Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:32 AM GMT

PDB ID	:	3P3W
Title	:	Structure of a dimeric GluA3 N-terminal domain (NTD) at 4.2 A resolution
Authors	:	Rossmann, M.; Sukumaran, M.; Greger, I.H.
Deposited on	:	2010-10-05
Resolution	:	4.20 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:

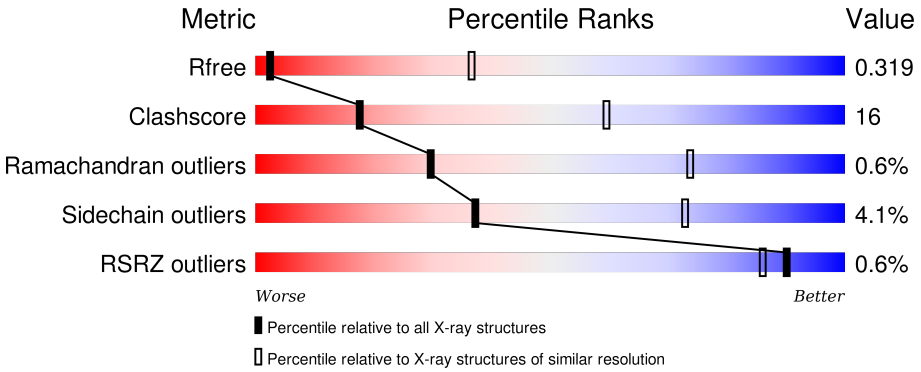
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	389	82% 12%
1	B	389	78% 16%
1	C	389	71% 20% 7%
1	D	389	2% 71% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11484 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 Glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2906	1853	491	546	16			
1	B	374	Total	C	N	O	S	0	0	0
			2914	1859	501	538	16			
1	C	362	Total	C	N	O	S	0	0	0
			2790	1788	463	523	16			
1	D	373	Total	C	N	O	S	0	0	0
			2874	1834	483	542	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	GLY	-	EXPRESSION TAG	UNP P19492
A	383	THR	-	EXPRESSION TAG	UNP P19492
A	384	HIS	-	EXPRESSION TAG	UNP P19492
A	385	HIS	-	EXPRESSION TAG	UNP P19492
A	386	HIS	-	EXPRESSION TAG	UNP P19492
A	387	HIS	-	EXPRESSION TAG	UNP P19492
A	388	HIS	-	EXPRESSION TAG	UNP P19492
A	389	HIS	-	EXPRESSION TAG	UNP P19492
B	382	GLY	-	EXPRESSION TAG	UNP P19492
B	383	THR	-	EXPRESSION TAG	UNP P19492
B	384	HIS	-	EXPRESSION TAG	UNP P19492
B	385	HIS	-	EXPRESSION TAG	UNP P19492
B	386	HIS	-	EXPRESSION TAG	UNP P19492
B	387	HIS	-	EXPRESSION TAG	UNP P19492
B	388	HIS	-	EXPRESSION TAG	UNP P19492
B	389	HIS	-	EXPRESSION TAG	UNP P19492
C	382	GLY	-	EXPRESSION TAG	UNP P19492
C	383	THR	-	EXPRESSION TAG	UNP P19492
C	384	HIS	-	EXPRESSION TAG	UNP P19492
C	385	HIS	-	EXPRESSION TAG	UNP P19492
C	386	HIS	-	EXPRESSION TAG	UNP P19492

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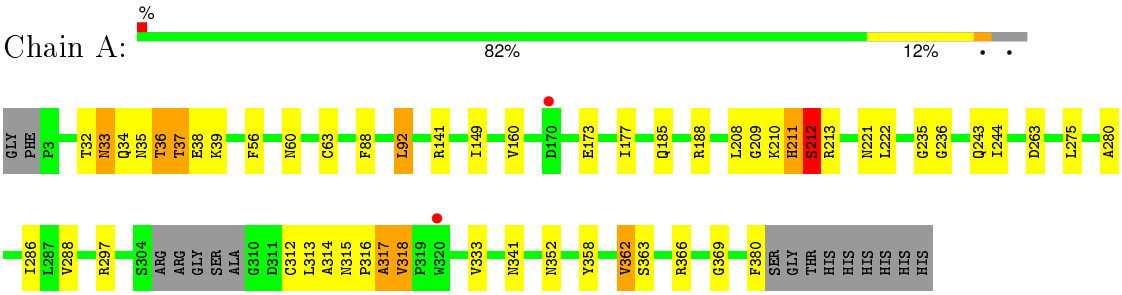
Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	EXPRESSION TAG	UNP P19492
C	388	HIS	-	EXPRESSION TAG	UNP P19492
C	389	HIS	-	EXPRESSION TAG	UNP P19492
D	382	GLY	-	EXPRESSION TAG	UNP P19492
D	383	THR	-	EXPRESSION TAG	UNP P19492
D	384	HIS	-	EXPRESSION TAG	UNP P19492
D	385	HIS	-	EXPRESSION TAG	UNP P19492
D	386	HIS	-	EXPRESSION TAG	UNP P19492
D	387	HIS	-	EXPRESSION TAG	UNP P19492
D	388	HIS	-	EXPRESSION TAG	UNP P19492
D	389	HIS	-	EXPRESSION TAG	UNP P19492

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.

