Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:24 am BST

PDB ID	:	1JJO
Title	:	Crystal Structure of Mouse Neuroserpin (Cleaved form)
Authors	:	Briand, C.; Kozlov, S.V.; Sonderegger, P.; Gruetter, M.G.
Deposited on	:	2001-07-09
Resolution	:	3.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

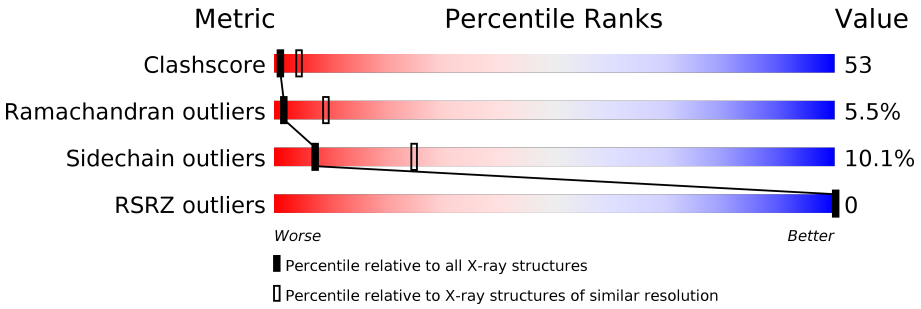
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.06 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))
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	40	43% 48% 10%
1	B	40	43% 48% 10%
2	C	261	31% 54% 8% • 7%
2	D	261	32% 53% 7% • 7%
3	E	33	27% 61% 12%
3	F	33	30% 58% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5074 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 NEUROSERPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	40	Total	C	N	O	S	0	0	0
			307	193	49	61	4			
1	B	40	Total	C	N	O	S	0	0	0
			307	193	49	61	4			

- Molecule 2 is a protein called NEUROSERPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	244	Total	C	N	O	S	0	0	0
			1950	1244	311	386	9			
2	D	244	Total	C	N	O	S	0	0	0
			1950	1244	311	386	9			

- Molecule 3 is a protein called NEUROSERPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	33	Total	C	N	O	S	0	0	0
			280	184	52	42	2			
3	F	33	Total	C	N	O	S	0	0	0
			280	184	52	42	2			

There are 4 discrepancies between the modelled and reference sequences:

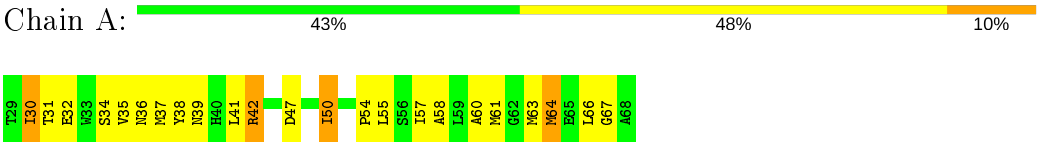
Chain	Residue	Modelled	Actual	Comment	Reference
E	392	HIS	-	SEE REMARK 999	UNP O35684
E	393	HIS	-	SEE REMARK 999	UNP O35684
F	392	HIS	-	SEE REMARK 999	UNP O35684
F	393	HIS	-	SEE REMARK 999	UNP O35684

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

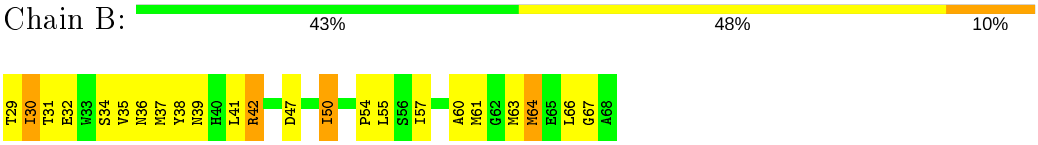
- Molecule 1: NEUROSERPIN

Chain A:



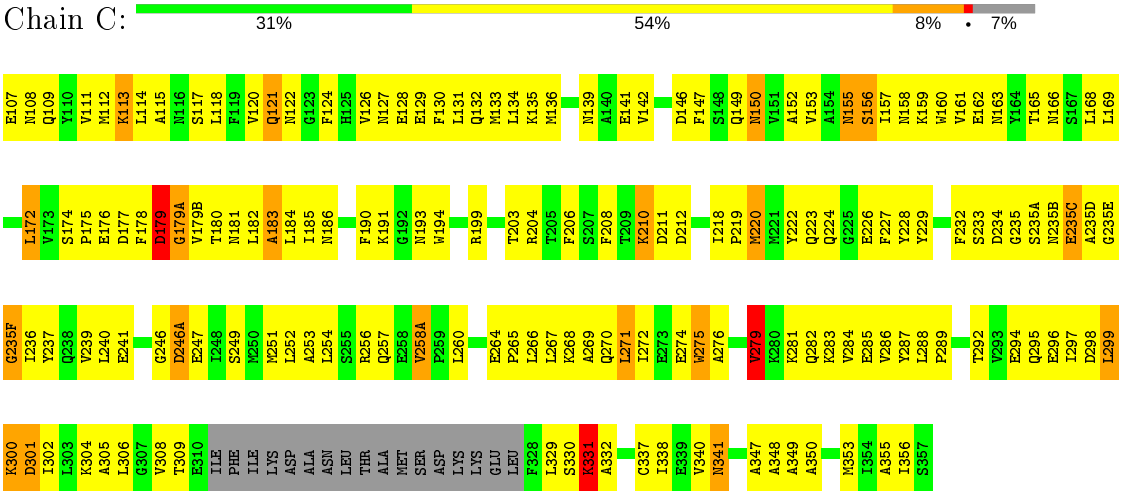
- Molecule 1: NEUROSERPIN

Chain B:



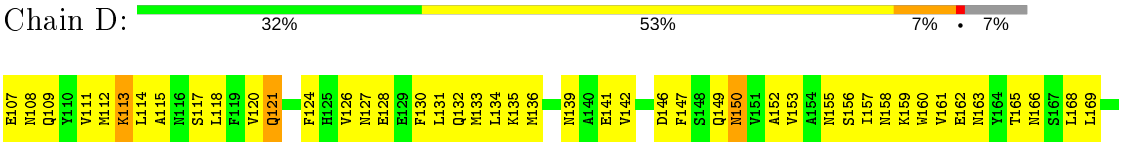
- Molecule 2: NEUROSERPIN

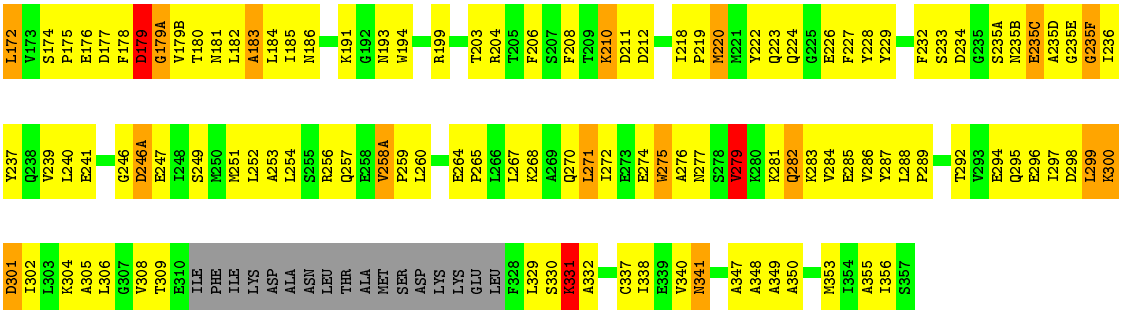
Chain C:



