Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:01 pm BST

PDB ID	:	1PFC
Title	:	MOLECULAR-REPLACEMENT STRUCTURE OF GUINEA PIG IGG1 P*FC(PRIME) REFINED AT 3.1 ANGSTROMS RESOLUTION
Authors	:	Bryant, S.H.; Amzel, L.M.; Poljak, R.J.; Phizackerley, R.P.
Deposited on	:	1981-10-28
Resolution	:	3.12 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 ⓘ) were used in the production of this report:

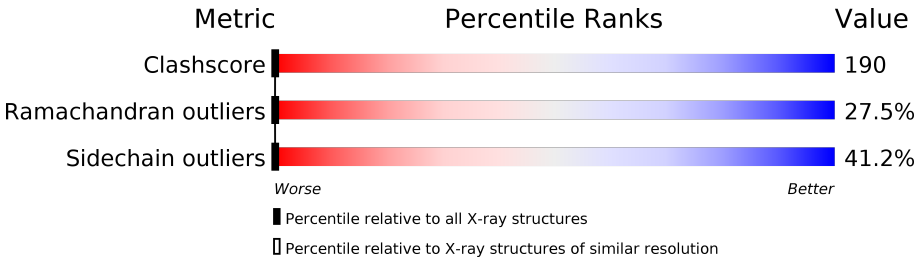
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.12 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	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)

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%

Mol	Chain	Length	Quality of chain
1	A	113	19% 39% 40%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 878 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 IGG1 PFC' FC.

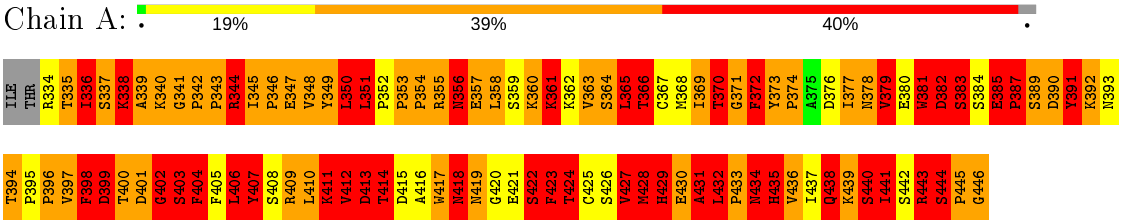
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	111	878	558	147	169	4	0	0	0

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. 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. 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: IGG1 PFC' FC

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	60.57Å 60.57Å 136.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 3.12 15.14 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-3.12) 95.5 (15.14-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.303 , (Not available) 0.357 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 225.6	EDS
L-test for twinning[1]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.63	EDS
Total number of atoms	878	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]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	2.41	30/904 (3.3%)	4.29	180/1230 (14.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	GLY	C-O	23.50	1.61	1.23
1	A	403	SER	C-O	18.91	1.59	1.23
1	A	398	PHE	C-O	17.07	1.55	1.23
1	A	370	THR	C-O	12.81	1.47	1.23
1	A	392	LYS	C-O	10.87	1.44	1.23
1	A	402	GLY	C-N	-10.40	1.10	1.34
1	A	398	PHE	C-N	-10.15	1.10	1.34
1	A	418	ASN	C-O	8.13	1.38	1.23
1	A	370	THR	C-N	-7.67	1.19	1.33
1	A	392	LYS	C-N	-7.58	1.16	1.34
1	A	409	ARG	CZ-NH2	6.88	1.42	1.33
1	A	341	GLY	N-CA	-6.41	1.36	1.46
1	A	428	MET	CA-CB	-6.30	1.40	1.53
1	A	349	TYR	CA-CB	6.14	1.67	1.53
1	A	399	ASP	N-CA	-5.93	1.34	1.46
1	A	392	LYS	N-CA	5.79	1.57	1.46
1	A	419	ASN	N-CA	-5.59	1.35	1.46
1	A	385	GLU	CB-CG	-5.51	1.41	1.52
1	A	371	GLY	CA-C	5.47	1.60	1.51
1	A	366	THR	CA-CB	5.42	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	SER	CB-OG	-5.42	1.35	1.42
1	A	418	ASN	C-N	-5.34	1.21	1.34
1	A	334	ARG	NE-CZ	-5.31	1.26	1.33
1	A	403	SER	CA-CB	-5.30	1.45	1.52
1	A	334	ARG	CD-NE	-5.29	1.37	1.46
1	A	385	GLU	CG-CD	-5.27	1.44	1.51
1	A	349	TYR	C-O	5.24	1.33	1.23
1	A	335	THR	CA-CB	5.22	1.67	1.53
1	A	446	GLY	N-CA	5.07	1.53	1.46
1	A	339	ALA	CA-CB	5.04	1.63	1.52