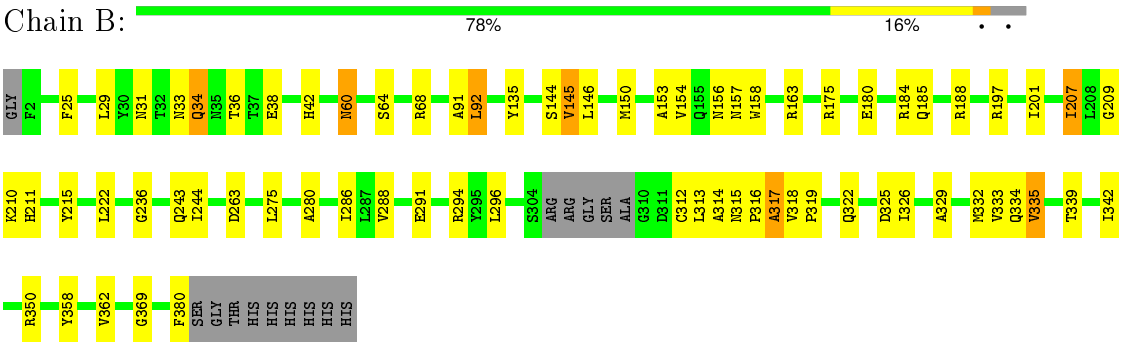
- Molecule 1: Glutamate receptor 3

Chain A:



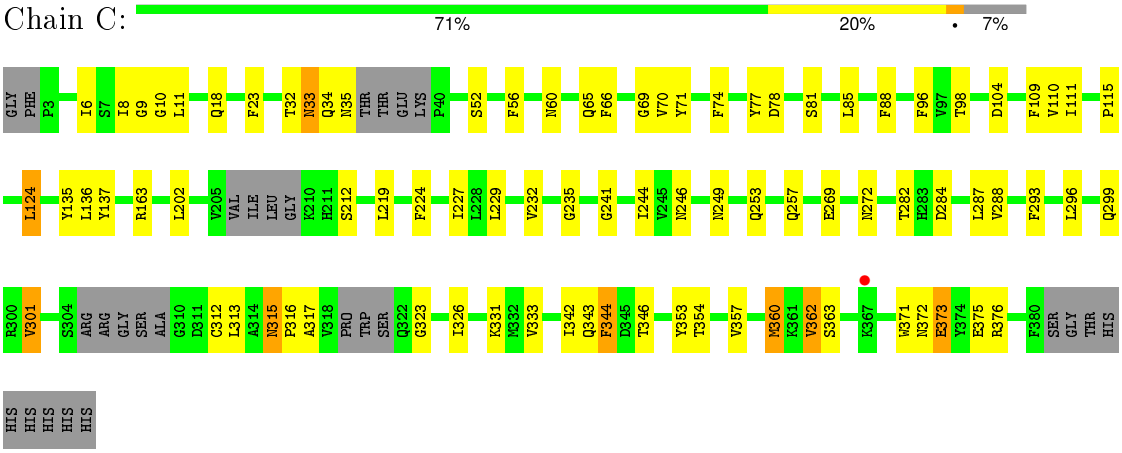
- Molecule 1: Glutamate receptor 3

Chain B:



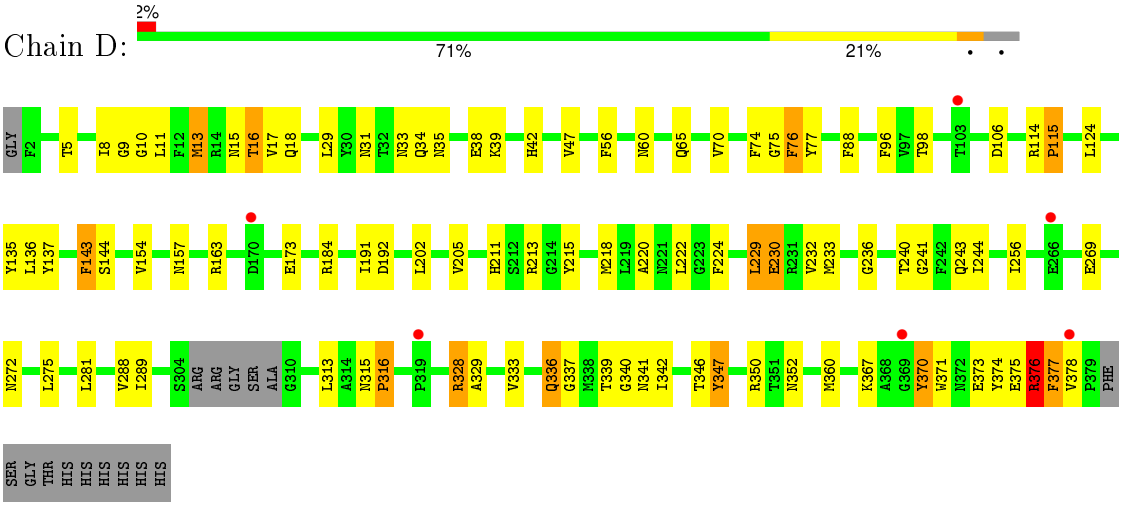
- Molecule 1: Glutamate receptor 3

Chain C:



• Molecule 1: Glutamate receptor 3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.96Å 127.92Å 130.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.41 – 4.20 55.41 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (55.41-4.20) 99.2 (55.41-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.32	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.306 , 0.338 0.297 , 0.319	Depositor DCC
R_{free} test set	688 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	104.7	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 66.8	EDS
Estimated twinning fraction	0.078 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 13917 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.01% 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