- Molecule 2: NEUROSERPIN

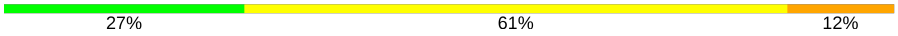
Chain D:

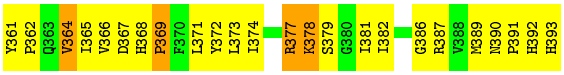




- Molecule 3: NEUROSERPIN

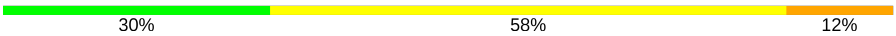
Chain E:

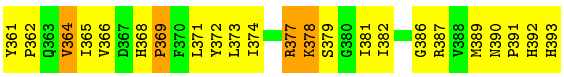




- Molecule 3: NEUROSERPIN

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.29Å 108.69Å 45.99Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	16.89 – 3.06 16.89 – 3.06	Depositor EDS
% Data completeness (in resolution range)	79.7 (16.89-3.06) 80.8 (16.89-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.08Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.232 , 0.308 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5074	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.42	0/312	0.64	0/420
1	B	0.42	0/312	0.64	0/420
2	C	0.46	1/1988 (0.1%)	0.70	1/2687 (0.0%)
2	D	0.46	1/1988 (0.1%)	0.70	1/2687 (0.0%)
3	E	0.45	0/289	0.76	1/389 (0.3%)
3	F	0.45	0/289	0.76	1/389 (0.3%)
All	All	0.45	2/5178 (0.0%)	0.70	4/6992 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	179(A)	GLY	CA-C	5.35	1.60	1.51
2	C	179(A)	GLY	CA-C	5.29	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	179	ASP	O-C-N	-6.56	112.05	123.20
2	C	179	ASP	O-C-N	-6.53	112.09	123.20
3	E	374	ILE	N-CA-C	-5.07	97.30	111.00
3	F	374	ILE	N-CA-C	-5.07	97.32	111.00

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	307	0	296	60	0
1	B	307	0	296	67	0
2	C	1950	0	1887	239	5
2	D	1950	0	1887	223	3
3	E	280	0	286	37	2
3	F	280	0	286	37	0
All	All	5074	0	4938	529	6

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 53.

