Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 04:19 AM EDT

PDB ID	:	2D26
Title	:	Active site distortion is sufficient for proteinase inhibit second crystal structure of covalent serpin-proteinase complex
Authors	:	Dementiev, A.; Dobo, J.; Gettins, P.G.
Deposited on	:	2005-09-03
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

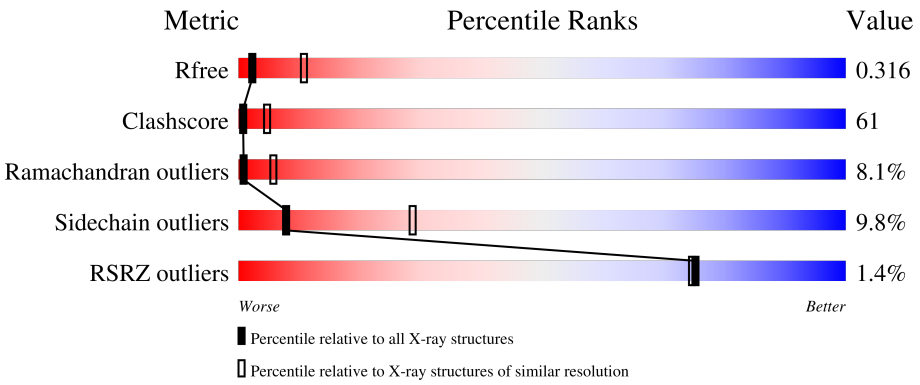
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of 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	358	.% 34% 50% 9% • 6%
2	B	36	3% 19% 47% 17% 17%
3	C	240	.% 35% 50% 8% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4189 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 Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2302	1474	394	429	5	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	GLU	engineered mutation	UNP P01009
A	51	LEU	PHE	engineered mutation	UNP P01009
A	59	ALA	THR	engineered mutation	UNP P01009
A	68	ALA	THR	engineered mutation	UNP P01009
A	70	GLY	ALA	engineered mutation	UNP P01009
A	101	HIS	ARG	engineered mutation	UNP P01009
A	232	SER	CYS	engineered mutation	UNP P01009

- Molecule 2 is a protein called Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	30	221	148	34	38	1	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	ILE	MET	engineered mutation	UNP P01009
B	381	ALA	SER	engineered mutation	UNP P01009
B	387	ARG	LYS	engineered mutation	UNP P01009

- Molecule 3 is a protein called Elastase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	223	1591	1001	288	292	10	0	0	0

- Molecule 4 is water.

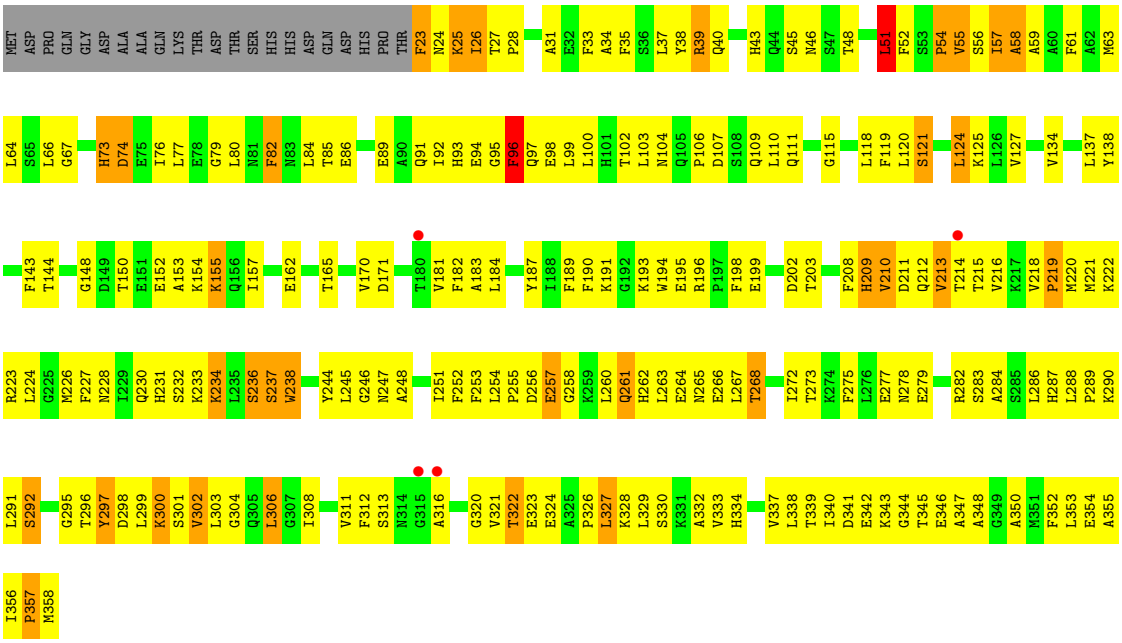
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	43	43	43	0	0
			Total	O		
4	B	3	3	3	0	0
			Total	O		
4	C	29	29	29	0	0

3 Residue-property plots (i)

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

- Molecule 1: Alpha-1-antitrypsin

Chain A:

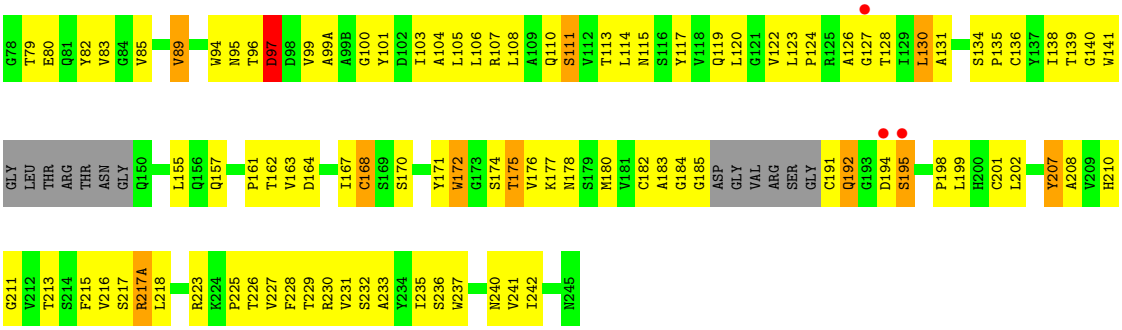


- Molecule 2: Alpha-1-antitrypsin

Chain B:

- Molecule 3: Elastase-1

Chain C:


