0.43
1:C:751:ILE:O	1:C:755:MET:HG3	2.18	0.43
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.41	0.43
1:D:147:ARG:HH11	1:D:147:ARG:CG	2.24	0.43
1:B:438:ASP:OD2	1:B:441:LYS:HG3	2.17	0.43
1:D:78:VAL:HG12	1:D:87:SER:O	2.17	0.43
1:C:95:PHE:O	1:C:96:ASP:C	2.56	0.43
1:C:40:ARG:HB2	1:C:506:ASN:O	2.18	0.43
1:C:271:VAL:HG22	1:C:272:ASN:N	2.33	0.43
1:A:109:PRO:HG2	1:A:161:GLY:O	2.18	0.43
1:C:244:GLU:CD	1:D:689:MET:HG3	2.38	0.43
1:D:535:ASP:O	1:D:537:SER:N	2.51	0.43
1:D:163:LYS:NZ	1:D:273:THR:OG1	2.50	0.43
1:C:110:ASP:OD2	1:C:162:HIS:HB3	2.18	0.43
1:B:600:THR:OG1	1:B:601:PHE:N	2.50	0.43
1:C:310:ARG:HD3	1:C:327:ILE:CG2	2.49	0.43
1:C:65:ASP:HA	1:C:462:SER:HB2	2.01	0.43
1:B:388:GLN:CB	1:B:391:LYS:HB2	2.48	0.43
1:B:567:LEU:O	1:B:571:GLU:HB2	2.18	0.43
1:D:703:ILE:HA	1:D:733:MET:O	2.19	0.43
1:A:634:TYR:HD1	1:A:656:VAL:O	2.02	0.43
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:OG	1:A:280:THR:CB	2.66	0.43
1:C:322:TYR:OH	1:C:346:ILE:HD13	2.18	0.43
1:B:415:LEU:HD13	1:B:415:LEU:C	2.39	0.43
1:C:153:GLN:HE22	1:C:170:ASN:HD22	1.60	0.43
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.19	0.43
1:A:478:PRO:HB2	1:A:497:ASN:ND2	2.34	0.43
1:C:520:ASN:O	1:C:521:GLU:HB2	2.19	0.43
1:B:661:TYR:CD2	1:B:715:GLN:HG2	2.53	0.43
1:A:524:PHE:CD2	1:A:580:GLY:HA2	2.53	0.43
1:C:546:VAL:CG2	1:C:547:TYR:N	2.81	0.43
1:D:651:ILE:CG2	1:D:755:MET:HE3	2.41	0.43
1:A:486:VAL:HG13	1:A:487:ASN:N	2.34	0.43
1:C:316:LEU:HD21	1:C:320:GLN:CG	2.49	0.43
1:C:203:TYR:HA	1:C:207:VAL:CG1	2.48	0.43
1:A:540:TYR:N	1:A:540:TYR:CD1	2.86	0.43
1:C:658:ARG:HD2	1:C:661:TYR:CE1	2.53	0.43
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.86	0.42
1:A:276:LEU:N	1:A:276:LEU:CD2	2.81	0.42
1:D:704:HIS:CE1	1:D:711:VAL:O	2.69	0.42
1:D:597:ARG:HG3	1:D:600:THR:HG21	2.01	0.42
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.19	0.42
1:B:661:TYR:HD2	1:B:715:GLN:HG2	1.84	0.42
1:B:651:ILE:HD13	1:B:755:MET:HE2	2.01	0.42
1:C:703:ILE:HG12	1:C:733:MET:HB3	2.01	0.42
1:B:171:ASP:HA	1:B:186:THR:HG21	2.01	0.42
1:A:75:ASN:N	1:A:92:ASN:HB3	2.34	0.42
1:D:115:LEU:HA	1:D:115:LEU:HD12	1.89	0.42
1:B:221:THR:HG23	1:B:274:ASP:OD2	2.19	0.42
1:C:177:GLU:HB2	1:C:180:LEU:HB2	2.00	0.42
1:A:426:PRO:O	1:A:553:GLN:NE2	2.50	0.42
1:D:367:ASP:OD2	1:D:369:ASN:OD1	2.37	0.42
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.01	0.42
1:A:270:VAL:HG11	1:A:337:TRP:CZ2	2.54	0.42