All (529) 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)
2:C:136:MET:CE	1:B:55:LEU:HD12	1.10	1.55
2:C:136:MET:CE	1:B:55:LEU:CD1	1.90	1.42
2:C:136:MET:HE2	1:B:55:LEU:CD1	1.46	1.41
1:A:55:LEU:HD12	2:D:136:MET:CE	1.50	1.39
1:A:30:ILE:CB	2:D:132:GLN:HG2	1.79	1.12
2:C:132:GLN:HG2	1:B:30:ILE:HB	1.26	1.09
1:B:50:ILE:HG22	2:D:295:GLN:HE22	1.11	1.09
2:C:136:MET:HE1	1:B:55:LEU:HD12	1.29	1.08
1:A:55:LEU:HD12	2:D:136:MET:HE2	1.20	1.07
2:C:132:GLN:HG2	1:B:30:ILE:CB	1.85	1.07
1:A:50:ILE:HG22	2:C:295:GLN:HE22	1.11	1.06
2:C:136:MET:HE3	1:B:55:LEU:CD1	1.84	1.06
1:A:55:LEU:CD1	2:D:136:MET:CE	2.32	1.06
1:A:30:ILE:HB	2:D:132:GLN:CG	1.86	1.04
1:A:30:ILE:HB	2:D:132:GLN:HG2	1.06	1.04
2:C:132:GLN:CG	1:B:30:ILE:HB	1.87	1.03
1:A:55:LEU:CD1	2:D:136:MET:HE2	1.88	1.01
2:C:136:MET:CE	1:B:55:LEU:HA	1.91	1.00
2:C:132:GLN:CD	1:B:30:ILE:CG2	2.35	0.94
1:A:30:ILE:HG23	1:A:31:THR:H	1.31	0.94
1:B:30:ILE:HG23	1:B:31:THR:H	1.31	0.94
2:C:161:VAL:HG11	2:C:172:LEU:HD12	1.50	0.90
2:D:288:LEU:HD12	3:F:366:VAL:HG11	1.52	0.90
2:C:132:GLN:HG2	1:B:30:ILE:CD1	2.02	0.90
2:C:132:GLN:HG2	1:B:30:ILE:HD12	1.53	0.90
2:C:288:LEU:HD12	3:E:366:VAL:HG11	1.52	0.90
2:D:161:VAL:HG11	2:D:172:LEU:HD12	1.50	0.90
2:D:121:GLN:HE21	2:D:121:GLN:HA	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:GLN:HA	2:C:121:GLN:HE21	1.36	0.89
2:C:136:MET:HE3	1:B:55:LEU:HA	1.55	0.87
2:D:287:TYR:HB2	3:F:365:ILE:HA	1.57	0.86
1:A:55:LEU:HA	2:D:136:MET:CE	2.05	0.86
2:C:136:MET:CE	1:B:55:LEU:HD13	2.05	0.85
2:C:228:TYR:HB2	2:C:241:GLU:HB3	1.58	0.85
2:C:136:MET:HE2	1:B:55:LEU:HD12	0.86	0.85
2:C:287:TYR:HB2	3:E:365:ILE:HA	1.57	0.85
2:D:228:TYR:HB2	2:D:241:GLU:HB3	1.58	0.85
2:C:132:GLN:CD	1:B:30:ILE:HG21	1.96	0.84
2:D:210:LYS:HD2	2:D:212:ASP:H	1.43	0.83
2:C:210:LYS:HD2	2:C:212:ASP:H	1.43	0.83
2:C:132:GLN:CG	1:B:30:ILE:HD12	2.07	0.83
1:A:66:LEU:HD12	2:C:134:LEU:HD23	1.60	0.82
1:A:55:LEU:HA	2:D:136:MET:HE3	1.62	0.81
1:B:50:ILE:HG22	2:D:295:GLN:NE2	1.93	0.80
1:B:66:LEU:HD12	2:D:134:LEU:HD23	1.60	0.80
1:A:50:ILE:HG22	2:C:295:GLN:NE2	1.93	0.80
2:D:147:PHE:HA	2:D:153:VAL:HG21	1.64	0.80
2:C:299:LEU:HD23	2:C:302:ILE:HD11	1.64	0.79
2:D:179(B):VAL:HB	2:D:356:ILE:HD11	1.65	0.79
1:A:55:LEU:HD12	2:D:136:MET:HE1	1.62	0.79
2:C:132:GLN:HG2	1:B:30:ILE:CG1	2.11	0.78
2:D:288:LEU:HA	3:F:366:VAL:CG1	2.14	0.78
2:D:299:LEU:HD23	2:D:302:ILE:HD11	1.64	0.78
2:C:179(B):VAL:HB	2:C:356:ILE:HD11	1.65	0.78
1:A:30:ILE:CG2	2:D:132:GLN:CD	2.51	0.78
1:A:55:LEU:HD12	2:D:136:MET:HE3	1.66	0.78
2:C:147:PHE:HA	2:C:153:VAL:HG21	1.64	0.77
2:C:288:LEU:HA	3:E:366:VAL:CG1	2.14	0.77
2:D:117:SER:HA	2:D:141:GLU:H	1.49	0.77
2:D:235(C):GLU:HG3	2:D:235(D):ALA:N	2.00	0.77
1:A:30:ILE:HD11	3:E:381:ILE:HA	1.66	0.77
2:C:136:MET:HE1	1:B:55:LEU:HA	1.65	0.77
2:C:117:SER:HA	2:C:141:GLU:H	1.49	0.77
2:C:235(C):GLU:HG3	2:C:235(D):ALA:N	1.99	0.76
2:C:300:LYS:H	2:C:332:ALA:HB3	1.51	0.76
2:D:300:LYS:H	2:D:332:ALA:HB3	1.51	0.76
2:D:218:ILE:HG13	2:D:219:PRO:HD2	1.68	0.76
2:C:206:PHE:HB2	2:C:220:MET:HG3	1.68	0.76
2:D:302:ILE:O	2:D:306:LEU:HB2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:MET:HE3	1:B:55:LEU:HD13	1.66	0.75
3:E:371:LEU:HA	3:E:387:ARG:HA	1.69	0.75
2:C:338:ILE:HG13	2:C:347:ALA:HB2	1.68	0.75
1:B:30:ILE:HD11	3:F:381:ILE:HA	1.66	0.75
2:C:132:GLN:OE1	1:B:30:ILE:HG22	1.85	0.75
2:C:302:ILE:O	2:C:306:LEU:HB2	1.86	0.74
2:C:218:ILE:HG13	2:C:219:PRO:HD2	1.67	0.74
2:D:338:ILE:HG13	2:D:347:ALA:HB2	1.68	0.74
2:D:206:PHE:HB2	2:D:220:MET:HG3	1.68	0.74
3:F:371:LEU:HA	3:F:387:ARG:HA	1.69	0.74
2:C:161:VAL:HG21	2:C:172:LEU:HB2	1.71	0.73
2:D:226:GLU:HB3	2:D:281:LYS:HE3	1.71	0.72
2:D:161:VAL:HG21	2:D:172:LEU:HB2	1.71	0.72
1:B:42:ARG:NH1	2:D:264:GLU:HB3	2.04	0.72
2:D:297:ILE:HG22	2:D:298:ASP:N	2.05	0.72
1:A:42:ARG:NH1	2:C:264:GLU:HB3	2.04	0.71
1:A:55:LEU:CD1	2:D:136:MET:HE3	2.17	0.71
2:C:186:ASN:O	2:C:350:ALA:HA	1.89	0.71
2:D:177:ASP:HA	2:D:331:LYS:HD3	1.72	0.71
2:D:186:ASN:O	2:D:350:ALA:HA	1.89	0.71
2:C:226:GLU:HB3	2:C:281:LYS:HE3	1.71	0.71
2:C:132:GLN:CG	1:B:30:ILE:CB	2.59	0.71
2:C:136:MET:CE	1:B:55:LEU:CA	2.69	0.71
2:C:297:ILE:HG22	2:C:298:ASP:N	2.05	0.70
2:C:229:TYR:CE2	3:E:362:PRO:HB3	2.27	0.70
2:D:294:GLU:HB3	2:D:337:CYS:HB3	1.73	0.70
2:C:177:ASP:HA	2:C:331:LYS:HD3	1.72	0.69
2:D:229:TYR:CE2	3:F:362:PRO:HB3	2.27	0.69
2:C:132:GLN:NE2	1:B:30:ILE:HG21	2.07	0.69
2:C:136:MET:HE1	1:B:55:LEU:O	1.92	0.69
2:C:294:GLU:HB3	2:C:337:CYS:HB3	1.73	0.68
2:C:184:LEU:HB2	2:C:353:MET:HB2	1.75	0.68
2:D:147:PHE:CD1	2:D:153:VAL:HG11	2.28	0.68
2:D:184:LEU:HB2	2:D:353:MET:HB2	1.75	0.68
1:B:63:MET:O	1:B:66:LEU:HB2	1.93	0.68
2:C:147:PHE:CD1	2:C:153:VAL:HG11	2.28	0.68
2:C:203:THR:HA	2:C:220:MET:O	1.93	0.68
2:D:203:THR:HA	2:D:220:MET:O	1.93	0.67
2:D:179:ASP:OD2	2:D:179(A):GLY:N	2.27	0.67
1:A:63:MET:O	1:A:66:LEU:HB2	1.93	0.67
2:C:237:TYR:HB2	2:C:254:LEU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:GLN:OE1	1:B:30:ILE:CG2	2.42	0.66
2:D:206:PHE:CB	2:D:220:MET:HG3	2.26	0.66
2:D:237:TYR:HB2	2:D:254:LEU:O	1.95	0.66
2:C:132:GLN:HA	2:C:135:LYS:HB2	1.78	0.66
2:C:178:PHE:O	2:C:179:ASP:HB2	1.96	0.66
2:C:299:LEU:O	2:C:301:ASP:N	2.28	0.66
2:D:299:LEU:O	2:D:301:ASP:N	2.28	0.66
2:D:275:TRP:O	2:D:279:VAL:HG22	1.96	0.66
2:C:272:ILE:O	2:C:275:TRP:HB2	1.96	0.66
2:D:264:GLU:N	2:D:265:PRO:HD2	2.11	0.66
2:C:264:GLU:N	2:C:265:PRO:HD2	2.11	0.65
2:C:147:PHE:CD2	2:C:180:THR:HG22	2.31	0.65
2:D:260:LEU:O	2:D:264:GLU:HG3	1.96	0.65
2:C:127:ASN:HD22	2:C:130:PHE:HB2	1.61	0.65
2:C:179(B):VAL:HB	2:C:356:ILE:CD1	2.27	0.65
2:C:206:PHE:CB	2:C:220:MET:HG3	2.26	0.65
1:A:55:LEU:HA	2:D:136:MET:HE1	1.76	0.65
2:C:275:TRP:O	2:C:279:VAL:HG22	1.96	0.65
2:C:240:LEU:HD21	2:C:286:VAL:HG11	1.79	0.65
2:D:147:PHE:CD2	2:D:180:THR:HG22	2.31	0.65
2:C:179:ASP:OD2	2:C:179(A):GLY:N	2.27	0.65
2:C:199:ARG:HH11	2:C:199:ARG:HG3	1.62	0.65
2:D:179(B):VAL:HB	2:D:356:ILE:CD1	2.27	0.65