G78 T79 E80 Q81 Y82 V83 G84 V85 V89 W94 N95 T96 D97 D98 V99 A99A A99B G100 Y101 D102 I103 A104 L105 L106 R107 L108 A109 Q110 S111 V112 T113 L114 N115 S116 Y117 V118 Q119 L120 G121 V122 L123 P124 R125 A126 G127 T128 I129 L130 A131 S134 P135 C136 Y137 I138 T139 G140 W141
GLY LEU THR ARG THR ASN GLY Q150 L155 Q156 Q157 P161 T162 V163 D164 I167 C168 S169 S170 Y171 W172 G173 S174 T175 V176 K177 N178 S179 M180 V181 C182 A183 G184 G185 ASP GLY VAL ARG SER GLY C191 Q192 G193 D194 S195 P198 L199 H200 C201 L202 Y207 A208 V209 H210
G211 V212 T213 S214 F215 V216 S217 R217A L218 R223 K224 P225 T226 V227 F228 T229 R230 V231 S232 A233 Y234 I235 S236 W237 N240 V241 I242 N245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.83Å 85.18Å 76.26Å 90.00° 121.01° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 39.16 – 2.93	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 91.3 (39.16-2.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.312 0.254 , 0.316	Depositor DCC
R_{free} test set	821 reflections (6.58%)	wwPDB-VP
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 184.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4189	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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 (i)

5.1 Standard geometry (i)

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	0.49	1/2353 (0.0%)	0.82	5/3222 (0.2%)
2	B	0.56	0/228	0.83	0/311
3	C	0.62	3/1628 (0.2%)	0.79	0/2229
All	All	0.55	4/4209 (0.1%)	0.81	5/5762 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TRP	NE1-CE2	8.70	1.48	1.37
3	C	38	TRP	NE1-CE2	8.69	1.48	1.37
3	C	27	TRP	NE1-CE2	8.67	1.48	1.37
3	C	172	TRP	NE1-CE2	8.66	1.48	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	LEU	CB-CG-CD2	10.07	128.12	111.00
1	A	278	ASN	N-CA-C	-9.67	84.90	111.00
1	A	278	ASN	CB-CA-C	-9.25	91.89	110.40
1	A	279	GLU	N-CA-CB	-9.00	94.40	110.60
1	A	51	LEU	CA-CB-CG	-6.20	101.04	115.30

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	2302	0	1920	271	2
2	B	221	0	198	39	0
3	C	1591	0	1401	171	1
4	A	43	0	0	5	0
4	B	3	0	0	0	0
4	C	29	0	0	5	1
All	All	4189	0	3519	468	2

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 61.