1:C:514:LEU:HD12	1:C:557:THR:CG2	2.48	0.42
1:C:386:TYR:O	1:C:394:CYS:HB2	2.19	0.42
1:C:331:ASP:CB	1:C:334:SER:HB2	2.44	0.42
1:D:289:ALA:HA	1:D:294:LEU:HG	2.02	0.42
1:C:171:ASP:HA	1:C:186:THR:CG2	2.49	0.42
1:D:90:LEU:O	1:D:90:LEU:HD22	2.19	0.42
1:B:486:VAL:HG13	1:B:487:ASN:N	2.35	0.42
1:A:415:LEU:HD13	1:A:415:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PHE:CE1	1:C:107:ILE:HD13	2.54	0.42
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.84	0.42
1:A:340:LEU:C	1:A:341:VAL:O	2.50	0.42
1:D:341:VAL:CG2	1:D:342:ALA:N	2.82	0.42
1:B:160:VAL:CG2	1:B:161:GLY:N	2.82	0.42
1:D:314:GLN:HE22	1:D:373:LYS:NZ	2.17	0.42
1:D:684:ARG:HA	1:D:684:ARG:HD3	1.85	0.42
1:C:614:SER:C	1:C:616:MET:H	2.23	0.42
1:A:600:THR:OG1	1:A:601:PHE:N	2.52	0.42
1:C:528:MET:HB3	1:C:528:MET:HE2	1.88	0.42
1:D:689:MET:HB3	1:D:722:ALA:HB2	2.00	0.42
1:C:551:CYS:HB2	1:C:591:MET:SD	2.60	0.42
1:C:369:ASN:C	1:C:389:ILE:HG23	2.39	0.42
1:B:270:VAL:HG11	1:B:337:TRP:CZ2	2.54	0.42
1:C:689:MET:HB3	1:C:722:ALA:HB2	2.01	0.42
1:D:540:TYR:CD1	1:D:540:TYR:N	2.87	0.42
1:D:277:SER:OG	1:D:280:THR:HB	2.20	0.42
1:C:675:THR:HB	1:C:676:PRO:HD2	2.02	0.42
1:C:177:GLU:CB	1:C:180:LEU:HD22	2.49	0.42
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.34	0.42
1:B:535:ASP:OD1	1:B:537:SER:HB3	2.19	0.42
1:A:736:THR:CG2	1:B:720:SER:OG	2.67	0.42
1:A:528:MET:HB3	1:A:528:MET:HE2	1.65	0.42
1:D:535:ASP:C	1:D:537:SER:H	2.23	0.42
1:C:259:ALA:HB3	1:C:660:GLU:HA	2.01	0.42
1:D:42:THR:HB	1:D:569:SER:OG	2.19	0.42
1:D:546:VAL:CG2	1:D:547:TYR:N	2.82	0.42
1:C:651:ILE:CG2	1:C:755:MET:HE3	2.40	0.42
1:C:74:ASN:O	1:C:92:ASN:HA	2.19	0.42
1:D:147:ARG:HG2	1:D:147:ARG:NH1	2.27	0.42
1:D:39:SER:C	1:D:40:ARG:HD2	2.40	0.42
1:C:704:HIS:CE1	1:C:711:VAL:O	2.72	0.42
1:C:603:VAL:HG22	1:C:604:GLU:N	2.35	0.42
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.19	0.42
1:A:627:TRP:HB2	1:A:651:ILE:HB	2.01	0.42
1:C:231:THR:HG22	1:C:232:GLU:HG3	2.00	0.42
1:B:540:TYR:N	1:B:540:TYR:CD1	2.87	0.42
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.40	0.42
1:D:186:THR:HG21	1:D:196:ASN:CB	2.50	0.42
1:D:276:LEU:H	1:D:276:LEU:HD23	1.77	0.42
1:D:108:SER:C	1:D:110:ASP:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:ASP:OD2	1:D:441:LYS:HG3	2.20	0.42
1:C:341:VAL:CG2	1:C:342:ALA:N	2.81	0.42
1:C:438:ASP:OD2	1:C:441:LYS:HG3	2.19	0.42
1:B:620:ASP:OD1	1:B:622:LYS:HB2	2.20	0.42