2:C:260:LEU:O	2:C:264:GLU:HG3	1.96	0.65
2:D:132:GLN:HA	2:D:135:LYS:HB2	1.78	0.65
2:D:127:ASN:HD22	2:D:130:PHE:HB2	1.61	0.65
2:C:121:GLN:HA	2:C:121:GLN:NE2	2.11	0.65
2:D:272:ILE:O	2:D:275:TRP:HB2	1.96	0.65
2:D:178:PHE:O	2:D:179:ASP:HB2	1.96	0.64
2:C:147:PHE:HD1	2:C:153:VAL:HG11	1.63	0.64
3:F:372:TYR:O	3:F:373:LEU:HD12	1.98	0.64
2:C:136:MET:HE1	1:B:55:LEU:CA	2.26	0.64
2:D:251:MET:CE	2:D:275:TRP:HB3	2.27	0.64
3:E:392:HIS:O	3:E:393:HIS:HB2	1.98	0.64
2:D:294:GLU:CB	2:D:337:CYS:HB3	2.28	0.64
2:D:240:LEU:HD21	2:D:286:VAL:HG11	1.79	0.63
2:D:199:ARG:HH11	2:D:199:ARG:HG3	1.62	0.63
1:B:30:ILE:HG23	1:B:31:THR:N	2.10	0.63
2:C:251:MET:CE	2:C:275:TRP:HB3	2.27	0.63
3:E:372:TYR:C	3:E:373:LEU:HD12	2.19	0.63
2:D:168:LEU:HB3	2:D:337:CYS:SG	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:372:TYR:O	3:E:373:LEU:HD12	1.98	0.63
2:C:168:LEU:HB3	2:C:337:CYS:SG	2.38	0.63
2:D:299:LEU:HA	2:D:302:ILE:HG12	1.81	0.63
1:A:30:ILE:HG23	1:A:31:THR:N	2.10	0.62
3:E:378:LYS:HD3	3:E:378:LYS:O	1.99	0.62
3:F:372:TYR:C	3:F:373:LEU:HD12	2.19	0.62
2:D:256:ARG:HB2	2:D:258(A):VAL:HG12	1.82	0.62
3:F:392:HIS:O	3:F:393:HIS:HB2	1.98	0.62
2:C:294:GLU:CB	2:C:337:CYS:HB3	2.28	0.62
2:D:147:PHE:HD1	2:D:153:VAL:HG11	1.63	0.62
2:D:251:MET:HE3	2:D:275:TRP:HB3	1.80	0.62
2:D:121:GLN:NE2	2:D:121:GLN:HA	2.11	0.62
3:F:378:LYS:HD3	3:F:378:LYS:O	1.99	0.62
2:C:114:LEU:HD23	2:C:115:ALA:N	2.15	0.62
2:D:114:LEU:HD23	2:D:115:ALA:N	2.15	0.61
2:D:287:TYR:O	3:F:366:VAL:HG12	2.00	0.61
2:C:136:MET:HE3	1:B:55:LEU:CA	2.28	0.61
2:C:299:LEU:HA	2:C:302:ILE:HG12	1.81	0.61
1:A:37:MET:HG2	2:C:306:LEU:HD21	1.83	0.61
2:D:121:GLN:HE22	2:D:146:ASP:HA	1.66	0.61
1:A:30:ILE:HG22	2:D:132:GLN:CD	2.21	0.61
2:C:132:GLN:CG	1:B:30:ILE:CD1	2.73	0.60
2:C:256:ARG:HB2	2:C:258(A):VAL:HG12	1.81	0.60
2:C:287:TYR:O	3:E:366:VAL:HG12	2.00	0.60
1:B:37:MET:HG2	2:D:306:LEU:HD21	1.83	0.60
2:C:129:GLU:OE2	1:B:29:THR:HG23	2.01	0.60
2:D:256:ARG:HB2	2:D:258(A):VAL:CG1	2.32	0.60
1:A:30:ILE:CB	2:D:132:GLN:CG	2.64	0.59
2:C:235(E):GLY:O	2:C:236:ILE:N	2.35	0.59
3:E:378:LYS:HD3	3:E:378:LYS:C	2.22	0.59
3:F:378:LYS:HD3	3:F:378:LYS:C	2.23	0.59
2:C:121:GLN:HE22	2:C:146:ASP:HA	1.66	0.59
2:C:174:SER:HB3	2:C:175:PRO:HD2	1.85	0.59
2:C:237:TYR:HH	2:C:275:TRP:HH2	1.50	0.59
2:D:235(E):GLY:O	2:D:236:ILE:N	2.35	0.59
2:C:131:LEU:CD2	2:C:142:VAL:HG21	2.32	0.59
2:C:294:GLU:HB3	2:C:337:CYS:CB	2.32	0.59
2:D:131:LEU:CD2	2:D:142:VAL:HG21	2.32	0.59
2:D:235(C):GLU:HG3	2:D:235(D):ALA:H	1.66	0.59
2:C:235(C):GLU:HG3	2:C:235(D):ALA:H	1.66	0.58
2:C:131:LEU:HD22	2:C:142:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:294:GLU:HB3	2:D:337:CYS:CB	2.32	0.58
2:C:121:GLN:NE2	2:C:146:ASP:HA	2.19	0.58
2:D:297:ILE:H	2:D:297:ILE:HD12	1.68	0.58
2:C:206:PHE:CG	2:C:220:MET:HG3	2.38	0.58
2:D:206:PHE:CG	2:D:220:MET:HG3	2.38	0.58
2:D:236:ILE:HG13	2:D:236:ILE:O	2.03	0.58
2:C:236:ILE:HG13	2:C:236:ILE:O	2.03	0.58
2:C:297:ILE:HD12	2:C:297:ILE:H	1.68	0.58
2:D:268:LYS:NZ	2:D:270:GLN:HE21	2.01	0.58
2:C:132:GLN:HG3	1:B:30:ILE:HD12	1.85	0.58
2:C:256:ARG:HB2	2:C:258(A):VAL:CG1	2.32	0.58
2:C:299:LEU:HB2	2:C:332:ALA:HB1	1.86	0.58
2:D:174:SER:HB3	2:D:175:PRO:HD2	1.85	0.58
2:C:268:LYS:NZ	2:C:270:GLN:HE21	2.01	0.57
2:D:299:LEU:HB2	2:D:332:ALA:HB1	1.86	0.57
2:D:131:LEU:HD22	2:D:142:VAL:HG21	1.85	0.57
2:D:271:LEU:HD12	2:D:275:TRP:CZ3	2.40	0.57
2:D:121:GLN:NE2	2:D:146:ASP:HA	2.19	0.57
1:B:41:LEU:HD21	2:D:297:ILE:HG12	1.87	0.57
2:C:271:LEU:HD12	2:C:275:TRP:CZ3	2.40	0.57
2:D:206:PHE:HB2	2:D:220:MET:CG	2.35	0.57
2:D:297:ILE:CG2	2:D:298:ASP:N	2.67	0.57
1:A:30:ILE:HG21	2:D:132:GLN:CD	2.23	0.56
3:F:366:VAL:O	3:F:366:VAL:HG22	2.04	0.56
2:C:239:VAL:HA	2:C:252:LEU:O	2.06	0.56
3:E:366:VAL:O	3:E:366:VAL:HG22	2.04	0.56
2:C:297:ILE:CG2	2:C:298:ASP:N	2.67	0.56
1:A:30:ILE:HG22	2:D:132:GLN:OE1	2.06	0.56
2:C:132:GLN:CD	1:B:30:ILE:HB	2.26	0.56
2:D:235(B):ASN:HA	2:D:235(F):GLY:HA3	1.87	0.56
2:C:206:PHE:HB2	2:C:220:MET:CG	2.35	0.55
2:C:235(B):ASN:HA	2:C:235(F):GLY:HA3	1.87	0.55
2:D:295:GLN:HG2	2:D:297:ILE:HD12	1.88	0.55
2:D:223:GLN:NE2	2:D:227:PHE:HZ	2.05	0.55
2:C:107:GLU:HG2	2:C:107:GLU:O	2.07	0.55
1:A:41:LEU:HD21	2:C:297:ILE:HG12	1.87	0.55
2:D:237:TYR:HH	2:D:275:TRP:HH2	1.54	0.55
2:C:253:ALA:HB3	3:E:371:LEU:HG	1.88	0.55
1:A:30:ILE:CG1	2:D:132:GLN:HG2	2.37	0.55
2:C:295:GLN:HG2	2:C:297:ILE:HD12	1.88	0.54
1:A:55:LEU:O	2:D:136:MET:HE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:VAL:HA	2:D:252:LEU:O	2.06	0.54
2:D:107:GLU:HG2	2:D:107:GLU:O	2.07	0.54
2:C:132:GLN:CD	1:B:30:ILE:CB	2.76	0.54
2:D:165:THR:HB	2:D:348:ALA:HB1	1.89	0.54
2:C:182:LEU:HB2	2:C:355:ALA:HB3	1.89	0.54
2:D:182:LEU:HB2	2:D:355:ALA:HB3	1.89	0.54
2:D:253:ALA:HB3	3:F:371:LEU:HG	1.87	0.54
2:C:223:GLN:NE2	2:C:227:PHE:HZ	2.05	0.54
2:C:228:TYR:HB3	2:C:279:VAL:HB	1.89	0.54
2:D:228:TYR:HB3	2:D:279:VAL:HB	1.90	0.54
2:C:338:ILE:CG1	2:C:347:ALA:HB2	2.37	0.53
2:C:165:THR:HB	2:C:348:ALA:HB1	1.89	0.53
2:D:235(B):ASN:HA	2:D:235(F):GLY:H	1.73	0.53
2:C:237:TYR:HE2	2:C:275:TRP:CH2	2.27	0.53
2:C:299:LEU:O	2:C:302:ILE:N	2.41	0.53
2:C:208:PHE:CG	3:E:391:PRO:HG3	2.44	0.53
2:C:305:ALA:O	2:C:306:LEU:HD12	2.09	0.53
2:D:338:ILE:CG1	2:D:347:ALA:HB2	2.37	0.53
2:D:237:TYR:HE2	2:D:275:TRP:CH2	2.27	0.53
2:D:299:LEU:O	2:D:302:ILE:N	2.41	0.53
2:C:251:MET:HE3	2:C:275:TRP:HB3	1.89	0.52
2:C:289:PRO:HD3	3:E:366:VAL:HG13	1.91	0.52
2:D:210:LYS:HG2	3:F:389:MET:O	2.10	0.52
2:C:177:ASP:HA	2:C:331:LYS:CD	2.39	0.52
1:A:31:THR:CG2	2:C:272:ILE:HD12	2.40	0.52
1:A:32:GLU:O	1:A:35:VAL:HG12	2.09	0.52
1:B:42:ARG:HB2	3:F:387:ARG:HH12	1.74	0.52
2:C:129:GLU:HG2	1:B:29:THR:N	2.25	0.52
2:C:235(B):ASN:HA	2:C:235(F):GLY:H	1.73	0.52
2:C:288:LEU:HA	3:E:366:VAL:HG13	1.90	0.52
2:C:179(B):VAL:HG12	2:C:356:ILE:O	2.10	0.52
2:D:149:GLN:HB3	2:D:152:ALA:HB3	1.92	0.52
2:D:208:PHE:CG	3:F:391:PRO:HG3	2.44	0.52