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	0.35	0/2973	0.61	7/4044 (0.2%)
1	B	0.33	0/2981	0.55	0/4054
1	C	0.33	0/2851	0.53	1/3869 (0.0%)
1	D	0.37	1/2938 (0.0%)	0.59	3/3999 (0.1%)
All	All	0.34	1/11743 (0.0%)	0.57	11/15966 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	115	PRO	N-CD	-6.64	1.38	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	ARG	N-CA-CB	-10.41	91.86	110.60
1	C	33	ASN	CB-CA-C	7.33	125.06	110.40
1	A	213	ARG	N-CA-C	7.24	130.54	111.00
1	D	230	GLU	N-CA-C	6.30	128.01	111.00
1	A	37	THR	N-CA-CB	-6.21	98.51	110.30
1	A	211	HIS	N-CA-C	-6.05	94.67	111.00
1	A	36	THR	CA-C-N	-5.80	104.43	117.20
1	D	143	PHE	N-CA-C	5.59	126.10	111.00
1	A	36	THR	CA-C-O	5.34	131.32	120.10
1	A	212	SER	CA-C-N	-5.09	105.99	117.20
1	D	229	LEU	N-CA-C	5.06	124.66	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	2906	0	2714	64	0
1	B	2914	0	2735	93	0
1	C	2790	0	2596	80	0
1	D	2874	0	2671	136	0
All	All	11484	0	10716	351	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 16.