All (468) 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:299:LEU:HB2	1:A:332:ALA:CB	1.54	1.37
1:A:299:LEU:CD1	1:A:332:ALA:HB1	1.57	1.33
3:C:122:VAL:O	3:C:208:ALA:HB1	1.43	1.16
1:A:45:SER:O	1:A:46:ASN:ND2	1.79	1.14
1:A:299:LEU:HB2	1:A:332:ALA:HB3	1.19	1.14
3:C:42:CYS:HA	3:C:195:SER:O	1.48	1.14
1:A:290:LYS:HE2	1:A:342:GLU:OE1	1.51	1.09
1:A:291:LEU:HD12	1:A:340:ILE:HD12	1.27	1.09
1:A:255:PRO:HG3	1:A:260:LEU:HD13	1.32	1.08
1:A:299:LEU:HD12	1:A:332:ALA:CB	1.83	1.06
1:A:299:LEU:HB3	1:A:303:LEU:HG	1.38	1.05
1:A:45:SER:C	1:A:46:ASN:HD22	1.57	1.04
1:A:221:MET:HG3	1:A:288:LEU:O	1.55	1.04
3:C:36(B):GLY:O	4:C:263:HOH:O	1.78	1.02
1:A:299:LEU:CB	1:A:332:ALA:CB	2.38	1.01
1:A:51:LEU:HG	1:A:51:LEU:O	1.50	1.00
1:A:299:LEU:CB	1:A:332:ALA:HB3	1.92	1.00
3:C:67:VAL:CG1	3:C:70:GLU:HG3	1.91	0.99
1:A:24:ASN:O	1:A:25:LYS:HG2	1.65	0.97
3:C:201:CYS:HB2	3:C:210:HIS:HD2	1.30	0.96
1:A:328:LYS:O	1:A:355:ALA:HA	1.67	0.95
1:A:327:LEU:HD23	1:A:327:LEU:H	1.29	0.94
3:C:216:VAL:HG12	3:C:226:THR:HG23	1.49	0.94
3:C:67:VAL:HG12	3:C:70:GLU:HG3	1.50	0.94
1:A:299:LEU:HB3	1:A:303:LEU:CG	1.99	0.92
1:A:302:VAL:HG13	1:A:303:LEU:N	1.82	0.92
1:A:226:MET:HA	1:A:283:SER:HA	1.50	0.92
1:A:238:TRP:HB2	1:A:254:LEU:HB3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:PRO:HB2	3:C:119:GLN:H	1.36	0.91
3:C:122:VAL:HG13	3:C:208:ALA:HA	1.49	0.91
1:A:297:TYR:CD1	1:A:297:TYR:N	2.40	0.89
1:A:264:GLU:HG3	1:A:265:ASN:ND2	1.88	0.88
3:C:122:VAL:O	3:C:208:ALA:CB	2.21	0.88
3:C:55:ALA:HB3	3:C:58:CYS:SG	2.14	0.87
1:A:299:LEU:HD12	1:A:332:ALA:HB1	0.88	0.86
3:C:72:ASN:ND2	3:C:75:GLN:HG2	1.91	0.85
1:A:302:VAL:CG1	1:A:303:LEU:H	1.89	0.85
1:A:302:VAL:CG1	1:A:303:LEU:N	2.39	0.84
1:A:255:PRO:HG3	1:A:260:LEU:CD1	2.06	0.84
1:A:45:SER:C	1:A:46:ASN:ND2	2.25	0.84
1:A:103:LEU:HD11	2:B:376:GLU:HG3	1.60	0.83
2:B:376:GLU:HB3	2:B:379:THR:O	1.79	0.83
3:C:136:CYS:HB3	3:C:199:LEU:HD11	1.61	0.83
3:C:42:CYS:CA	3:C:195:SER:O	2.27	0.82
1:A:255:PRO:CG	1:A:260:LEU:HD13	2.09	0.82
1:A:299:LEU:CD1	1:A:332:ALA:CB	2.51	0.81
2:B:369:PRO:HA	2:B:388:VAL:O	1.81	0.81
3:C:67:VAL:HG11	3:C:70:GLU:HG3	1.63	0.81
1:A:290:LYS:CE	1:A:342:GLU:OE1	2.29	0.80
1:A:216:VAL:HA	4:A:396:HOH:O	1.81	0.80
1:A:244:TYR:HB2	1:A:248:ALA:HB3	1.64	0.79
1:A:290:LYS:HE2	1:A:342:GLU:CD	2.03	0.79
1:A:194:TRP:NE1	1:A:344:GLY:HA2	1.97	0.78
3:C:217(A):ARG:HD2	3:C:217(A):ARG:N	1.99	0.78
1:A:221:MET:CG	1:A:288:LEU:O	2.31	0.77
1:A:109:GLN:NE2	1:A:245:LEU:HD13	2.00	0.77
3:C:124:PRO:O	3:C:235:ILE:CD1	2.33	0.76
1:A:299:LEU:CG	1:A:332:ALA:HB1	2.15	0.76
3:C:122:VAL:HG13	3:C:208:ALA:CA	2.15	0.76
3:C:72:ASN:ND2	3:C:75:GLN:CG	2.49	0.76
1:A:231:HIS:HB2	1:A:238:TRP:CZ3	2.21	0.75
1:A:299:LEU:HB3	1:A:303:LEU:CD1	2.17	0.75
1:A:24:ASN:O	1:A:25:LYS:CG	2.36	0.74
1:A:299:LEU:HA	1:A:302:VAL:HG12	1.69	0.74
3:C:72:ASN:HD22	3:C:75:GLN:CG	2.01	0.74
1:A:299:LEU:HB2	1:A:332:ALA:HB2	1.64	0.74
3:C:33:LEU:HD12	3:C:66:VAL:HG12	1.70	0.73
2:B:379:THR:O	2:B:381:ALA:N	2.19	0.72
3:C:230:ARG:CZ	3:C:233:ALA:HB2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ARG:NE	3:C:233:ALA:HB2	2.05	0.72
3:C:63:LEU:HD12	3:C:63:LEU:H	1.54	0.71
1:A:327:LEU:H	1:A:327:LEU:CD2	2.03	0.71
1:A:219:PRO:HG2	1:A:290:LYS:HB2	1.73	0.71
1:A:124:LEU:HG	1:A:125:LYS:N	2.06	0.71
1:A:265:ASN:N	1:A:265:ASN:HD22	1.87	0.70
3:C:171:TYR:HA	3:C:223:ARG:O	1.92	0.70
1:A:203:THR:HG23	1:A:221:MET:HA	1.74	0.70
2:B:377:GLN:HE21	2:B:377:GLN:CA	2.02	0.70
1:A:120:LEU:O	1:A:144:THR:HA	1.92	0.70
1:A:291:LEU:O	1:A:292:SER:HB2	1.92	0.69
1:A:256:ASP:O	1:A:258:GLY:N	2.26	0.69
1:A:311:VAL:HG22	1:A:329:LEU:CB	2.23	0.69
3:C:23:GLN:HB2	3:C:26:SER:OG	1.92	0.69
1:A:80:LEU:HD12	1:A:80:LEU:O	1.93	0.69
1:A:254:LEU:HD11	2:B:368:LYS:HE2	1.75	0.68
1:A:299:LEU:O	1:A:300:LYS:C	2.32	0.68
3:C:140:GLY:O	3:C:155:LEU:HD12	1.93	0.68
1:A:291:LEU:HD12	1:A:340:ILE:CD1	2.17	0.68
1:A:296:THR:C	1:A:297:TYR:CG	2.67	0.68
3:C:172:TRP:HB3	3:C:176:VAL:HG23	1.75	0.68
1:A:184:LEU:HD22	1:A:353:LEU:HD12	1.74	0.67
3:C:211:GLY:HA2	3:C:231:VAL:HG13	1.76	0.67
1:A:27:THR:N	1:A:28:PRO:HD2	2.07	0.67
1:A:51:LEU:O	1:A:51:LEU:CG	2.35	0.67
3:C:124:PRO:HB2	3:C:128:THR:HG21	1.77	0.67
1:A:238:TRP:HD1	1:A:254:LEU:HD23	1.60	0.66
3:C:130:LEU:HD13	3:C:162:THR:HG21	1.77	0.66
1:A:39:ARG:HH12	1:A:265:ASN:HA	1.61	0.66
3:C:124:PRO:HG3	3:C:210:HIS:ND1	2.10	0.66
1:A:26:ILE:HB	1:A:82:PHE:CZ	2.31	0.65
1:A:247:ASN:O	2:B:377:GLN:HB2	1.96	0.65
3:C:104:ALA:O	3:C:105:LEU:HD23	1.97	0.65
1:A:223:ARG:HD3	1:A:227:PHE:CZ	2.32	0.64
1:A:61:PHE:CZ	1:A:303:LEU:HD13	2.33	0.64
3:C:178:ASN:O	3:C:230:ARG:HD3	1.98	0.64
2:B:376:GLU:OE2	2:B:378:ASN:HB2	1.98	0.64
1:A:265:ASN:ND2	1:A:265:ASN:N	2.44	0.63
3:C:167:ILE:HG23	3:C:171:TYR:CZ	2.33	0.63
3:C:74:ASN:C	3:C:74:ASN:OD1	2.36	0.63
3:C:23:GLN:O	3:C:24:ARG:C	2.36	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:ASN:HD22	3:C:75:GLN:HG2	1.59	0.63
1:A:103:LEU:CD1	2:B:376:GLU:HG3	2.28	0.63
1:A:341:ASP:OD1	1:A:343:LYS:N	2.32	0.63
2:B:369:PRO:HB3	2:B:389:VAL:HG22	1.79	0.63