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.35	0.42
1:D:319:ILE:C	1:D:321:ASN:H	2.23	0.42
1:C:703:ILE:HA	1:C:733:MET:O	2.19	0.42
1:C:684:ARG:HD3	1:C:684:ARG:HA	1.85	0.42
1:B:332:GLU:HA	1:B:332:GLU:OE1	2.19	0.42
1:C:312:SER:HA	1:C:326:ASP:O	2.20	0.41
1:C:381:TYR:N	1:C:381:TYR:CD1	2.87	0.41
1:B:285:ILE:CD1	1:B:285:ILE:N	2.83	0.41
1:A:567:LEU:O	1:A:571:GLU:HB2	2.20	0.41
1:A:741:GLY:O	1:A:742:ILE:C	2.58	0.41
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.82	0.41
1:B:242:SER:CB	1:B:246:LEU:HD12	2.44	0.41
1:A:528:MET:HE3	1:A:618:PHE:CE1	2.55	0.41
1:B:60:LEU:O	1:B:60:LEU:HD12	2.18	0.41
1:D:726:VAL:O	1:D:726:VAL:CG1	2.67	0.41
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.55	0.41
1:B:502:LYS:O	1:B:505:GLN:HG2	2.20	0.41
1:A:77:LEU:HD23	1:A:88:VAL:HA	2.01	0.41
1:B:175:LYS:NZ	1:B:182:SER:HB2	2.35	0.41
1:A:285:ILE:N	1:A:285:ILE:CD1	2.83	0.41
1:C:330:TYR:HE1	1:C:335:GLY:O	2.03	0.41
1:D:422:TYR:CE2	1:D:423:LYS:HD3	2.55	0.41
1:B:598:LEU:HD22	1:B:631:TYR:OH	2.20	0.41
1:B:76:ILE:CD1	1:B:90:LEU:HD11	2.42	0.41
1:C:124:TRP:HB2	1:C:204:GLU:OE2	2.19	0.41
1:C:551:CYS:O	1:C:551:CYS:SG	2.78	0.41
1:A:725:ASP:HA	1:B:746:THR:HG21	2.03	0.41
1:B:75:ASN:N	1:B:92:ASN:HB3	2.35	0.41
1:D:751:ILE:O	1:D:755:MET:HG3	2.19	0.41
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.86	0.41
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.20	0.41
1:A:242:SER:CB	1:A:246:LEU:HD12	2.44	0.41
1:D:39:SER:CB	1:D:40:ARG:HE	2.33	0.41
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.41
1:B:422:TYR:C	1:B:424:GLY:N	2.72	0.41
1:C:136:ASP:O	1:C:140:ARG:N	2.54	0.41
1:D:523:LYS:H	1:D:523:LYS:HG2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:C	1:A:542:LEU:HD23	2.40	0.41
1:B:39:SER:O	1:B:40:ARG:C	2.59	0.41
1:A:92:ASN:ND2	1:A:93:SER:H	2.11	0.41
1:D:92:ASN:ND2	1:D:93:SER:H	2.18	0.41
1:C:377:ASN:N	1:C:381:TYR:O	2.52	0.41
1:A:422:TYR:C	1:A:424:GLY:N	2.72	0.41
1:B:66:HIS:ND1	1:B:66:HIS:N	2.69	0.41
1:D:200:ASP:O	1:D:201:TRP:C	2.57	0.41
1:D:454:CYS:HB3	1:D:457:TYR:CZ	2.56	0.41
1:A:118:TYR:CD2	1:A:119:ASN:ND2	2.88	0.41
1:C:540:TYR:N	1:C:540:TYR:CD1	2.88	0.41
1:D:170:ASN:HD22	1:D:170:ASN:H	1.67	0.41
1:B:340:LEU:C	1:B:341:VAL:O	2.54	0.41
1:A:293:MET:HG3	1:A:298:HIS:HB3	2.03	0.41
1:C:74:ASN:C	1:C:92:ASN:HB3	2.39	0.41
1:A:736:THR:O	1:A:737:ASP:HB2	2.21	0.41
1:C:756:SER:O	1:C:760:LYS:CG	2.69	0.41
1:D:291:ALA:O	1:D:295:ILE:HG23	2.21	0.41