All (351) 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:236:GLY:CA	1:A:362:VAL:HG11	1.57	1.32
1:A:236:GLY:HA2	1:A:362:VAL:CG1	1.61	1.29
1:A:33:ASN:HA	1:A:34:GLN:CB	1.53	1.26
1:B:33:ASN:HA	1:B:34:GLN:CB	1.61	1.23
1:B:319:PRO:HG2	1:B:322:GLN:OE1	1.45	1.15
1:B:33:ASN:HA	1:B:34:GLN:HB3	1.25	1.14
1:D:15:ASN:ND2	1:D:16:THR:H	1.44	1.14
1:C:111:ILE:CG2	1:C:344:PHE:HE1	1.61	1.14
1:B:33:ASN:CA	1:B:34:GLN:HB3	1.79	1.12
1:C:111:ILE:CG2	1:C:344:PHE:CE1	2.31	1.12
1:B:318:VAL:HG13	1:B:319:PRO:HD2	1.15	1.11
1:A:33:ASN:HD22	1:A:35:ASN:N	1.50	1.08
1:C:111:ILE:HG23	1:C:344:PHE:CE1	1.85	1.08
1:B:312:CYS:C	1:B:313:LEU:HD12	1.72	1.08
1:A:36:THR:HG23	1:A:37:THR:HG23	1.35	1.06
1:A:33:ASN:CA	1:A:34:GLN:CB	2.33	1.06
1:D:376:ARG:CG	1:D:376:ARG:HH11	1.68	1.06
1:D:336:GLN:HA	1:D:336:GLN:OE1	1.43	1.05
1:B:319:PRO:HG2	1:B:322:GLN:CD	1.78	1.03
1:B:33:ASN:HA	1:B:34:GLN:HB2	1.43	1.01
1:B:156:ASN:ND2	1:B:158:TRP:CZ2	2.30	1.00
1:C:111:ILE:HG23	1:C:344:PHE:CD1	1.96	1.00
1:D:370:TYR:O	1:D:370:TYR:HD1	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:OD1	1:B:34:GLN:HB3	1.61	0.99
1:D:222:LEU:HD22	1:D:244:ILE:CD1	1.93	0.99
1:C:111:ILE:HG22	1:C:344:PHE:HE1	1.28	0.99
1:D:15:ASN:CG	1:D:16:THR:H	1.64	0.98
1:B:314:ALA:C	1:B:316:PRO:HD2	1.86	0.96
1:D:11:LEU:CD2	1:D:65:GLN:HE21	1.77	0.96
1:C:353:TYR:CE1	1:C:373:GLU:OE2	2.16	0.96
1:C:315:ASN:CB	1:C:316:PRO:HD3	1.96	0.96
1:B:154:VAL:CG1	1:D:184:ARG:HH12	1.79	0.96
1:B:33:ASN:CA	1:B:34:GLN:CB	2.38	0.95
1:D:371:TRP:CD2	1:D:371:TRP:CZ3	2.41	0.95
1:D:15:ASN:O	1:D:16:THR:HG23	1.67	0.95
1:B:33:ASN:CB	1:B:34:GLN:HB3	1.98	0.94
1:B:154:VAL:HG12	1:D:184:ARG:HH12	1.30	0.94
1:B:33:ASN:CG	1:B:34:GLN:HB3	1.88	0.93
1:C:96:PHE:HB3	1:C:110:VAL:HG12	1.49	0.93
1:D:222:LEU:HD22	1:D:244:ILE:HD11	1.48	0.92
1:D:370:TYR:CE1	1:D:378:VAL:HB	2.04	0.92
1:D:346:THR:HG23	1:D:347:TYR:CD1	2.05	0.91
1:B:319:PRO:CG	1:B:322:GLN:OE1	2.20	0.89
1:B:314:ALA:HB3	1:D:60:ASN:CB	2.03	0.89
1:C:343:GLN:C	1:C:344:PHE:HD2	1.77	0.88
1:D:376:ARG:HG2	1:D:376:ARG:HH11	1.34	0.88
1:C:315:ASN:HB2	1:C:316:PRO:HD3	1.52	0.88
1:B:318:VAL:HG13	1:B:319:PRO:CD	2.03	0.88
1:D:315:ASN:HB2	1:D:316:PRO:HD3	1.56	0.87
1:B:197:ARG:O	1:B:201:ILE:HD12	1.74	0.87
1:B:315:ASN:N	1:B:316:PRO:CD	2.39	0.86
1:C:11:LEU:HD11	1:C:65:GLN:HG3	1.55	0.85
1:D:15:ASN:CG	1:D:16:THR:N	2.31	0.84
1:A:33:ASN:ND2	1:A:34:GLN:C	2.30	0.84
1:D:15:ASN:C	1:D:16:THR:HG23	1.94	0.84
1:D:11:LEU:CD2	1:D:65:GLN:NE2	2.40	0.84
1:D:106:ASP:HB3	1:D:347:TYR:CD2	2.12	0.84
1:D:10:GLY:C	1:D:11:LEU:HD23	1.98	0.83
1:A:236:GLY:HA2	1:A:362:VAL:HG11	0.83	0.82
1:B:33:ASN:OD1	1:B:34:GLN:CB	2.27	0.81
1:B:318:VAL:CG1	1:B:319:PRO:HD2	2.05	0.81
1:A:92:LEU:HD12	1:A:318:VAL:HG21	1.61	0.81
1:B:313:LEU:HB2	1:B:316:PRO:HG3	1.60	0.81
1:A:236:GLY:CA	1:A:362:VAL:CG1	2.35	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ARG:HG3	1:D:376:ARG:HH11	1.46	0.80
1:A:32:THR:HG23	1:A:32:THR:O	1.80	0.80
1:B:313:LEU:HD12	1:B:313:LEU:N	1.96	0.79
1:A:33:ASN:ND2	1:A:35:ASN:N	2.30	0.79
1:A:212:SER:HB3	1:A:235:GLY:HA3	1.65	0.79
1:C:32:THR:O	1:C:33:ASN:OD1	2.01	0.78
1:D:229:LEU:HD13	1:D:360:MET:SD	2.24	0.78
1:D:75:GLY:C	1:D:76:PHE:HD2	1.86	0.78
1:B:313:LEU:O	1:B:316:PRO:CG	2.32	0.78
1:D:346:THR:HG23	1:D:347:TYR:CE1	2.20	0.77
1:B:313:LEU:CB	1:B:316:PRO:HG3	2.15	0.77
1:A:212:SER:HB3	1:A:235:GLY:CA	2.14	0.77
1:A:236:GLY:C	1:A:362:VAL:CG1	2.53	0.77
1:D:370:TYR:O	1:D:370:TYR:CD1	2.33	0.77
1:C:353:TYR:HE1	1:C:373:GLU:OE2	1.62	0.77
1:B:339:THR:HG22	1:B:339:THR:O	1.84	0.77
1:B:222:LEU:HD22	1:B:244:ILE:HG23	1.67	0.76
1:A:236:GLY:C	1:A:362:VAL:HG11	2.05	0.76
1:C:315:ASN:CG	1:C:316:PRO:HD3	2.06	0.76
1:A:316:PRO:O	1:A:317:ALA:HB3	1.86	0.75
1:B:154:VAL:HG12	1:D:184:ARG:NH1	2.02	0.74
1:D:376:ARG:NH1	1:D:376:ARG:CG	2.39	0.74
1:C:342:ILE:HG22	1:C:344:PHE:HE2	1.50	0.73
1:D:315:ASN:CB	1:D:316:PRO:HD3	2.18	0.73
1:A:314:ALA:C	1:A:316:PRO:HD2	2.09	0.73