1:A:110:LEU:HD11	1:A:190:PHE:HE1	1.63	0.63
3:C:47:ILE:HA	4:C:252:HOH:O	1.99	0.63
3:C:141:TRP:H	3:C:194:ASP:CB	2.12	0.63
3:C:172:TRP:CB	3:C:176:VAL:HG23	2.28	0.63
1:A:230:GLN:O	1:A:238:TRP:HE3	1.82	0.62
1:A:313:SER:O	1:A:328:LYS:HE3	1.99	0.62
1:A:221:MET:HE3	1:A:288:LEU:CB	2.30	0.61
1:A:54:PRO:O	1:A:55:VAL:C	2.37	0.61
2:B:376:GLU:HB2	2:B:383:LEU:HD21	1.82	0.61
1:A:119:PHE:CD2	1:A:143:PHE:HB2	2.35	0.61
1:A:119:PHE:HA	1:A:143:PHE:O	2.01	0.61
1:A:224:LEU:HD12	1:A:284:ALA:O	2.01	0.61
2:B:376:GLU:OE1	2:B:377:GLN:N	2.34	0.61
3:C:49:GLN:HG2	3:C:114:LEU:HD21	1.82	0.61
1:A:57:ILE:O	1:A:59:ALA:N	2.32	0.60
3:C:47:ILE:O	3:C:48:ARG:HG3	2.02	0.60
1:A:253:PHE:O	2:B:370:PHE:HB2	2.01	0.60
1:A:230:GLN:O	1:A:238:TRP:CE3	2.55	0.60
1:A:194:TRP:CD1	1:A:344:GLY:HA2	2.37	0.60
3:C:185:GLY:CA	3:C:225:PRO:HB3	2.31	0.60
1:A:299:LEU:CG	1:A:332:ALA:CB	2.78	0.60
1:A:33:PHE:CE2	1:A:58:ALA:HB2	2.36	0.60
1:A:220:MET:HA	1:A:289:PRO:HA	1.83	0.60
1:A:198:PHE:HB2	1:A:342:GLU:HA	1.82	0.60
1:A:301:SER:O	1:A:302:VAL:C	2.40	0.59
1:A:184:LEU:HD22	1:A:353:LEU:CD1	2.32	0.59
2:B:377:GLN:HA	2:B:377:GLN:NE2	2.17	0.59
3:C:44:GLY:HA3	3:C:54:THR:HG22	1.84	0.59
3:C:124:PRO:HB3	3:C:210:HIS:CE1	2.37	0.59
1:A:301:SER:O	1:A:304:GLY:N	2.36	0.58
3:C:215:PHE:CZ	3:C:227:VAL:HG11	2.38	0.58
1:A:313:SER:C	1:A:328:LYS:HZ2	2.07	0.58
3:C:122:VAL:C	3:C:208:ALA:HB1	2.23	0.58
3:C:82:TYR:N	3:C:82:TYR:CD2	2.71	0.58
3:C:122:VAL:HG13	3:C:208:ALA:CB	2.34	0.58
1:A:272:ILE:O	1:A:275:PHE:N	2.37	0.58
3:C:126:ALA:HB1	4:C:248:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:ILE:HG22	3:C:168:CYS:N	2.18	0.58
1:A:26:ILE:HB	1:A:82:PHE:HZ	1.67	0.58
1:A:64:LEU:HD22	1:A:76:ILE:CD1	2.34	0.58
3:C:31:ILE:HB	3:C:44:GLY:O	2.04	0.57
1:A:296:THR:C	1:A:297:TYR:CD1	2.78	0.57
3:C:37:SER:OG	4:C:274:HOH:O	2.17	0.57
1:A:298:ASP:HA	1:A:332:ALA:O	2.05	0.57
3:C:122:VAL:HG22	3:C:208:ALA:HB2	1.87	0.57
1:A:31:ALA:O	1:A:34:ALA:HB3	2.05	0.57
1:A:261:GLN:CD	1:A:261:GLN:H	2.08	0.57
3:C:138:ILE:HG23	3:C:138:ILE:O	2.04	0.57
2:B:377:GLN:CA	2:B:377:GLN:NE2	2.68	0.57
3:C:70:GLU:HG2	3:C:80:GLU:HG2	1.86	0.56
1:A:260:LEU:O	1:A:262:HIS:N	2.37	0.56
1:A:80:LEU:HD12	1:A:82:PHE:HB2	1.88	0.56
1:A:208:PHE:O	1:A:210:VAL:N	2.37	0.56
3:C:27:TRP:CE2	3:C:139:THR:HG21	2.39	0.56
3:C:161:PRO:O	3:C:184:GLY:N	2.37	0.56
1:A:313:SER:C	1:A:328:LYS:NZ	2.59	0.56
3:C:27:TRP:NE1	3:C:139:THR:HG21	2.21	0.56
3:C:183:ALA:O	3:C:225:PRO:HB2	2.05	0.56
1:A:26:ILE:C	1:A:26:ILE:HD12	2.26	0.56
1:A:226:MET:CA	1:A:283:SER:HA	2.31	0.56
3:C:174:SER:O	3:C:175:THR:C	2.42	0.56
3:C:194:ASP:O	3:C:195:SER:C	2.44	0.56
3:C:123:LEU:HD12	3:C:123:LEU:N	2.20	0.56
3:C:135:PRO:O	3:C:136:CYS:SG	2.64	0.56
1:A:66:LEU:HD21	1:A:138:TYR:CE1	2.41	0.55
1:A:184:LEU:HB3	1:A:353:LEU:HB2	1.88	0.55
1:A:275:PHE:C	1:A:277:GLU:H	2.09	0.55
1:A:302:VAL:HG12	1:A:303:LEU:H	1.66	0.55
1:A:233:LYS:O	1:A:234:LYS:C	2.43	0.55
2:B:369:PRO:CB	2:B:389:VAL:HA	2.36	0.55
3:C:31:ILE:HD11	3:C:46:LEU:HD13	1.88	0.55
3:C:35:TYR:CB	3:C:63:LEU:HD23	2.36	0.55
1:A:39:ARG:NH1	1:A:265:ASN:HA	2.21	0.55
3:C:124:PRO:HG2	3:C:232:SER:HB3	1.88	0.55
1:A:110:LEU:HD11	1:A:190:PHE:CE1	2.42	0.55
1:A:118:LEU:HD12	1:A:182:PHE:CE1	2.41	0.55
1:A:299:LEU:O	1:A:301:SER:N	2.39	0.55
1:A:210:VAL:CG2	1:A:216:VAL:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:CYS:HB2	3:C:210:HIS:CD2	2.23	0.55
1:A:110:LEU:HB2	1:A:246:GLY:HA3	1.88	0.54
1:A:209:HIS:HB2	2:B:367:ASN:O	2.07	0.54
1:A:221:MET:CB	1:A:288:LEU:O	2.55	0.54
3:C:168:CYS:HB3	3:C:176:VAL:HG11	1.88	0.54
1:A:92:ILE:O	1:A:96:PHE:HD2	1.90	0.54
1:A:308:ILE:HG22	1:A:308:ILE:O	2.06	0.54
3:C:61:ARG:HB3	3:C:63:LEU:CD1	2.37	0.54
3:C:185:GLY:HA3	3:C:225:PRO:HB3	1.89	0.54
3:C:236:SER:O	3:C:240:ASN:ND2	2.41	0.54
1:A:61:PHE:CZ	1:A:303:LEU:CD1	2.91	0.54
3:C:33:LEU:CD1	3:C:66:VAL:HG12	2.36	0.54
1:A:327:LEU:HD23	1:A:327:LEU:N	2.09	0.54
3:C:51:TRP:CZ2	3:C:107:ARG:HD3	2.43	0.54
1:A:98:GLU:O	1:A:102:THR:HG22	2.07	0.54
1:A:110:LEU:HB2	1:A:245:LEU:O	2.08	0.54
1:A:295:GLY:HA3	1:A:297:TYR:OH	2.07	0.54
3:C:46:LEU:HD23	3:C:119:GLN:O	2.08	0.54
1:A:67:GLY:HA2	1:A:320:GLY:HA3	1.89	0.54
1:A:77:LEU:O	1:A:80:LEU:HG	2.08	0.54
3:C:163:VAL:N	3:C:182:CYS:O	2.41	0.54
1:A:251:ILE:HG22	1:A:253:PHE:CE1	2.42	0.54
3:C:72:ASN:ND2	3:C:75:GLN:HB3	2.22	0.54
3:C:85:VAL:HG12	3:C:108:LEU:HD23	1.89	0.54
3:C:30:GLN:HE22	3:C:198:PRO:CD	2.21	0.54
3:C:44:GLY:H	3:C:198:PRO:HD3	1.72	0.54
1:A:234:LYS:O	1:A:262:HIS:CE1	2.61	0.54
1:A:327:LEU:CD2	1:A:327:LEU:N	2.70	0.54
3:C:161:PRO:O	3:C:183:ALA:HA	2.07	0.54
1:A:208:PHE:CE1	2:B:368:LYS:HA	2.43	0.53
1:A:299:LEU:HB3	1:A:303:LEU:HD12	1.91	0.53
1:A:121:SER:O	1:A:124:LEU:HB2	2.08	0.53
1:A:339:THR:O	1:A:345:THR:HG23	2.08	0.53
1:A:64:LEU:O	1:A:64:LEU:HD23	2.09	0.53
1:A:119:PHE:CE1	1:A:157:ILE:HG12	2.43	0.53
1:A:134:VAL:O	1:A:138:TYR:HB2	2.08	0.53
1:A:326:PRO:O	1:A:357:PRO:HA	2.08	0.53
3:C:72:ASN:ND2	3:C:75:GLN:CB	2.72	0.53
3:C:177:LYS:HG2	3:C:180:MET:HE1	1.89	0.53
2:B:379:THR:C	2:B:381:ALA:H	2.09	0.53