2:C:210:LYS:HG2	3:E:389:MET:O	2.10	0.52
1:B:31:THR:CG2	2:D:272:ILE:HD12	2.40	0.52
1:B:32:GLU:O	1:B:35:VAL:HG12	2.09	0.52
1:B:42:ARG:CZ	2:D:264:GLU:HB3	2.40	0.51
2:C:149:GLN:HB3	2:C:152:ALA:HB3	1.92	0.51
2:D:289:PRO:HD3	3:F:366:VAL:HG13	1.91	0.51
1:A:42:ARG:HB2	3:E:387:ARG:HH12	1.74	0.51
2:D:179(B):VAL:HG12	2:D:356:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:ALA:O	2:D:306:LEU:HD12	2.09	0.51
2:D:177:ASP:HA	2:D:331:LYS:CD	2.39	0.51
2:C:177:ASP:HA	2:C:331:LYS:CE	2.41	0.51
2:C:108:ASN:OD1	2:C:109:GLN:NE2	2.43	0.51
1:A:42:ARG:CZ	2:C:264:GLU:HB3	2.40	0.51
2:C:300:LYS:H	2:C:332:ALA:CB	2.23	0.51
2:D:108:ASN:OD1	2:D:109:GLN:NE2	2.43	0.51
2:D:169:LEU:HD12	2:D:169:LEU:N	2.25	0.51
2:D:177:ASP:HA	2:D:331:LYS:CE	2.41	0.51
1:B:32:GLU:HA	1:B:35:VAL:HG12	1.93	0.51
2:C:169:LEU:N	2:C:169:LEU:HD12	2.25	0.51
2:C:246:GLY:O	2:C:247:GLU:N	2.43	0.51
2:C:299:LEU:HB2	2:C:332:ALA:CB	2.41	0.51
2:D:299:LEU:HB2	2:D:332:ALA:CB	2.41	0.51
1:A:30:ILE:CD1	2:D:132:GLN:HG2	2.41	0.51
2:D:246:GLY:C	2:D:247:GLU:H	2.14	0.51
3:F:392:HIS:O	3:F:393:HIS:CB	2.59	0.51
1:A:32:GLU:HA	1:A:35:VAL:HG12	1.93	0.51
2:C:264:GLU:O	2:C:267:LEU:HB2	2.11	0.51
3:E:392:HIS:O	3:E:393:HIS:CB	2.59	0.51
2:C:232:PHE:O	2:C:236:ILE:HA	2.12	0.50
2:D:264:GLU:O	2:D:267:LEU:HB2	2.11	0.50
1:A:42:ARG:HB2	3:E:387:ARG:NH1	2.27	0.50
2:D:232:PHE:O	2:D:236:ILE:HA	2.12	0.50
2:D:224:GLN:NE2	2:D:283:LYS:HE2	2.27	0.50
2:D:297:ILE:CG2	2:D:298:ASP:H	2.25	0.50
2:C:246:GLY:C	2:C:247:GLU:H	2.14	0.50
2:D:150:ASN:H	2:D:150:ASN:HD22	1.60	0.50
1:A:47:ASP:CB	2:C:210:LYS:HZ3	2.25	0.49
2:C:127:ASN:ND2	2:C:130:PHE:HB2	2.26	0.49
2:C:224:GLN:NE2	2:C:283:LYS:HE2	2.27	0.49
1:A:31:THR:HG23	3:E:382:ILE:HD11	1.94	0.49
1:A:35:VAL:O	1:A:35:VAL:HG22	2.12	0.49
1:B:31:THR:HG23	3:F:382:ILE:HD11	1.93	0.49
2:C:299:LEU:HD13	2:C:353:MET:CE	2.42	0.49
2:D:127:ASN:ND2	2:D:130:PHE:HB2	2.26	0.49
1:A:30:ILE:CG2	2:D:132:GLN:CG	2.90	0.49
2:C:150:ASN:N	2:C:150:ASN:HD22	2.11	0.49
1:B:35:VAL:HG22	1:B:35:VAL:O	2.12	0.49
2:C:111:VAL:HB	2:C:191:LYS:HB3	1.95	0.49
2:D:117:SER:HB3	2:D:160:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:LEU:HA	3:F:366:VAL:HG13	1.90	0.49
2:D:299:LEU:HD13	2:D:353:MET:CE	2.42	0.49
2:C:150:ASN:H	2:C:150:ASN:HD22	1.60	0.49
2:D:237:TYR:CE2	2:D:275:TRP:CH2	3.00	0.49
2:D:153:VAL:HB	2:D:178:PHE:CE1	2.48	0.49
2:D:210:LYS:HD2	2:D:212:ASP:N	2.20	0.49
1:B:42:ARG:HB2	3:F:387:ARG:NH1	2.27	0.49
1:B:60:ALA:O	1:B:64:MET:HB2	2.13	0.48
1:A:30:ILE:CG2	2:D:132:GLN:HG2	2.41	0.48
2:C:211:ASP:H	3:E:369:PRO:HG2	1.78	0.48
2:D:211:ASP:H	3:F:369:PRO:HG2	1.78	0.48
1:B:50:ILE:HG12	3:F:387:ARG:HG2	1.95	0.48
2:C:237:TYR:CE2	2:C:275:TRP:CH2	3.00	0.48
2:D:199:ARG:NH1	2:D:199:ARG:HG3	2.27	0.48
2:D:268:LYS:HZ1	2:D:270:GLN:HE21	1.61	0.48
1:A:60:ALA:O	1:A:64:MET:HB2	2.13	0.48
2:C:117:SER:HB3	2:C:160:TRP:CZ2	2.48	0.48
2:D:246:GLY:O	2:D:247:GLU:N	2.43	0.48
3:E:371:LEU:HD12	3:E:371:LEU:C	2.34	0.48
2:C:224:GLN:NE2	3:E:361:TYR:OH	2.46	0.48
2:C:297:ILE:CG2	2:C:298:ASP:H	2.25	0.48
2:D:111:VAL:HB	2:D:191:LYS:HB3	1.95	0.48
2:D:297:ILE:HD12	2:D:297:ILE:N	2.28	0.48
2:C:260:LEU:O	2:C:260:LEU:HG	2.13	0.48
2:C:297:ILE:HG22	2:C:298:ASP:H	1.76	0.48
2:D:159:LYS:O	2:D:159:LYS:HD3	2.14	0.48
2:C:153:VAL:HB	2:C:178:PHE:CE1	2.48	0.48
2:C:210:LYS:HD2	2:C:212:ASP:N	2.20	0.48
2:C:268:LYS:HZ1	2:C:270:GLN:HE21	1.62	0.48
2:D:299:LEU:O	2:D:300:LYS:C	2.52	0.48
2:D:297:ILE:HG22	2:D:298:ASP:H	1.76	0.48
1:A:50:ILE:HG12	3:E:387:ARG:HG2	1.95	0.48
2:D:224:GLN:NE2	3:F:361:TYR:OH	2.46	0.48
2:D:177:ASP:CA	2:D:331:LYS:HD3	2.42	0.48
3:F:371:LEU:C	3:F:371:LEU:HD12	2.34	0.48
1:B:38:TYR:HE1	1:B:42:ARG:NH1	2.11	0.48
2:C:224:GLN:OE1	3:E:361:TYR:HE2	1.97	0.48
1:A:38:TYR:HE1	1:A:42:ARG:NH1	2.11	0.47
2:C:288:LEU:HG	2:C:289:PRO:HD2	1.95	0.47
2:D:235(C):GLU:CG	2:D:235(D):ALA:N	2.72	0.47
1:A:50:ILE:O	3:E:386:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:GLN:OE1	3:F:361:TYR:HE2	1.97	0.47
1:B:50:ILE:O	3:F:386:GLY:HA3	2.14	0.47
2:D:288:LEU:HG	2:D:289:PRO:HD2	1.95	0.47
1:A:30:ILE:HG21	2:D:132:GLN:NE2	2.29	0.47
3:E:364:VAL:HG22	3:E:364:VAL:O	2.14	0.47
2:C:237:TYR:CE2	2:C:275:TRP:HH2	2.33	0.47
2:C:340:VAL:O	2:C:341:ASN:HB3	2.15	0.47
2:C:159:LYS:O	2:C:159:LYS:HD3	2.14	0.47
2:C:169:LEU:HD21	2:C:349:ALA:HA	1.97	0.47
3:E:377:ARG:O	3:E:378:LYS:C	2.53	0.47
2:C:299:LEU:O	2:C:300:LYS:C	2.52	0.47
2:D:150:ASN:HD22	2:D:150:ASN:N	2.11	0.47
3:F:390:ASN:HD22	3:F:391:PRO:HD2	1.80	0.47
2:D:112:MET:O	2:D:113:LYS:C	2.53	0.47
2:C:330:SER:HB3	2:C:356:ILE:HB	1.98	0.46
2:D:237:TYR:CE2	2:D:275:TRP:HH2	2.33	0.46
2:C:199:ARG:NH1	2:C:199:ARG:HG3	2.28	0.46
2:D:300:LYS:H	2:D:332:ALA:CB	2.23	0.46
3:F:364:VAL:O	3:F:364:VAL:HG22	2.14	0.46
2:D:268:LYS:NZ	2:D:270:GLN:NE2	2.63	0.46
2:C:297:ILE:HD12	2:C:297:ILE:N	2.28	0.46
1:A:30:ILE:HD12	2:D:132:GLN:HG2	1.96	0.46
2:D:120:VAL:HA	2:D:181:ASN:O	2.14	0.46
2:C:112:MET:O	2:C:113:LYS:C	2.53	0.46
2:C:179(B):VAL:CG1	2:C:356:ILE:HG13	2.45	0.46
2:C:234:ASP:OD2	2:C:235(A):SER:O	2.33	0.46
2:D:240:LEU:CD2	2:D:286:VAL:HG11	2.45	0.46
3:E:390:ASN:HD22	3:E:391:PRO:HD2	1.80	0.46
3:F:377:ARG:O	3:F:378:LYS:C	2.53	0.46
2:C:120:VAL:HA	2:C:181:ASN:O	2.15	0.46
2:D:204:ARG:O	2:D:220:MET:HB2	2.16	0.46
2:D:235(B):ASN:HA	2:D:235(F):GLY:CA	2.46	0.46
2:C:268:LYS:NZ	2:C:270:GLN:NE2	2.63	0.46
2:C:235(B):ASN:HA	2:C:235(F):GLY:CA	2.46	0.46
2:D:184:LEU:C	2:D:185:ILE:HD12	2.36	0.46
2:C:229:TYR:CE2	3:E:362:PRO:CB	2.98	0.46
2:D:260:LEU:O	2:D:260:LEU:HG	2.13	0.46
2:D:340:VAL:O	2:D:341:ASN:HB3	2.15	0.46
2:D:330:SER:HB3	2:D:356:ILE:HB	1.98	0.46
2:C:177:ASP:CA	2:C:331:LYS:HD3	2.42	0.46
2:D:169:LEU:HD21	2:D:349:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:234:ASP:OD2	2:D:235(A):SER:O	2.33	0.45
2:D:210:LYS:HZ2	2:D:212:ASP:HB2	1.81	0.45
3:F:377:ARG:HH11	3:F:377:ARG:HG3	1.81	0.45
2:C:204:ARG:O	2:C:220:MET:HB2	2.16	0.45
2:C:240:LEU:CD2	2:C:286:VAL:HG11	2.45	0.45