1:A:33:ASN:HD22	1:A:35:ASN:CB	2.02	0.72
1:D:377:PHE:HD1	1:D:378:VAL:N	1.87	0.72
1:C:371:TRP:CD1	1:C:376:ARG:O	2.43	0.72
1:B:163:ARG:NH2	1:B:180:GLU:OE1	2.19	0.72
1:C:315:ASN:CB	1:C:316:PRO:CD	2.68	0.72
1:A:33:ASN:ND2	1:A:35:ASN:CB	2.53	0.72
1:A:315:ASN:N	1:A:316:PRO:HD2	2.04	0.72
1:A:33:ASN:HD22	1:A:35:ASN:CA	2.03	0.72
1:D:370:TYR:CD1	1:D:370:TYR:C	2.62	0.72
1:D:370:TYR:C	1:D:370:TYR:HD1	1.93	0.71
1:D:106:ASP:HB3	1:D:347:TYR:CE2	2.25	0.71
1:B:135:TYR:OH	1:B:145:VAL:CG2	2.39	0.71
1:A:33:ASN:HD22	1:A:34:GLN:C	1.88	0.71
1:B:64:SER:O	1:B:68:ARG:HG3	1.90	0.71
1:D:11:LEU:HD23	1:D:11:LEU:N	2.06	0.70
1:A:210:LYS:HG2	1:A:210:LYS:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ASN:N	1:B:316:PRO:HD2	2.05	0.70
1:D:15:ASN:ND2	1:D:16:THR:N	2.30	0.70
1:B:313:LEU:N	1:B:313:LEU:CD1	2.55	0.70
1:C:343:GLN:C	1:C:344:PHE:CD2	2.64	0.70
1:D:222:LEU:HD22	1:D:244:ILE:HD12	1.73	0.69
1:D:15:ASN:O	1:D:16:THR:CG2	2.41	0.69
1:D:222:LEU:CD2	1:D:244:ILE:HD11	2.20	0.69
1:A:315:ASN:N	1:A:316:PRO:CD	2.56	0.69
1:B:209:GLY:O	1:B:211:HIS:ND1	2.24	0.69
1:B:31:ASN:ND2	1:B:42:HIS:CE1	2.60	0.69
1:B:33:ASN:OD1	1:B:34:GLN:CG	2.41	0.69
1:B:313:LEU:O	1:B:316:PRO:HG2	1.92	0.68
1:A:316:PRO:O	1:A:317:ALA:CB	2.40	0.68
1:D:347:TYR:N	1:D:347:TYR:HD1	1.92	0.68
1:A:314:ALA:HB3	1:C:60:ASN:CB	2.24	0.67
1:D:11:LEU:HD22	1:D:65:GLN:HE21	1.58	0.67
1:D:347:TYR:N	1:D:347:TYR:CD1	2.60	0.66
1:A:35:ASN:CB	1:A:38:GLU:HB2	2.24	0.66
1:B:314:ALA:HB2	1:D:56:PHE:CE2	2.30	0.66
1:A:275:LEU:HD11	1:A:280:ALA:HB2	1.78	0.66
1:D:315:ASN:HB2	1:D:316:PRO:CD	2.25	0.66
1:A:212:SER:CB	1:A:235:GLY:HA3	2.26	0.66
1:B:313:LEU:O	1:B:316:PRO:CD	2.44	0.65
1:A:209:GLY:O	1:A:211:HIS:ND1	2.29	0.65
1:D:337:GLY:N	1:D:340:GLY:O	2.30	0.65
1:A:33:ASN:CG	1:A:34:GLN:CB	2.65	0.64
1:D:352:ASN:N	1:D:373:GLU:OE1	2.25	0.64
1:C:8:ILE:HD11	1:C:23:PHE:HZ	1.62	0.63
1:D:337:GLY:O	1:D:340:GLY:N	2.31	0.63
1:D:76:PHE:N	1:D:76:PHE:CD2	2.64	0.63
1:B:334:GLN:O	1:B:334:GLN:CG	2.47	0.63
1:B:156:ASN:ND2	1:B:158:TRP:CH2	2.61	0.63
1:B:275:LEU:HD11	1:B:280:ALA:HB2	1.79	0.63
1:C:315:ASN:ND2	1:C:316:PRO:HD3	2.14	0.62
1:D:376:ARG:HG3	1:D:376:ARG:NH1	2.09	0.62
1:D:213:ARG:O	1:D:215:TYR:HD2	1.83	0.62
1:B:312:CYS:O	1:B:313:LEU:HD12	1.99	0.62
1:D:370:TYR:HE1	1:D:378:VAL:HB	1.60	0.62
1:C:372:ASN:OD1	1:C:375:GLU:HB2	2.00	0.61
1:B:339:THR:HG21	1:B:350:ARG:HH12	1.66	0.60
1:A:313:LEU:O	1:A:316:PRO:HD2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:HG22	1:C:344:PHE:CE1	2.18	0.60
1:A:208:LEU:HD23	1:A:211:HIS:CE1	2.37	0.60
1:B:33:ASN:OD1	1:B:34:GLN:HG2	2.01	0.60
1:B:156:ASN:HB2	1:B:158:TRP:CE2	2.36	0.60
1:C:115:PRO:HG2	1:C:244:ILE:HG21	1.84	0.59
1:D:11:LEU:HD23	1:D:65:GLN:NE2	2.17	0.59
1:B:314:ALA:CB	1:D:60:ASN:CB	2.80	0.59
1:B:315:ASN:N	1:B:316:PRO:HD3	2.18	0.59
1:B:184:ARG:HH21	1:D:157:ASN:HA	1.67	0.59
1:D:376:ARG:HG2	1:D:376:ARG:NH1	2.12	0.59
1:A:222:LEU:HD22	1:A:244:ILE:HG23	1.85	0.59
1:D:76:PHE:HD2	1:D:76:PHE:N	1.98	0.59
1:D:47:VAL:O	1:D:47:VAL:HG13	2.01	0.59
1:A:212:SER:HB3	1:A:235:GLY:C	2.24	0.58
1:C:74:PHE:HZ	1:C:282:THR:HG22	1.68	0.58
1:A:173:GLU:O	1:A:177:ILE:HG12	2.03	0.58
1:D:124:LEU:HD21	1:D:377:PHE:HE2	1.69	0.58
1:D:135:TYR:CE2	1:D:137:TYR:HB3	2.37	0.58
1:D:288:VAL:HG23	1:D:333:VAL:HG21	1.86	0.58
1:A:288:VAL:HG13	1:A:333:VAL:HG21	1.86	0.57
1:D:377:PHE:CD1	1:D:378:VAL:N	2.70	0.57
1:C:10:GLY:C	1:C:11:LEU:HD12	2.25	0.57
1:C:342:ILE:CG2	1:C:344:PHE:HE2	2.18	0.57
1:D:15:ASN:C	1:D:16:THR:CG2	2.66	0.57
1:C:32:THR:O	1:C:33:ASN:CG	2.43	0.57
1:C:342:ILE:HG22	1:C:344:PHE:CE2	2.37	0.56
1:D:136:LEU:HD12	1:D:191:ILE:HG12	1.86	0.56
1:A:314:ALA:CB	1:C:60:ASN:CB	2.83	0.56
1:B:153:ALA:O	1:B:157:ASN:N	2.38	0.56
1:A:141:ARG:NH2	1:A:221:ASN:HD22	2.02	0.56
1:D:18:GLN:CB	1:D:269:GLU:HB2	2.36	0.56
1:D:74:PHE:CZ	1:D:76:PHE:HE2	2.23	0.56
1:C:344:PHE:N	1:C:344:PHE:CD2	2.74	0.56
1:B:313:LEU:O	1:B:316:PRO:HD2	2.06	0.56