1:B:718:GLN:HE21	1:B:718:GLN:HA	1.85	0.41
1:C:336:ARG:HG2	1:C:336:ARG:HH11	1.86	0.41
1:B:289:ALA:HA	1:B:294:LEU:CD1	2.51	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HB3	2.03	0.41
1:B:140:ARG:NH1	1:B:140:ARG:CG	2.84	0.41
1:A:487:ASN:HD22	1:A:487:ASN:HA	1.64	0.41
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.36	0.41
1:B:110:ASP:C	1:B:112:GLN:N	2.73	0.41
1:D:65:ASP:HA	1:D:462:SER:HB2	2.03	0.41
1:D:514:LEU:HD22	1:D:525:TRP:HE3	1.85	0.41
1:C:689:MET:HE3	1:C:718:GLN:HB3	2.02	0.41
1:A:118:TYR:CE2	1:A:119:ASN:ND2	2.88	0.41
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.81	0.41
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.55	0.41
1:A:122:LYS:CG	1:A:123:GLN:N	2.84	0.41
1:B:167:VAL:HG21	1:B:198:ILE:HG23	2.02	0.41
1:A:74:ASN:C	1:A:92:ASN:CB	2.88	0.41
1:D:612:GLN:HE21	1:D:612:GLN:HB3	1.65	0.41
1:D:89:PHE:HD1	1:D:90:LEU:HD12	1.85	0.41
1:B:487:ASN:O	1:B:488:ASP:HB2	2.21	0.41
1:D:654:ALA:N	1:D:655:PRO:CD	2.84	0.41
1:D:193:ILE:HG22	1:D:194:ILE:HG13	2.03	0.41
1:C:535:ASP:C	1:C:537:SER:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:SER:OG	1:B:280:THR:HB	2.21	0.41
1:B:310:ARG:HH12	1:B:343:ARG:NH1	2.18	0.41
1:A:662:TYR:HB3	1:A:667:THR:OG1	2.21	0.41
1:C:334:SER:HB3	1:C:336:ARG:HD2	2.00	0.40
1:A:171:ASP:HA	1:A:186:THR:HG21	2.04	0.40
1:C:92:ASN:ND2	1:C:93:SER:H	2.18	0.40
1:C:39:SER:C	1:C:40:ARG:HD2	2.41	0.40
1:A:127:SER:HB3	1:A:211:TYR:CG	2.56	0.40
1:A:62:TRP:CG	1:A:462:SER:HA	2.56	0.40
1:D:152:THR:HG23	1:D:167:VAL:O	2.21	0.40
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.86	0.40
1:C:319:ILE:O	1:C:321:ASN:N	2.47	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.93	0.40
1:B:118:TYR:CD2	1:B:119:ASN:ND2	2.90	0.40
1:B:236:ILE:O	1:B:253:ARG:HA	2.22	0.40
1:D:95:PHE:O	1:D:96:ASP:C	2.59	0.40
1:D:110:ASP:C	1:D:112:GLN:H	2.21	0.40
1:B:301:CYS:O	1:B:302:ASP:HB2	2.21	0.40
1:C:115:LEU:HD12	1:C:134:ILE:HG12	2.02	0.40
1:A:272:ASN:C	1:A:272:ASN:ND2	2.74	0.40
1:B:422:TYR:C	1:B:424:GLY:H	2.25	0.40
1:A:71:LYS:HZ1	1:A:105:TYR:HB2	1.86	0.40
1:C:448:GLU:O	1:C:449:LEU:C	2.59	0.40
1:D:536:LYS:HB3	1:D:536:LYS:NZ	2.35	0.40
1:D:231:THR:HG22	1:D:232:GLU:HG3	2.03	0.40
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.81	0.40
1:C:74:ASN:HB3	1:C:92:ASN:HB3	2.04	0.40
1:C:39:SER:HB2	1:C:40:ARG:HE	1.86	0.40
1:A:301:CYS:O	1:A:302:ASP:HB2	2.20	0.40