2:D:193:ASN:O	2:D:194:TRP:C	2.55	0.45
2:D:237:TYR:OH	2:D:275:TRP:HH2	1.98	0.45
2:C:264:GLU:N	2:C:265:PRO:CD	2.79	0.45
1:A:34:SER:HB3	1:A:54:PRO:HB3	1.99	0.45
2:C:268:LYS:HZ2	2:C:270:GLN:NE2	2.15	0.45
2:D:179(B):VAL:CG1	2:D:356:ILE:HG13	2.45	0.45
2:C:135:LYS:O	2:C:139:ASN:HA	2.17	0.45
2:C:193:ASN:O	2:C:194:TRP:C	2.55	0.45
1:B:34:SER:HB3	1:B:54:PRO:HB3	1.98	0.45
2:C:184:LEU:C	2:C:185:ILE:HD12	2.36	0.45
2:C:132:GLN:CG	1:B:30:ILE:CG2	2.94	0.45
2:D:234:ASP:OD2	2:D:235(F):GLY:HA3	2.17	0.45
2:D:341:ASN:HD22	2:D:341:ASN:N	2.15	0.45
2:C:341:ASN:N	2:C:341:ASN:HD22	2.15	0.45
2:D:268:LYS:HZ2	2:D:270:GLN:NE2	2.15	0.45
1:A:47:ASP:HB3	2:C:210:LYS:HZ3	1.82	0.44
2:C:237:TYR:OH	2:C:275:TRP:HH2	1.98	0.44
2:C:300:LYS:N	2:C:332:ALA:HB3	2.27	0.44
2:D:218:ILE:CG1	2:D:219:PRO:HD2	2.45	0.44
2:D:222:TYR:HE1	2:D:285:GLU:HG2	1.83	0.44
2:D:295:GLN:CG	2:D:296:GLU:N	2.81	0.44
2:C:161:VAL:C	2:C:163:ASN:H	2.21	0.44
2:C:234:ASP:OD2	2:C:235(F):GLY:HA3	2.17	0.44
2:D:149:GLN:O	2:D:150:ASN:C	2.55	0.44
2:D:229:TYR:CE2	3:F:362:PRO:CB	2.98	0.44
2:D:135:LYS:O	2:D:139:ASN:HA	2.17	0.44
3:E:377:ARG:O	3:E:379:SER:N	2.51	0.44
2:C:183:ALA:O	2:C:185:ILE:HD12	2.18	0.44
2:C:222:TYR:HE1	2:C:285:GLU:HG2	1.83	0.44
2:D:131:LEU:O	2:D:135:LYS:HG3	2.18	0.44
2:D:159:LYS:O	2:D:163:ASN:HB2	2.17	0.44
2:D:158:ASN:O	2:D:162:GLU:CB	2.66	0.44
2:D:235(E):GLY:O	2:D:236:ILE:HG12	2.18	0.44
2:D:330:SER:O	2:D:331:LYS:CB	2.66	0.44
2:C:158:ASN:O	2:C:162:GLU:CB	2.66	0.44
2:C:295:GLN:CG	2:C:296:GLU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:ALA:O	2:D:185:ILE:HD12	2.18	0.44
2:D:292:THR:O	2:D:292:THR:HG23	2.18	0.44
2:C:159:LYS:O	2:C:163:ASN:HB2	2.17	0.44
3:F:377:ARG:NH1	3:F:377:ARG:HG3	2.33	0.44
2:C:235(B):ASN:HA	2:C:235(F):GLY:N	2.33	0.43
2:C:228:TYR:N	2:C:228:TYR:CD1	2.86	0.43
2:C:235(E):GLY:O	2:C:236:ILE:HG12	2.18	0.43
3:F:377:ARG:O	3:F:379:SER:N	2.51	0.43
2:C:136:MET:HE1	1:B:55:LEU:C	2.38	0.43
2:C:136:MET:HE3	1:B:55:LEU:CB	2.48	0.43
2:C:330:SER:O	2:C:331:LYS:CB	2.66	0.43
2:D:228:TYR:CD1	2:D:228:TYR:N	2.86	0.43
3:E:377:ARG:HG3	3:E:377:ARG:HH11	1.81	0.43
3:F:368:HIS:HB2	3:F:369:PRO:HD2	2.00	0.43
2:C:131:LEU:O	2:C:135:LYS:HG3	2.18	0.43
2:C:292:THR:HG23	2:C:292:THR:O	2.18	0.43
2:D:118:LEU:CD1	2:D:184:LEU:HD13	2.49	0.43
1:A:55:LEU:CA	2:D:136:MET:HE1	2.47	0.43
1:B:41:LEU:HD21	2:D:297:ILE:CG1	2.48	0.43
2:C:160:TRP:O	2:C:163:ASN:HB3	2.18	0.43
2:D:121:GLN:HB3	2:D:124:PHE:HB2	2.00	0.43
2:D:161:VAL:C	2:D:163:ASN:H	2.21	0.43
2:C:118:LEU:CD1	2:C:184:LEU:HD13	2.49	0.43
2:C:149:GLN:O	2:C:150:ASN:C	2.55	0.43
2:D:235(B):ASN:HA	2:D:235(F):GLY:N	2.33	0.43
1:A:57:ILE:HG22	1:A:61:MET:SD	2.59	0.43
3:E:377:ARG:HG3	3:E:377:ARG:NH1	2.33	0.43
1:A:41:LEU:HD21	2:C:297:ILE:CG1	2.48	0.43
2:D:149:GLN:O	2:D:152:ALA:N	2.52	0.42
2:D:233:SER:HA	2:D:235(F):GLY:O	2.19	0.42
2:D:264:GLU:N	2:D:265:PRO:CD	2.79	0.42
2:C:149:GLN:O	2:C:152:ALA:N	2.52	0.42
2:D:181:ASN:C	2:D:182:LEU:HD12	2.40	0.42
3:E:368:HIS:HB2	3:E:369:PRO:HD2	2.00	0.42
2:C:168:LEU:C	2:C:169:LEU:HD12	2.39	0.42
2:D:126:VAL:O	2:D:127:ASN:C	2.58	0.42
2:D:160:TRP:O	2:D:163:ASN:HB3	2.19	0.42
2:D:168:LEU:C	2:D:169:LEU:HD12	2.39	0.42
2:C:121:GLN:HB3	2:C:124:PHE:HB2	2.00	0.42
2:C:181:ASN:C	2:C:182:LEU:HD12	2.40	0.42
1:B:32:GLU:O	1:B:36:ASN:OD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:VAL:O	2:C:127:ASN:C	2.58	0.42
2:D:147:PHE:CE1	2:D:153:VAL:HG11	2.54	0.42
2:C:233:SER:HA	2:C:235(F):GLY:O	2.20	0.41
2:C:182:LEU:HD12	2:C:182:LEU:N	2.35	0.41
2:C:287:TYR:O	3:E:366:VAL:CG1	2.68	0.41
1:A:55:LEU:CA	2:D:136:MET:CE	2.90	0.41
1:B:47:ASP:CB	2:D:210:LYS:HZ3	2.33	0.41
1:A:47:ASP:HB2	2:C:210:LYS:NZ	2.35	0.41
1:B:57:ILE:HG22	1:B:61:MET:SD	2.59	0.41
2:D:330:SER:O	2:D:331:LYS:HB2	2.20	0.41
1:A:30:ILE:HD12	2:D:132:GLN:CG	2.50	0.41
2:D:182:LEU:N	2:D:182:LEU:HD12	2.35	0.41
2:D:126:VAL:HG22	2:D:127:ASN:N	2.35	0.41
2:D:130:PHE:O	2:D:133:MET:HB3	2.21	0.41
2:D:229:TYR:HB3	2:D:282:GLN:HG3	2.03	0.41
2:C:147:PHE:CE1	2:C:153:VAL:HG11	2.54	0.41
2:C:276:ALA:HA	2:C:279:VAL:HG22	2.02	0.41
2:D:258(A):VAL:HA	2:D:259:PRO:HD3	1.91	0.41
2:D:271:LEU:CD1	2:D:275:TRP:CZ3	3.03	0.41
2:C:132:GLN:CD	1:B:30:ILE:HG22	2.22	0.41
2:D:276:ALA:HA	2:D:279:VAL:HG22	2.02	0.41
1:A:58:ALA:CB	2:D:136:MET:SD	3.09	0.41
2:C:160:TRP:CZ3	2:C:185:ILE:HG22	2.56	0.41
2:C:178:PHE:O	2:C:179:ASP:CB	2.67	0.41
2:C:271:LEU:CD1	2:C:275:TRP:CZ3	3.03	0.41
1:A:32:GLU:O	1:A:36:ASN:OD1	2.38	0.41
2:C:150:ASN:H	2:C:150:ASN:ND2	2.19	0.41
2:C:157:ILE:HD12	2:C:178:PHE:HZ	1.86	0.41
2:C:330:SER:O	2:C:331:LYS:HB2	2.20	0.41
2:D:160:TRP:CZ3	2:D:185:ILE:HG22	2.56	0.41
2:C:130:PHE:O	2:C:133:MET:HB3	2.21	0.41
2:C:118:LEU:HD13	2:C:184:LEU:HD13	2.03	0.41
1:A:32:GLU:CA	2:C:269:ALA:HB2	2.51	0.41
2:C:222:TYR:CE1	2:C:285:GLU:HG2	2.56	0.41
2:C:212:ASP:OD2	2:C:212:ASP:O	2.39	0.40
2:D:157:ILE:HD12	2:D:178:PHE:HZ	1.86	0.40
2:C:210:LYS:C	2:C:212:ASP:N	2.75	0.40
2:C:235(A):SER:O	2:C:235(F):GLY:HA3	2.22	0.40
2:C:266:LEU:O	2:C:271:LEU:HD23	2.21	0.40
2:C:190:PHE:N	2:C:347:ALA:O	2.48	0.40
2:C:147:PHE:HD2	2:C:180:THR:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:256:ARG:O	2:C:258(A):VAL:HG13	2.22	0.40
2:C:177:ASP:HA	2:C:331:LYS:NZ	2.36	0.40
1:A:55:LEU:HD13	2:D:136:MET:HE3	1.98	0.40
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.97	0.40
2:D:150:ASN:H	2:D:150:ASN:ND2	2.19	0.40
1:B:47:ASP:HB2	2:D:210:LYS:NZ	2.35	0.40
2:C:155:ASN:O	2:C:156:SER:C	2.60	0.40
2:D:235(A):SER:O	2:D:235(F):GLY:HA3	2.22	0.40
2:D:287:TYR:O	3:F:366:VAL:CG1	2.68	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:235(B):ASN:ND2	2:D:309:THR:OG1[2_655]	1.82	0.38
2:C:109:GLN:NE2	2:C:309:THR:OG1[1_556]	1.95	0.25
3:E:392:HIS:CD2	2:D:277:ASN:O[2_555]	1.98	0.22
2:C:235:GLY:O	2:D:304:LYS:CE[2_655]	2.09	0.11
2:C:109:GLN:CG	2:C:304:LYS:NZ[1_556]	2.13	0.07
2:C:122:ASN:ND2	3:E:367:ASP:OD1[2_545]	2.17	0.03