1:C:331:LYS:HD3	1:C:346:THR:O	2.06	0.56
1:D:222:LEU:HD13	1:D:244:ILE:HD11	1.88	0.55
1:D:11:LEU:HD21	1:D:65:GLN:HG3	1.87	0.55
1:B:154:VAL:HG13	1:D:184:ARG:HH12	1.65	0.55
1:B:211:HIS:O	1:B:215:TYR:CG	2.59	0.55
1:B:60:ASN:HD21	1:D:313:LEU:HA	1.71	0.55
1:B:329:ALA:HA	1:B:332:MET:HG2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:O	1:B:154:VAL:HG23	2.06	0.55
1:A:313:LEU:O	1:A:316:PRO:CG	2.55	0.55
1:D:281:LEU:HD23	1:D:339:THR:HG21	1.88	0.55
1:D:315:ASN:CB	1:D:316:PRO:CD	2.83	0.55
1:B:339:THR:HG22	1:B:350:ARG:HH22	1.72	0.55
1:A:313:LEU:O	1:A:316:PRO:CD	2.55	0.55
1:D:230:GLU:HA	1:D:233:MET:HB2	1.88	0.55
1:B:334:GLN:HG2	1:B:334:GLN:O	2.06	0.54
1:C:66:PHE:O	1:C:69:GLY:N	2.40	0.54
1:C:315:ASN:HB2	1:C:316:PRO:CD	2.32	0.54
1:C:8:ILE:HD11	1:C:23:PHE:CZ	2.42	0.54
1:A:36:THR:CG2	1:A:37:THR:HG23	2.23	0.54
1:C:344:PHE:N	1:C:344:PHE:HD2	2.03	0.54
1:C:315:ASN:OD1	1:C:315:ASN:N	2.32	0.54
1:C:18:GLN:HG2	1:C:269:GLU:HB3	1.89	0.54
1:D:336:GLN:CA	1:D:336:GLN:OE1	2.32	0.53
1:D:74:PHE:CE2	1:D:76:PHE:HE2	2.26	0.53
1:B:319:PRO:CG	1:B:322:GLN:CD	2.65	0.53
1:C:315:ASN:CG	1:C:316:PRO:CD	2.74	0.53
1:D:328:ARG:HH21	1:D:329:ALA:HA	1.74	0.53
1:C:372:ASN:OD1	1:C:375:GLU:CB	2.57	0.53
1:B:184:ARG:NH2	1:D:157:ASN:HA	2.24	0.53
1:D:346:THR:C	1:D:347:TYR:HD1	2.11	0.53
1:D:74:PHE:CE2	1:D:76:PHE:CE2	2.97	0.53
1:D:11:LEU:HD21	1:D:65:GLN:NE2	2.22	0.52
1:A:362:VAL:CG2	1:A:363:SER:N	2.72	0.52
1:D:124:LEU:HD21	1:D:377:PHE:CE2	2.44	0.52
1:D:33:ASN:HB2	1:D:35:ASN:N	2.24	0.52
1:C:219:LEU:HD13	1:C:227:ILE:HD13	1.91	0.52
1:B:319:PRO:HG2	1:B:322:GLN:CG	2.39	0.52
1:C:111:ILE:HG23	1:C:344:PHE:HD1	1.67	0.52
1:C:253:GLN:O	1:C:257:GLN:HG2	2.10	0.52
1:B:156:ASN:CB	1:B:158:TRP:CE2	2.93	0.52
1:B:145:VAL:CG2	1:B:146:LEU:N	2.73	0.52
1:C:8:ILE:CD1	1:C:23:PHE:HZ	2.23	0.52
1:C:10:GLY:O	1:C:11:LEU:HD12	2.10	0.52
1:C:96:PHE:CB	1:C:110:VAL:HG12	2.33	0.51
1:D:375:GLU:O	1:D:376:ARG:HB2	2.10	0.51
1:C:313:LEU:HB3	1:C:315:ASN:OD1	2.10	0.51
1:D:35:ASN:HB3	1:D:38:GLU:HB2	1.93	0.51
1:C:269:GLU:HA	1:C:272:ASN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ASN:ND2	1:D:39:LYS:HB2	2.25	0.51
1:C:202:LEU:HD12	1:C:232:VAL:HG21	1.92	0.51
1:B:312:CYS:C	1:B:313:LEU:CD1	2.64	0.51
1:C:9:GLY:HA3	1:C:70:VAL:HG21	1.93	0.51
1:D:106:ASP:CB	1:D:347:TYR:CD2	2.92	0.50
1:D:15:ASN:O	1:D:16:THR:CB	2.57	0.50
1:B:210:LYS:C	1:B:211:HIS:HD1	2.14	0.50
1:B:154:VAL:HG21	1:D:163:ARG:HD3	1.93	0.50
1:D:218:MET:HG3	1:D:240:THR:HB	1.94	0.50
1:D:224:PHE:CD1	1:D:241:GLY:HA3	2.47	0.50
1:D:18:GLN:CB	1:D:269:GLU:CB	2.90	0.50
1:D:336:GLN:OE1	1:D:341:ASN:HA	2.11	0.49
1:A:149:ILE:HD13	1:A:160:VAL:HG11	1.93	0.49
1:B:335:VAL:HG12	1:B:342:ILE:HD12	1.93	0.49
1:B:163:ARG:NH2	1:D:154:VAL:HG21	2.27	0.49
1:B:135:TYR:OH	1:B:145:VAL:HG23	2.12	0.49
1:B:236:GLY:HA2	1:B:362:VAL:HB	1.95	0.49
1:A:92:LEU:HD12	1:A:318:VAL:CG2	2.38	0.48
1:D:337:GLY:O	1:D:340:GLY:HA2	2.13	0.48
1:D:8:ILE:HD11	1:D:289:ILE:HG21	1.95	0.48
1:B:92:LEU:HD12	1:B:318:VAL:HG21	1.95	0.48
1:D:74:PHE:CZ	1:D:76:PHE:CE2	3.01	0.48
1:C:6:ILE:HG23	1:C:71:TYR:CD2	2.48	0.48
1:C:66:PHE:C	1:C:69:GLY:H	2.16	0.48
1:B:291:GLU:OE1	1:B:294:ARG:NH2	2.44	0.48
1:B:314:ALA:HA	1:D:56:PHE:HE2	1.79	0.48
1:D:47:VAL:CG1	1:D:47:VAL:O	2.62	0.48
1:D:256:ILE:HD13	1:D:275:LEU:HD22	1.95	0.48
1:C:246:ASN:HB3	1:C:249:ASN:HB2	1.95	0.47
1:D:337:GLY:O	1:D:340:GLY:CA	2.62	0.47
1:A:369:GLY:HA2	1:A:380:PHE:CE2	2.50	0.47
1:B:296:LEU:HD21	1:B:326:ILE:HG22	1.96	0.47
1:D:114:ARG:HA	1:D:115:PRO:HD3	1.69	0.47
1:B:369:GLY:HA2	1:B:380:PHE:CE2	2.50	0.47
1:A:88:PHE:HA	1:C:56:PHE:HD2	1.80	0.47
1:D:346:THR:CG2	1:D:347:TYR:CE1	2.95	0.47
1:B:145:VAL:HG22	1:B:146:LEU:N	2.30	0.47
1:B:313:LEU:C	1:B:316:PRO:CD	2.83	0.47
1:B:163:ARG:HH12	1:D:154:VAL:HG11	1.80	0.46
1:B:154:VAL:CG1	1:D:184:ARG:NH1	2.61	0.46
1:D:31:ASN:HA	1:D:39:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PHE:HE1	1:C:323:GLY:O	1.98	0.46