1:D:125:ARG:HG2	1:D:126:HIS:CE1	2.55	0.40
1:A:519:LEU:O	1:A:520:ASN:C	2.60	0.40
1:C:522:THR:CG2	1:C:523:LYS:N	2.85	0.40
1:C:689:MET:HG3	1:D:244:GLU:CD	2.42	0.40
1:B:662:TYR:HB3	1:B:667:THR:OG1	2.21	0.40
1:B:741:GLY:O	1:B:742:ILE:C	2.59	0.40
1:B:756:SER:O	1:B:760:LYS:HG2	2.21	0.40
1:C:477:LEU:HD12	1:C:501:ASP:HB2	2.02	0.40
1:D:183:TYR:CD2	1:D:276:LEU:HG	2.56	0.40
1:D:69:LEU:CD1	1:D:107:ILE:HD12	2.52	0.40
1:A:514:LEU:HD12	1:A:557:THR:CG2	2.48	0.40
1:C:316:LEU:HD21	1:C:320:GLN:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:GLN:NE2	1:C:373:LYS:HZ1	2.20	0.40
1:C:750:HIS:CD2	1:D:724:VAL:HA	2.56	0.40
1:C:286:GLN:HE21	1:C:288:THR:HG22	1.86	0.40
1:B:581:ARG:NE	1:B:605:ASP:OD2	2.47	0.40
1:A:70:TYR:HB3	1:A:79:PHE:CE2	2.57	0.40
1:D:160:VAL:HG23	1:D:161:GLY:N	2.36	0.40
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.56	0.40
1:D:95:PHE:HB3	1:D:98:PHE:HB2	2.02	0.40
1:A:334:SER:HB2	1:A:336:ARG:HD2	2.04	0.40
1:B:336:ARG:H	1:B:336:ARG:HD2	1.86	0.40
1:B:325:MET:HE2	1:B:327:ILE:HD11	2.03	0.40
1:A:459:VAL:CG2	1:A:460:SER:N	2.82	0.40
1:D:522:THR:CG2	1:D:523:LYS:N	2.85	0.40
1:C:55:LEU:HD23	1:C:500:LEU:HD22	2.04	0.40
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.57	0.40
1:C:514:LEU:HD23	1:C:526:TYR:O	2.22	0.40
1:A:598:LEU:HD22	1:A:631:TYR:OH	2.21	0.40
1:D:330:TYR:HE1	1:D:335:GLY:O	2.04	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	724/728 (100%)	647 (89%)	69 (10%)	8 (1%)	17	50
1	B	724/728 (100%)	650 (90%)	65 (9%)	9 (1%)	16	47
1	C	724/728 (100%)	643 (89%)	68 (9%)	13 (2%)	11	34
1	D	724/728 (100%)	643 (89%)	67 (9%)	14 (2%)	10	32
All	All	2896/2912 (100%)	2583 (89%)	269 (9%)	44 (2%)	13	40

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	277	SER
1	A	278	SER
1	B	40	ARG
1	B	277	SER
1	B	278	SER
1	C	40	ARG
1	C	278	SER
1	D	40	ARG
1	D	278	SER
1	A	289	ALA
1	A	320	GLN
1	A	520	ASN
1	B	289	ALA
1	B	520	ASN
1	C	289	ALA
1	C	320	GLN
1	C	486	VAL
1	C	520	ASN
1	C	536	LYS
1	D	289	ALA
1	D	320	GLN
1	D	486	VAL
1	D	520	ASN
1	D	536	LYS
1	A	94	THR
1	A	583	SER
1	B	320	GLN
1	C	138	ASN
1	C	282	ALA
1	C	412	SER
1	C	463	LYS
1	D	138	ASN
1	D	282	ALA
1	D	412	SER
1	B	583	SER
1	C	334	SER
1	D	334	SER
1	D	463	LYS
1	B	94	THR
1	B	273	THR
1	C	218	PRO
1	D	450	ASN

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Mol	Chain	Res	Type
1	D	218	PRO

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	651/653 (100%)	600 (92%)	51 (8%)	16	41