3:C:94:TRP:CH2	3:C:99:VAL:HG23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:OE1	1:A:257:GLU:N	2.42	0.53
1:A:261:GLN:O	1:A:264:GLU:HG2	2.09	0.53
3:C:66:VAL:HG22	3:C:83:VAL:HG13	1.90	0.53
1:A:124:LEU:CG	1:A:125:LYS:N	2.72	0.53
1:A:290:LYS:HE2	1:A:342:GLU:OE2	2.09	0.52
2:B:369:PRO:HB3	2:B:389:VAL:HA	1.91	0.52
3:C:72:ASN:HD22	3:C:75:GLN:CD	2.13	0.52
3:C:122:VAL:CG1	3:C:208:ALA:HA	2.33	0.52
3:C:140:GLY:O	3:C:155:LEU:HA	2.10	0.52
1:A:184:LEU:HB3	1:A:353:LEU:HD12	1.91	0.52
3:C:167:ILE:HG23	3:C:171:TYR:CE2	2.44	0.52
1:A:308:ILE:O	1:A:312:PHE:HD2	1.92	0.52
3:C:96:THR:O	3:C:97:ASP:C	2.47	0.52
1:A:342:GLU:CD	1:A:342:GLU:H	2.13	0.52
2:B:388:VAL:O	2:B:388:VAL:HG12	2.09	0.52
3:C:72:ASN:C	3:C:72:ASN:OD1	2.48	0.52
1:A:212:GLN:O	1:A:213:VAL:CB	2.56	0.52
1:A:84:LEU:O	1:A:86:GLU:N	2.43	0.51
3:C:31:ILE:HD11	3:C:46:LEU:CD1	2.41	0.51
1:A:299:LEU:HD13	1:A:303:LEU:HD11	1.93	0.51
1:A:115:GLY:HA3	1:A:187:TYR:CE2	2.46	0.51
2:B:379:THR:O	2:B:379:THR:OG1	2.29	0.51
2:B:383:LEU:N	2:B:383:LEU:HD22	2.26	0.51
1:A:328:LYS:N	1:A:356:ILE:O	2.43	0.51
1:A:38:TYR:C	1:A:40:GLN:H	2.14	0.51
1:A:184:LEU:HD23	1:A:184:LEU:C	2.31	0.51
1:A:261:GLN:H	1:A:261:GLN:NE2	2.08	0.51
1:A:38:TYR:O	1:A:40:GLN:N	2.44	0.51
3:C:94:TRP:HB2	3:C:101:TYR:O	2.10	0.51
1:A:26:ILE:HG12	1:A:95:GLY:O	2.11	0.50
3:C:191:CYS:SG	3:C:192:GLN:HG2	2.51	0.50
1:A:153:ALA:O	1:A:155:LYS:N	2.38	0.50
1:A:223:ARG:HD3	1:A:227:PHE:HZ	1.76	0.50
1:A:226:MET:HA	1:A:283:SER:CA	2.34	0.50
1:A:264:GLU:C	1:A:265:ASN:HD22	2.14	0.50
3:C:61:ARG:HB3	3:C:63:LEU:HD12	1.92	0.50
3:C:72:ASN:OD1	3:C:74:ASN:N	2.44	0.50
3:C:124:PRO:O	3:C:235:ILE:HD11	2.10	0.50
1:A:165:THR:HA	1:A:189:PHE:HB2	1.94	0.50
1:A:313:SER:O	1:A:328:LYS:CE	2.59	0.50
1:A:337:VAL:CG2	1:A:348:ALA:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:CYS:C	3:C:60:ASP:H	2.13	0.50
3:C:48:ARG:O	3:C:50:ASN:N	2.44	0.50
3:C:168:CYS:SG	3:C:176:VAL:HG21	2.52	0.50
1:A:236:SER:O	1:A:237:SER:CB	2.59	0.49
1:A:333:VAL:HB	1:A:352:PHE:HB3	1.92	0.49
1:A:35:PHE:O	1:A:39:ARG:N	2.30	0.49
1:A:268:THR:O	1:A:272:ILE:HG13	2.12	0.49
1:A:273:THR:HG22	1:A:277:GLU:OE2	2.12	0.49
3:C:94:TRP:HH2	3:C:99:VAL:HG23	1.75	0.49
3:C:171:TYR:N	3:C:171:TYR:CD1	2.81	0.49
3:C:201:CYS:O	3:C:207:TYR:HA	2.11	0.49
1:A:233:LYS:O	1:A:236:SER:N	2.45	0.49
1:A:260:LEU:C	1:A:262:HIS:N	2.65	0.49
1:A:26:ILE:HD12	1:A:26:ILE:O	2.12	0.49
1:A:221:MET:O	1:A:287:HIS:HA	2.11	0.49
3:C:48:ARG:CD	3:C:242:ILE:HD12	2.43	0.49
1:A:251:ILE:HG22	1:A:253:PHE:CZ	2.47	0.49
3:C:35:TYR:CB	3:C:63:LEU:CD2	2.90	0.49
3:C:100:GLY:O	3:C:101:TYR:HB2	2.13	0.49
3:C:113:THR:HA	4:C:259:HOH:O	2.12	0.49
1:A:338:LEU:HD12	1:A:347:ALA:HB2	1.96	0.48
1:A:27:THR:H	1:A:28:PRO:HD2	1.75	0.48
1:A:193:LYS:O	1:A:244:TYR:HA	2.13	0.48
1:A:223:ARG:CD	1:A:227:PHE:HZ	2.27	0.48
1:A:299:LEU:CB	1:A:303:LEU:CD1	2.91	0.48
3:C:59:VAL:HG11	3:C:106:LEU:CD2	2.42	0.48
1:A:37:LEU:O	1:A:37:LEU:HD12	2.14	0.48
1:A:38:TYR:C	1:A:40:GLN:N	2.67	0.48
1:A:330:SER:CB	1:A:354:GLU:HG2	2.43	0.48
3:C:38:TRP:CE3	3:C:65(A):ARG:HG2	2.49	0.48
2:B:369:PRO:HG3	2:B:389:VAL:O	2.14	0.47
3:C:128:THR:HG23	3:C:128:THR:O	2.14	0.47
1:A:231:HIS:HB2	1:A:238:TRP:CE3	2.49	0.47
3:C:123:LEU:N	3:C:123:LEU:CD1	2.77	0.47
3:C:163:VAL:HB	3:C:182:CYS:HB2	1.95	0.47
1:A:63:MET:HE2	1:A:184:LEU:HD11	1.97	0.47
3:C:202:LEU:O	3:C:202:LEU:HG	2.14	0.47
3:C:230:ARG:HH21	3:C:233:ALA:HA	1.79	0.47
1:A:48:THR:CB	4:A:362:HOH:O	2.63	0.47
2:B:377:GLN:HE21	2:B:377:GLN:HA	1.69	0.47
3:C:99:VAL:HG13	3:C:99(A):ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG13	1:A:76:ILE:O	2.14	0.47
1:A:181:VAL:N	1:A:355:ALA:O	2.48	0.47
1:A:253:PHE:HD1	2:B:371:VAL:O	1.98	0.47
2:B:377:GLN:HE21	2:B:377:GLN:N	2.12	0.47
1:A:73:HIS:ND1	1:A:73:HIS:C	2.68	0.47
1:A:73:HIS:NE2	1:A:89:GLU:OE2	2.48	0.47
3:C:115:ASN:C	3:C:117:TYR:N	2.69	0.47
3:C:192:GLN:HE21	3:C:192:GLN:HB3	1.37	0.47
1:A:63:MET:HE3	1:A:184:LEU:HG	1.97	0.47
1:A:221:MET:N	1:A:288:LEU:O	2.38	0.46
1:A:162:GLU:CB	1:A:170:VAL:HA	2.46	0.46
1:A:322:THR:CG2	1:A:327:LEU:HD22	2.46	0.46
3:C:141:TRP:CD1	3:C:155:LEU:N	2.83	0.46
3:C:172:TRP:CB	3:C:176:VAL:CG2	2.92	0.46
1:A:247:ASN:C	2:B:377:GLN:HB2	2.36	0.46
1:A:260:LEU:O	1:A:261:GLN:C	2.53	0.46
1:A:238:TRP:CD1	1:A:254:LEU:HD23	2.45	0.46
1:A:183:ALA:HA	1:A:353:LEU:O	2.15	0.46
1:A:203:THR:HG23	1:A:221:MET:CA	2.45	0.46
1:A:299:LEU:CB	1:A:303:LEU:HG	2.27	0.46
3:C:67:VAL:HG11	3:C:70:GLU:CG	2.39	0.46
1:A:208:PHE:HB3	1:A:216:VAL:HG23	1.97	0.46
3:C:218:LEU:N	3:C:218:LEU:HD22	2.31	0.46
1:A:124:LEU:HG	1:A:125:LYS:H	1.77	0.46
1:A:182:PHE:HB3	1:A:355:ALA:HB3	1.98	0.46
3:C:99(A):ALA:HB1	3:C:175:THR:HG23	1.97	0.46
3:C:232:SER:HA	3:C:235:ILE:HG13	1.98	0.46
1:A:25:LYS:HA	4:A:400:HOH:O	2.16	0.45
1:A:191:LYS:HA	1:A:346:GLU:HA	1.99	0.45
1:A:218:VAL:O	1:A:220:MET:N	2.49	0.45
1:A:299:LEU:CA	1:A:332:ALA:HB3	2.43	0.45
1:A:52:PHE:CD1	1:A:52:PHE:N	2.85	0.45
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.79	0.45
3:C:235:ILE:O	3:C:236:SER:C	2.55	0.45
1:A:52:PHE:CZ	2:B:385:MET:HG2	2.52	0.45