1:D:9:GLY:CA	1:D:65:GLN:OE1	2.63	0.46
1:C:372:ASN:OD1	1:C:375:GLU:N	2.44	0.46
1:C:136:LEU:HD23	1:C:163:ARG:HB2	1.96	0.46
1:A:92:LEU:HD13	1:C:56:PHE:CZ	2.51	0.46
1:D:341:ASN:OD1	1:D:342:ILE:N	2.49	0.45
1:A:56:PHE:HD2	1:C:88:PHE:HA	1.81	0.45
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.52	0.45
1:D:341:ASN:O	1:D:350:ARG:NH2	2.50	0.45
1:C:34:GLN:O	1:C:35:ASN:CB	2.64	0.45
1:C:212:SER:HB2	1:C:235:GLY:HA3	1.99	0.45
1:A:33:ASN:CB	1:A:34:GLN:CB	2.94	0.45
1:D:205:VAL:HG13	1:D:211:HIS:O	2.16	0.45
1:D:75:GLY:C	1:D:76:PHE:CD2	2.77	0.45
1:C:9:GLY:CA	1:C:65:GLN:OE1	2.65	0.45
1:B:31:ASN:HD21	1:B:42:HIS:CE1	2.33	0.45
1:C:224:PHE:CD1	1:C:241:GLY:HA3	2.51	0.45
1:D:9:GLY:N	1:D:70:VAL:HG11	2.32	0.44
1:B:288:VAL:HG13	1:B:333:VAL:HG21	1.99	0.44
1:A:297:ARG:O	1:A:297:ARG:HG2	2.16	0.44
1:D:13:MET:HB3	1:D:13:MET:HE3	1.82	0.44
1:D:222:LEU:HD13	1:D:244:ILE:CD1	2.47	0.44
1:A:32:THR:CG2	1:A:32:THR:O	2.53	0.44
1:B:316:PRO:CD	1:B:317:ALA:H	2.30	0.44
1:D:143:PHE:O	1:D:144:SER:C	2.55	0.44
1:D:222:LEU:CD1	1:D:244:ILE:HD11	2.47	0.44
1:A:236:GLY:CA	1:A:362:VAL:HG12	2.39	0.44
1:A:212:SER:HB3	1:A:235:GLY:O	2.16	0.44
1:C:362:VAL:HG22	1:C:363:SER:N	2.32	0.44
1:A:208:LEU:HD23	1:A:211:HIS:NE2	2.33	0.44
1:C:293:PHE:HA	1:C:296:LEU:HD12	2.00	0.43
1:A:341:ASN:HB3	1:A:352:ASN:O	2.18	0.43
1:B:38:GLU:O	1:B:294:ARG:HD3	2.19	0.43
1:B:314:ALA:CB	1:D:56:PHE:CE2	3.00	0.43
1:D:337:GLY:C	1:D:340:GLY:H	2.19	0.43
1:D:370:TYR:HE1	1:D:378:VAL:CB	2.30	0.43
1:C:353:TYR:CZ	1:C:373:GLU:OE2	2.69	0.43
1:D:192:ASP:HB3	1:D:220:ALA:HB3	2.00	0.43
1:A:35:ASN:CB	1:A:39:LYS:H	2.32	0.43
1:A:56:PHE:CD2	1:C:88:PHE:HA	2.53	0.43
1:C:74:PHE:CZ	1:C:282:THR:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ARG:HA	1:D:376:ARG:HD2	1.48	0.42
1:C:299:GLN:HB2	1:C:301:VAL:HG23	2.01	0.42
1:D:13:MET:O	1:D:16:THR:CG2	2.67	0.42
1:D:337:GLY:HA3	1:D:342:ILE:HD11	2.01	0.42
1:C:135:TYR:CE2	1:C:137:TYR:HB3	2.55	0.42
1:A:63:CYS:HG	1:A:312:CYS:HG	0.99	0.42
1:D:340:GLY:O	1:D:342:ILE:HG13	2.19	0.42
1:A:208:LEU:CD2	1:A:211:HIS:CE1	3.03	0.42
1:C:284:ASP:HA	1:C:287:LEU:HD12	2.01	0.42
1:D:5:THR:HG23	1:D:42:HIS:HB3	2.01	0.42
1:B:243:GLN:HB2	1:B:358:TYR:HE2	1.85	0.42
1:C:343:GLN:O	1:C:344:PHE:CD2	2.73	0.42
1:B:318:VAL:CG1	1:B:319:PRO:CD	2.82	0.41
1:B:91:ALA:O	1:B:318:VAL:HG11	2.19	0.41
1:C:81:SER:O	1:C:85:LEU:HD12	2.20	0.41
1:D:75:GLY:CA	1:D:96:PHE:CZ	3.03	0.41
1:D:377:PHE:C	1:D:377:PHE:CD1	2.93	0.41
1:C:371:TRP:CD1	1:C:376:ARG:C	2.94	0.41
1:D:33:ASN:N	1:D:34:GLN:HA	2.34	0.41
1:B:211:HIS:O	1:B:215:TYR:CD2	2.74	0.41
1:C:66:PHE:O	1:C:69:GLY:HA2	2.21	0.41
1:D:224:PHE:HB3	1:D:243:GLN:HG3	2.02	0.41
1:D:202:LEU:HD22	1:D:232:VAL:HG21	2.03	0.41
1:D:75:GLY:HA3	1:D:96:PHE:CZ	2.55	0.41
1:C:224:PHE:HZ	1:C:360:MET:HG3	1.86	0.41
1:B:25:PHE:CE2	1:B:29:LEU:HD23	2.55	0.41
1:D:244:ILE:HG22	1:D:339:THR:HA	2.03	0.41
1:B:150:MET:O	1:B:154:VAL:CG2	2.69	0.41
1:A:313:LEU:C	1:A:316:PRO:HD2	2.40	0.41
1:D:33:ASN:HB2	1:D:34:GLN:HA	2.03	0.41
1:C:77:TYR:CE2	1:C:98:THR:HG21	2.56	0.41
1:D:33:ASN:HB2	1:D:35:ASN:H	1.86	0.40
1:A:243:GLN:HB2	1:A:358:TYR:HE2	1.86	0.40
1:B:175:ARG:NH1	1:B:207:ILE:HG21	2.36	0.40
1:D:9:GLY:HA3	1:D:65:GLN:OE1	2.21	0.40
1:C:288:VAL:HG13	1:C:333:VAL:HG21	2.03	0.40
1:C:124:LEU:HD11	1:C:357:VAL:HG11	2.03	0.40
1:D:213:ARG:HA	1:D:236:GLY:O	2.22	0.40
1:C:52:SER:HB2	1:C:78:ASP:HB2	2.04	0.40
1:D:244:ILE:HG21	1:D:339:THR:HB	2.02	0.40
1:A:141:ARG:HH22	1:A:221:ASN:HD22	1.68	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	369/389 (95%)	353 (96%)	14 (4%)	2 (0%)	34	77
1	B	370/389 (95%)	356 (96%)	12 (3%)	2 (0%)	34	77
1	C	352/389 (90%)	329 (94%)	21 (6%)	2 (1%)	30	74
1	D	369/389 (95%)	351 (95%)	15 (4%)	3 (1%)	24	69
All	All	1460/1556 (94%)	1389 (95%)	62 (4%)	9 (1%)	30	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	17	VAL
1	D	316	PRO
1	A	317	ALA
1	B	34	GLN
1	B	317	ALA
1	C	301	VAL
1	D	376	ARG
1	A	212	SER
1	C	317	ALA