1	B	651/653 (100%)	600 (92%)	51 (8%)	16	41
1	C	651/653 (100%)	599 (92%)	52 (8%)	15	40
1	D	651/653 (100%)	598 (92%)	53 (8%)	15	39
All	All	2604/2612 (100%)	2397 (92%)	207 (8%)	15	40

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	41	LYS
1	A	51	ASN
1	A	61	ARG
1	A	66	HIS
1	A	75	ASN
1	A	90	LEU
1	A	92	ASN
1	A	110	ASP
1	A	125	ARG
1	A	140	ARG
1	A	141	GLN
1	A	170	ASN
1	A	184	ARG
1	A	207	VAL
1	A	209	SER
1	A	214	LEU
1	A	246	LEU
1	A	253	ARG

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Mol	Chain	Res	Type
1	A	254	VAL
1	A	272	ASN
1	A	276	LEU
1	A	293	MET
1	A	303	VAL
1	A	313	LEU
1	A	326	ASP
1	A	336	ARG
1	A	376	SER
1	A	385	CYS
1	A	388	GLN
1	A	413	ASP
1	A	436	LEU
1	A	440	THR
1	A	442	VAL
1	A	448	GLU
1	A	482	LEU
1	A	487	ASN
1	A	514	LEU
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	581	ARG
1	A	603	VAL
1	A	608	GLU
1	A	679	ASN
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	736	THR
1	A	761	GLN
1	B	39	SER
1	B	40	ARG
1	B	41	LYS
1	B	51	ASN
1	B	61	ARG
1	B	66	HIS
1	B	75	ASN
1	B	90	LEU
1	B	92	ASN
1	B	110	ASP
1	B	125	ARG

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Mol	Chain	Res	Type
1	B	140	ARG
1	B	141	GLN
1	B	170	ASN
1	B	184	ARG
1	B	207	VAL
1	B	209	SER
1	B	214	LEU
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	272	ASN
1	B	276	LEU
1	B	293	MET
1	B	303	VAL
1	B	313	LEU
1	B	326	ASP
1	B	336	ARG
1	B	376	SER
1	B	385	CYS
1	B	388	GLN
1	B	413	ASP
1	B	436	LEU
1	B	440	THR
1	B	448	GLU
1	B	482	LEU
1	B	485	SER
1	B	487	ASN
1	B	514	LEU
1	B	536	LYS
1	B	543	LEU
1	B	561	LEU
1	B	581	ARG
1	B	603	VAL
1	B	608	GLU
1	B	679	ASN
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	736	THR
1	B	761	GLN
1	C	40	ARG
1	C	41	LYS

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Mol	Chain	Res	Type
1	C	75	ASN
1	C	90	LEU
1	C	91	GLU
1	C	92	ASN
1	C	110	ASP
1	C	140	ARG
1	C	141	GLN
1	C	145	GLU
1	C	147	ARG
1	C	170	ASN
1	C	184	ARG
1	C	207	VAL
1	C	209	SER
1	C	214	LEU
1	C	246	LEU
1	C	253	ARG
1	C	272	ASN
1	C	276	LEU
1	C	293	MET
1	C	313	LEU
1	C	326	ASP
1	C	336	ARG
1	C	385	CYS
1	C	388	GLN
1	C	390	ASP
1	C	436	LEU
1	C	440	THR
1	C	448	GLU
1	C	472	CYS
1	C	482	LEU
1	C	498	SER
1	C	507	VAL
1	C	514	LEU
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU
1	C	546	VAL
1	C	561	LEU
1	C	581	ARG
1	C	597	ARG
1	C	603	VAL
1	C	608	GLU

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Mol	Chain	Res	Type
1	C	658	ARG