2:B:374:ILE:C	2:B:375:ILE:HG13	2.37	0.45
3:C:99(A):ALA:CB	3:C:175:THR:HG23	2.47	0.45
3:C:115:ASN:C	3:C:117:TYR:H	2.19	0.45
1:A:97:GLN:HB3	1:A:137:LEU:O	2.16	0.45
1:A:299:LEU:N	1:A:332:ALA:HB3	2.32	0.45
1:A:100:LEU:O	1:A:104:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HA	1:A:302:VAL:CG1	2.42	0.44
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.82	0.44
1:A:111:GLN:O	1:A:190:PHE:HA	2.17	0.44
1:A:264:GLU:HG3	1:A:265:ASN:N	2.31	0.44
2:B:369:PRO:HG3	2:B:389:VAL:HA	2.00	0.44
3:C:49:GLN:CG	3:C:114:LEU:HD21	2.46	0.44
3:C:124:PRO:HB3	3:C:210:HIS:HE1	1.82	0.44
3:C:130:LEU:HD22	3:C:134:SER:CB	2.47	0.44
1:A:194:TRP:CE2	1:A:344:GLY:HA2	2.52	0.44
1:A:299:LEU:CB	1:A:303:LEU:HD12	2.48	0.44
3:C:139:THR:HA	3:C:157:GLN:HA	2.00	0.44
1:A:214:THR:HG22	1:A:215:THR:N	2.32	0.44
1:A:262:HIS:O	1:A:266:GLU:CB	2.64	0.44
3:C:48:ARG:HD2	3:C:242:ILE:HD12	1.99	0.44
3:C:130:LEU:HD22	3:C:134:SER:HB2	1.98	0.44
1:A:55:VAL:O	1:A:56:SER:C	2.55	0.44
1:A:26:ILE:HB	1:A:82:PHE:CE2	2.53	0.44
1:A:237:SER:HA	1:A:254:LEU:O	2.17	0.44
1:A:255:PRO:HB3	1:A:260:LEU:HA	1.98	0.44
3:C:216:VAL:HG12	3:C:226:THR:CG2	2.32	0.44
1:A:25:LYS:O	1:A:26:ILE:HG13	2.18	0.44
1:A:34:ALA:HB1	2:B:385:MET:HE2	1.99	0.44
1:A:82:PHE:HE1	1:A:96:PHE:HE2	1.65	0.44
1:A:210:VAL:HG12	1:A:211:ASP:N	2.32	0.44
3:C:89:VAL:HG13	3:C:105:LEU:O	2.18	0.44
1:A:64:LEU:HD23	1:A:64:LEU:C	2.38	0.43
3:C:216:VAL:CG1	3:C:226:THR:HG23	2.34	0.43
3:C:59:VAL:HG11	3:C:106:LEU:HD22	1.99	0.43
3:C:192:GLN:HG2	3:C:192:GLN:H	1.41	0.43
3:C:213:THR:HA	3:C:228:PHE:CD1	2.54	0.43
1:A:109:GLN:HB3	1:A:245:LEU:HB3	2.01	0.43
1:A:251:ILE:CG2	1:A:253:PHE:CZ	3.01	0.43
3:C:59:VAL:O	3:C:59:VAL:HG23	2.18	0.43
3:C:164:ASP:O	3:C:167:ILE:HB	2.18	0.43
3:C:63:LEU:HB2	3:C:65:PHE:CE2	2.54	0.43
1:A:61:PHE:HE1	1:A:308:ILE:HG21	1.82	0.43
1:A:91:GLN:O	1:A:92:ILE:C	2.55	0.43
1:A:304:GLY:C	1:A:306:LEU:N	2.71	0.43
1:A:328:LYS:CG	1:A:329:LEU:N	2.81	0.43
1:A:48:THR:HA	4:A:394:HOH:O	2.18	0.43
1:A:25:LYS:O	1:A:27:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:CD1	1:A:252:PHE:N	2.86	0.43
3:C:110:GLN:C	3:C:111:SER:O	2.57	0.43
1:A:80:LEU:O	1:A:80:LEU:CD1	2.64	0.43
1:A:284:ALA:HB1	2:B:362:PRO:O	2.19	0.43
2:B:372:PHE:CZ	2:B:386:GLY:HA3	2.54	0.42
2:B:383:LEU:HD22	2:B:383:LEU:H	1.83	0.42
1:A:77:LEU:C	1:A:79:GLY:N	2.72	0.42
1:A:198:PHE:O	1:A:342:GLU:HB2	2.19	0.42
1:A:221:MET:SD	1:A:341:ASP:C	2.97	0.42
1:A:313:SER:O	1:A:328:LYS:NZ	2.51	0.42
3:C:110:GLN:O	3:C:111:SER:O	2.37	0.42
1:A:27:THR:N	1:A:28:PRO:CD	2.77	0.42
2:B:383:LEU:H	2:B:383:LEU:CD2	2.32	0.42
3:C:30:GLN:HE22	3:C:198:PRO:HD2	1.84	0.42
3:C:130:LEU:HD23	3:C:131:ALA:H	1.85	0.42
2:B:379:THR:C	2:B:381:ALA:N	2.71	0.42
3:C:167:ILE:O	3:C:170:SER:N	2.53	0.42
1:A:223:ARG:HG2	1:A:227:PHE:HZ	1.84	0.42
1:A:286:LEU:HA	2:B:364:VAL:O	2.19	0.42
1:A:208:PHE:CD1	1:A:208:PHE:C	2.92	0.42
1:A:302:VAL:HG13	1:A:303:LEU:H	1.52	0.42
3:C:114:LEU:HD22	3:C:114:LEU:N	2.35	0.42
1:A:195:GLU:HB3	1:A:245:LEU:HD23	2.02	0.41
1:A:93:HIS:HB3	1:A:137:LEU:HD13	2.03	0.41
1:A:260:LEU:O	1:A:263:LEU:N	2.53	0.41
3:C:56:ALA:HB2	3:C:103:ILE:H	1.85	0.41
1:A:124:LEU:CG	1:A:125:LYS:H	2.31	0.41
1:A:261:GLN:O	1:A:264:GLU:CG	2.68	0.41
1:A:322:THR:OG1	1:A:323:GLU:N	2.54	0.41
1:A:334:HIS:ND1	1:A:350:ALA:O	2.51	0.41
3:C:49:GLN:O	3:C:111:SER:HA	2.19	0.41
1:A:222:LYS:HE2	1:A:287:HIS:HD2	1.86	0.41
1:A:255:PRO:CB	1:A:260:LEU:HA	2.51	0.41
3:C:95:ASN:HB3	3:C:97:ASP:OD2	2.20	0.41
3:C:215:PHE:O	3:C:227:VAL:HG12	2.20	0.41
3:C:231:VAL:CG2	3:C:232:SER:N	2.83	0.41
1:A:275:PHE:C	1:A:277:GLU:N	2.74	0.41
3:C:47:ILE:HG12	3:C:51:TRP:O	2.21	0.41
3:C:48:ARG:HA	3:C:120:LEU:CD1	2.51	0.41
3:C:128:THR:O	3:C:128:THR:CG2	2.68	0.41
3:C:230:ARG:NH2	3:C:233:ALA:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:PRO:CG	2:B:389:VAL:HG13	2.51	0.41
3:C:67:VAL:HG11	3:C:70:GLU:OE2	2.21	0.41
3:C:122:VAL:O	3:C:208:ALA:CA	2.68	0.41
1:A:25:LYS:N	4:A:400:HOH:O	2.53	0.41
1:A:236:SER:HB2	1:A:262:HIS:ND1	2.36	0.41
1:A:43:HIS:N	1:A:43:HIS:CD2	2.86	0.41
1:A:57:ILE:C	1:A:59:ALA:H	2.23	0.41
3:C:48:ARG:HA	3:C:120:LEU:HD11	2.02	0.41
3:C:65(A):ARG:CZ	3:C:82:TYR:HD1	2.34	0.41
1:A:73:HIS:HD1	1:A:74:ASP:N	2.19	0.41
1:A:127:VAL:HG22	1:A:323:GLU:HG3	2.03	0.41
1:A:292:SER:HA	1:A:338:LEU:O	2.21	0.41
3:C:167:ILE:CG2	3:C:171:TYR:CE2	3.04	0.41
1:A:109:GLN:HE21	1:A:245:LEU:HD13	1.80	0.40
1:A:199:GLU:CB	1:A:202:ASP:OD1	2.69	0.40
3:C:72:ASN:C	3:C:74:ASN:H	2.24	0.40
3:C:72:ASN:HB3	3:C:75:GLN:HG2	2.02	0.40
3:C:85:VAL:O	3:C:85:VAL:HG23	2.21	0.40
3:C:230:ARG:CZ	3:C:233:ALA:CB	2.93	0.40
1:A:99:LEU:O	1:A:103:LEU:HB2	2.21	0.40
3:C:172:TRP:CD1	3:C:225:PRO:HD2	2.57	0.40
1:A:80:LEU:CD1	1:A:82:PHE:HB2	2.50	0.40
1:A:94:GLU:O	1:A:97:GLN:HG2	2.21	0.40
3:C:77:ASP:C	3:C:79:THR:H	2.23	0.40
3:C:235:ILE:C	3:C:237:TRP:N	2.73	0.40
1:A:150:THR:C	1:A:152:GLU:H	2.24	0.40
1:A:223:ARG:HD3	1:A:227:PHE:CE1	2.56	0.40
1:A:194:TRP:C	1:A:196:ARG:N	2.73	0.40
3:C:72:ASN:HD21	3:C:75:GLN:HB3	1.85	0.40
3:C:72:ASN:CG	3:C:75:GLN:HG2	2.41	0.40