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	38/40 (95%)	32 (84%)	4 (10%)	2 (5%)	2 10
1	B	38/40 (95%)	32 (84%)	4 (10%)	2 (5%)	2 10
2	C	240/261 (92%)	189 (79%)	38 (16%)	13 (5%)	2 9
2	D	240/261 (92%)	189 (79%)	38 (16%)	13 (5%)	2 9
3	E	31/33 (94%)	26 (84%)	3 (10%)	2 (6%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	31/33 (94%)	26 (84%)	3 (10%)	2 (6%)	1 6
All	All	618/668 (92%)	494 (80%)	90 (15%)	34 (6%)	2 9

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
2	C	235(C)	GLU
2	C	299	LEU
2	C	300	LYS
1	B	30	ILE
2	D	235(C)	GLU
2	D	299	LEU
2	D	300	LYS
2	C	113	LYS
2	C	150	ASN
2	C	156	SER
2	C	235(F)	GLY
2	C	246(A)	ASP
2	D	113	LYS
2	D	150	ASN
2	D	156	SER
2	D	235(F)	GLY
2	D	246(A)	ASP
1	A	67	GLY
2	C	331	LYS
3	E	378	LYS
1	B	67	GLY
2	D	331	LYS
3	F	378	LYS
2	C	179	ASP
3	E	369	PRO
2	D	179	ASP
3	F	369	PRO
2	C	183	ALA
2	D	183	ALA
2	C	279	VAL
2	D	279	VAL
2	C	308	VAL
2	D	308	VAL