1	C	679	ASN
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	736	THR
1	C	760	LYS
1	C	761	GLN
1	D	40	ARG
1	D	41	LYS
1	D	75	ASN
1	D	90	LEU
1	D	91	GLU
1	D	92	ASN
1	D	103	ASN
1	D	110	ASP
1	D	125	ARG
1	D	140	ARG
1	D	141	GLN
1	D	145	GLU
1	D	147	ARG
1	D	170	ASN
1	D	184	ARG
1	D	207	VAL
1	D	209	SER
1	D	214	LEU
1	D	246	LEU
1	D	253	ARG
1	D	272	ASN
1	D	275	SER
1	D	276	LEU
1	D	293	MET
1	D	326	ASP
1	D	336	ARG
1	D	385	CYS
1	D	388	GLN
1	D	390	ASP
1	D	436	LEU
1	D	440	THR
1	D	448	GLU
1	D	482	LEU
1	D	498	SER

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Mol	Chain	Res	Type
1	D	507	VAL
1	D	514	LEU
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	546	VAL
1	D	561	LEU
1	D	581	ARG
1	D	597	ARG
1	D	603	VAL
1	D	608	GLU
1	D	658	ARG
1	D	679	ASN
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	736	THR
1	D	760	LYS
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	92	ASN
1	A	119	ASN
1	A	123	GLN
1	A	169	ASN
1	A	170	ASN
1	A	227	GLN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	369	ASN
1	A	483	HIS
1	A	487	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN

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Mol	Chain	Res	Type
1	B	72	GLN
1	B	92	ASN
1	B	119	ASN
1	B	123	GLN
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	369	ASN
1	B	388	GLN
1	B	483	HIS
1	B	487	ASN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	GLN
1	C	72	GLN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	286	GLN
1	C	314	GLN
1	C	369	ASN
1	C	388	GLN
1	C	483	HIS
1	C	487	ASN
1	C	505	GLN
1	C	520	ASN
1	C	533	HIS
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	761	GLN
1	D	72	GLN
1	D	169	ASN

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Mol	Chain	Res	Type
1	D	170	ASN
1	D	247	GLN
1	D	272	ASN
1	D	286	GLN
1	D	314	GLN
1	D	369	ASN
1	D	388	GLN
1	D	483	HIS
1	D	487	ASN
1	D	505	GLN
1	D	533	HIS
1	D	572	ASN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	761	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

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	GGO	B	901	-	31,31,31	1.85	5 (16%)	40,45,45	1.16	5 (12%)

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	GGO	B	901	-	-	0/9/31/31	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	GGO	O-C10	-2.06	1.35	1.38
2	B	901	GGO	C20-C27	3.39	1.43	1.38
2	B	901	GGO	C8-C7	3.89	1.47	1.38
2	B	901	GGO	C18-C16	4.13	1.57	1.51