All (2) 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)
1:A:23:PHE:N	3:C:127:GLY:CA[3_445]	1.71	0.49
1:A:24:ASN:ND2	4:C:269:HOH:O[3_445]	1.80	0.40

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	334/358 (93%)	244 (73%)	57 (17%)	33 (10%)	0 3
2	B	28/36 (78%)	18 (64%)	7 (25%)	3 (11%)	0 3
3	C	217/240 (90%)	152 (70%)	54 (25%)	11 (5%)	2 13
All	All	579/634 (91%)	414 (72%)	118 (20%)	47 (8%)	1 6

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	55	VAL
1	A	210	VAL
1	A	213	VAL
1	A	257	GLU
1	A	292	SER
1	A	316	ALA
1	A	357	PRO
2	B	380	LYS
3	C	111	SER
1	A	51	LEU
1	A	58	ALA
1	A	85	THR
1	A	121	SER
1	A	154	LYS
1	A	155	LYS
1	A	171	ASP
1	A	209	HIS
1	A	261	GLN
1	A	300	LYS
1	A	302	VAL
3	C	24	ARG
3	C	49	GLN
3	C	217	SER

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Mol	Chain	Res	Type
1	A	39	ARG
1	A	54	PRO
1	A	96	PHE
1	A	124	LEU
1	A	219	PRO
1	A	234	LYS
1	A	324	GLU
3	C	97	ASP
1	A	236	SER
2	B	373	LEU
3	C	195	SER
1	A	237	SER
1	A	321	VAL
2	B	382	PRO
3	C	175	THR
1	A	148	GLY
3	C	62	GLU
1	A	26	ILE
3	C	59	VAL
3	C	241	VAL
1	A	57	ILE
3	C	43	GLY
1	A	106	PRO