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	300/340 (88%)	290 (97%)	10 (3%)	45	78
1	B	299/340 (88%)	287 (96%)	12 (4%)	38	73
1	C	285/340 (84%)	274 (96%)	11 (4%)	39	74
1	D	294/340 (86%)	279 (95%)	15 (5%)	29	68
All	All	1178/1360 (87%)	1130 (96%)	48 (4%)	37	73

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	ASN
1	A	92	LEU
1	A	185	GLN
1	A	188	ARG
1	A	263	ASP
1	A	286	ILE
1	A	318	VAL
1	A	362	VAL
1	A	366	ARG
1	B	36	THR
1	B	60	ASN
1	B	92	LEU
1	B	144	SER
1	B	145	VAL
1	B	185	GLN
1	B	188	ARG
1	B	207	ILE
1	B	263	ASP
1	B	286	ILE
1	B	325	ASP
1	B	335	VAL
1	C	104	ASP
1	C	124	LEU
1	C	229	LEU
1	C	312	CYS
1	C	315	ASN
1	C	326	ILE
1	C	344	PHE
1	C	354	THR
1	C	360	MET
1	C	362	VAL
1	C	373	GLU

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Mol	Chain	Res	Type
1	D	13	MET
1	D	16	THR
1	D	29	LEU
1	D	76	PHE
1	D	88	PHE
1	D	173	GLU
1	D	272	ASN
1	D	328	ARG
1	D	336	GLN
1	D	347	TYR
1	D	367	LYS
1	D	370	TYR
1	D	374	TYR
1	D	376	ARG
1	D	377	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	322	GLN
1	B	42	HIS
1	C	343	GLN
1	D	15	ASN
1	D	65	GLN
1	D	79	GLN
1	D	112	GLN
1	D	254	GLN
1	D	272	ASN

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

There are no ligands in this entry.

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	373/389 (95%)	-0.26	2 (0%) 91 88	79, 111, 180, 222	0
1	B	374/389 (96%)	-0.17	0 100 100	85, 119, 163, 211	0
1	C	362/389 (93%)	-0.14	1 (0%) 94 92	76, 108, 161, 207	0
1	D	373/389 (95%)	-0.15	6 (1%) 74 65	79, 112, 150, 217	0
All	All	1482/1556 (95%)	-0.18	9 (0%) 90 86	76, 112, 165, 222	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	319	PRO	2.7
1	A	170	ASP	2.7
1	D	369	GLY	2.4
1	D	266	GLU	2.3
1	D	378	VAL	2.3
1	A	320	TRP	2.3
1	D	103	THR	2.1
1	C	367	LYS	2.0
1	D	170	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.