2	B	901	GGO	C16-N4	5.28	1.40	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	GGO	C12-O13-C14	-2.18	102.22	105.35
2	B	901	GGO	C12-O-C10	-2.16	102.24	105.35
2	B	901	GGO	C5-N4-C3	2.00	118.92	116.98
2	B	901	GGO	C-C3-N4	2.24	113.74	110.89
2	B	901	GGO	O13-C12-O	2.28	111.98	108.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	GGO	1	0

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	726/728 (99%)	-0.05	17 (2%)	64	52	3, 27, 62, 153	0
1	B	726/728 (99%)	0.07	31 (4%)	39	27	6, 28, 68, 116	0
1	C	726/728 (99%)	-0.04	20 (2%)	56	44	5, 33, 69, 111	0
1	D	726/728 (99%)	-0.06	23 (3%)	51	39	10, 31, 66, 146	0
All	All	2904/2912 (99%)	-0.02	91 (3%)	52	40	3, 29, 67, 153	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	13.0
1	A	278	SER	10.8
1	C	39	SER	7.5
1	A	280	THR	7.4
1	A	277	SER	6.3
1	D	39	SER	5.7
1	B	39	SER	5.5
1	D	278	SER	5.0
1	B	71	LYS	4.9
1	A	282	ALA	4.8
1	D	88	VAL	4.7
1	A	39	SER	4.3
1	A	281	ASN	4.2
1	A	73	GLU	3.9
1	D	91	GLU	3.8
1	C	73	GLU	3.7
1	D	87	SER	3.7
1	B	111	GLY	3.7
1	B	280	THR	3.7
1	B	105	TYR	3.5
1	C	98	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	89	PHE	3.5
1	B	96	ASP	3.5
1	A	74	ASN	3.4
1	D	92	ASN	3.4
1	B	92	ASN	3.4
1	B	99	GLY	3.4
1	C	105	TYR	3.3
1	B	98	PHE	3.2
1	D	99	GLY	3.1
1	C	89	PHE	3.1
1	D	86	SER	3.0
1	A	502	LYS	3.0
1	C	71	LYS	3.0
1	B	73	GLU	2.9
1	C	142	LEU	2.9
1	C	138	ASN	2.9
1	B	93	SER	2.8
1	C	277	SER	2.8
1	B	76	ILE	2.8
1	D	101	SER	2.8
1	D	83	TYR	2.8
1	D	77	LEU	2.7
1	D	98	PHE	2.7
1	C	90	LEU	2.7
1	B	278	SER	2.6
1	A	333	SER	2.6
1	B	142	LEU	2.6
1	C	392	LYS	2.6
1	B	89	PHE	2.6
1	B	141	GLN	2.6
1	C	74	ASN	2.6
1	C	82	GLU	2.6
1	A	72	GLN	2.5
1	B	491	LEU	2.5
1	C	88	VAL	2.5
1	C	504	LEU	2.5
1	B	95	PHE	2.5
1	B	74	ASN	2.5
1	D	85	ASN	2.5
1	D	333	SER	2.5
1	C	140	ARG	2.5
1	B	114	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	97	GLU	2.4
1	B	277	SER	2.4
1	B	91	GLU	2.4
1	D	105	TYR	2.4
1	D	289	ALA	2.3
1	C	173	TYR	2.3
1	D	281	ASN	2.3
1	B	90	LEU	2.3
1	C	94	THR	2.3
1	D	97	GLU	2.3
1	C	72	GLN	2.2
1	D	40	ARG	2.2
1	A	142	LEU	2.2
1	B	101	SER	2.2
1	A	138	ASN	2.2
1	D	74	ASN	2.1
1	B	61	ARG	2.1
1	B	102	ILE	2.1
1	A	90	LEU	2.1
1	B	40	ARG	2.1
1	C	87	SER	2.1
1	B	487	ASN	2.1
1	D	96	ASP	2.1
1	A	505	GLN	2.1
1	B	135	TYR	2.1
1	A	489	LYS	2.0
1	B	289	ALA	2.0
1	D	93	SER	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	GGO	B	901	28/28	0.90	0.25	2.63	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.