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	33/33 (100%)	29 (88%)	4 (12%)	5 17
1	B	33/33 (100%)	29 (88%)	4 (12%)	5 17
2	C	214/229 (93%)	192 (90%)	22 (10%)	7 24
2	D	214/229 (93%)	192 (90%)	22 (10%)	7 24
3	E	31/31 (100%)	29 (94%)	2 (6%)	17 44
3	F	31/31 (100%)	29 (94%)	2 (6%)	17 44
All	All	556/586 (95%)	500 (90%)	56 (10%)	7 25

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	42	ARG
1	A	50	ILE
1	A	64	MET
2	C	121	GLN
2	C	128	GLU
2	C	155	ASN
2	C	166	ASN
2	C	172	LEU
2	C	176	GLU
2	C	210	LYS
2	C	220	MET
2	C	246(A)	ASP
2	C	249	SER
2	C	257	GLN
2	C	258(A)	VAL
2	C	271	LEU
2	C	274	GLU
2	C	275	TRP
2	C	279	VAL
2	C	282	GLN
2	C	284	VAL

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Mol	Chain	Res	Type
2	C	301	ASP
2	C	329	LEU
2	C	331	LYS
2	C	341	ASN
3	E	364	VAL
3	E	377	ARG
1	B	39	ASN
1	B	42	ARG
1	B	50	ILE
1	B	64	MET
2	D	121	GLN
2	D	128	GLU
2	D	155	ASN
2	D	166	ASN
2	D	172	LEU
2	D	176	GLU
2	D	210	LYS
2	D	220	MET
2	D	246(A)	ASP
2	D	249	SER
2	D	257	GLN
2	D	258(A)	VAL
2	D	271	LEU
2	D	274	GLU
2	D	275	TRP
2	D	279	VAL
2	D	282	GLN
2	D	284	VAL
2	D	301	ASP
2	D	329	LEU
2	D	331	LYS
2	D	341	ASN
3	F	364	VAL
3	F	377	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
2	C	116	ASN
2	C	121	GLN
2	C	139	ASN

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Mol	Chain	Res	Type
2	C	150	ASN
2	C	158	ASN
2	C	163	ASN
2	C	166	ASN
2	C	186	ASN
2	C	223	GLN
2	C	224	GLN
2	C	270	GLN
2	C	282	GLN
2	C	341	ASN
3	E	390	ASN
1	B	36	ASN
2	D	121	GLN
2	D	139	ASN
2	D	150	ASN
2	D	158	ASN
2	D	163	ASN
2	D	166	ASN
2	D	223	GLN
2	D	224	GLN
2	D	270	GLN
2	D	282	GLN
2	D	341	ASN
3	F	390	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	40/40 (100%)	-0.47	0	100	100	16, 29, 50, 51	0
1	B	40/40 (100%)	-0.50	0	100	100	16, 29, 50, 51	0
2	C	244/261 (93%)	-0.49	0	100	100	9, 27, 51, 60	0
2	D	244/261 (93%)	-0.47	0	100	100	9, 27, 51, 60	0
3	E	33/33 (100%)	-0.70	0	100	100	11, 20, 33, 47	0
3	F	33/33 (100%)	-0.77	0	100	100	11, 20, 33, 47	0
All	All	634/668 (94%)	-0.51	0	100	100	9, 26, 51, 60	0

There are no RSRZ outliers to report.

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.