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	182/311 (58%)	166 (91%)	16 (9%)	10 33
2	B	21/34 (62%)	15 (71%)	6 (29%)	0 1
3	C	144/198 (73%)	132 (92%)	12 (8%)	11 36
All	All	347/543 (64%)	313 (90%)	34 (10%)	8 29

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	51	LEU
1	A	73	HIS
1	A	74	ASP
1	A	82	PHE
1	A	96	PHE
1	A	107	ASP
1	A	228	ASN
1	A	232	SER
1	A	268	THR
1	A	282	ARG
1	A	297	TYR
1	A	306	LEU
1	A	322	THR
1	A	327	LEU
1	A	358	MET
2	B	367	ASN
2	B	376	GLU
2	B	377	GLN
2	B	382	PRO
2	B	385	MET
2	B	388	VAL
3	C	45	THR
3	C	63	LEU
3	C	70	GLU
3	C	74	ASN
3	C	89	VAL
3	C	97	ASP
3	C	130	LEU
3	C	168	CYS
3	C	192	GLN
3	C	207	TYR
3	C	217(A)	ARG
3	C	229	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	97	GLN
1	A	109	GLN
1	A	111	GLN
1	A	228	ASN

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Mol	Chain	Res	Type
1	A	261	GLN
1	A	265	ASN
1	A	287	HIS
2	B	367	ASN
2	B	377	GLN
3	C	23	GLN
3	C	30	GLN
3	C	74	ASN
3	C	119	GLN
3	C	192	GLN
3	C	200	HIS
3	C	210	HIS
3	C	240	ASN
3	C	245	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	336/358 (93%)	-0.27	4 (1%)	79	78	31, 71, 96, 98	0
2	B	30/36 (83%)	-0.28	1 (3%)	46	44	29, 52, 86, 92	0
3	C	223/240 (92%)	-0.26	3 (1%)	77	77	28, 54, 91, 99	5 (2%)
All	All	589/634 (92%)	-0.26	8 (1%)	75	75	28, 62, 95, 99	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	THR	3.8
1	A	315	GLY	3.1
2	B	367	ASN	2.7
3	C	194	ASP	2.5
1	A	316	ALA	2.3
3	C	127	GLY	2.2
3	C	195	SER	2.2
1	A	214	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.