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	370	THR	CA-C-N	27.22	170.64	116.20
1	A	402	GLY	CA-C-N	26.88	176.34	117.20
1	A	402	GLY	O-C-N	-24.75	83.10	122.70
1	A	402	GLY	C-N-CA	22.31	177.47	121.70
1	A	370	THR	O-C-N	-22.07	85.67	123.20
1	A	334	ARG	NE-CZ-NH1	20.93	130.76	120.30
1	A	443	ARG	NE-CZ-NH1	-20.18	110.21	120.30
1	A	334	ARG	CD-NE-CZ	19.98	151.58	123.60
1	A	398	PHE	O-C-N	-19.53	91.45	122.70
1	A	392	LYS	C-N-CA	19.33	170.04	121.70
1	A	398	PHE	CA-C-N	18.91	158.81	117.20
1	A	392	LYS	O-C-N	-18.22	93.55	122.70
1	A	403	SER	CA-C-N	17.48	155.65	117.20
1	A	394	THR	N-CA-CB	17.40	143.35	110.30
1	A	409	ARG	CD-NE-CZ	16.48	146.68	123.60
1	A	334	ARG	NE-CZ-NH2	-15.97	112.31	120.30
1	A	422	SER	C-N-CA	15.62	160.74	121.70
1	A	365	LEU	C-N-CA	15.30	159.95	121.70
1	A	418	ASN	C-N-CA	15.22	159.75	121.70
1	A	402	GLY	CA-C-O	-14.84	93.89	120.60
1	A	403	SER	CA-C-O	-14.26	90.16	120.10
1	A	392	LYS	CA-C-N	14.16	148.36	117.20
1	A	398	PHE	C-N-CA	14.04	156.81	121.70
1	A	370	THR	CA-C-O	-13.36	92.05	120.10
1	A	418	ASN	CA-C-N	13.16	146.15	117.20
1	A	409	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	A	409	ARG	NE-CZ-NH2	-12.07	114.27	120.30
1	A	401	ASP	CB-CG-OD2	-11.99	107.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	347	GLU	C-N-CA	11.84	151.30	121.70
1	A	414	THR	C-N-CA	11.76	151.11	121.70
1	A	443	ARG	NH1-CZ-NH2	11.65	132.22	119.40
1	A	446	GLY	CA-C-O	-11.50	99.89	120.60
1	A	355	ARG	NE-CZ-NH2	11.40	126.00	120.30
1	A	371	GLY	N-CA-C	-11.38	84.66	113.10
1	A	382	ASP	CB-CG-OD1	11.31	128.48	118.30
1	A	385	GLU	CA-CB-CG	11.25	138.15	113.40
1	A	394	THR	O-C-N	11.23	142.45	121.10
1	A	355	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	A	381	TRP	CA-CB-CG	10.66	133.95	113.70
1	A	418	ASN	O-C-N	-10.49	105.92	122.70
1	A	435	HIS	CA-CB-CG	10.43	131.34	113.60
1	A	339	ALA	N-CA-CB	-10.39	95.55	110.10
1	A	398	PHE	CA-C-O	-9.97	99.16	120.10
1	A	382	ASP	C-N-CA	9.82	146.25	121.70
1	A	428	MET	CB-CA-C	9.74	129.88	110.40
1	A	385	GLU	CB-CG-CD	9.72	140.44	114.20
1	A	339	ALA	N-CA-C	9.64	137.03	111.00
1	A	391	TYR	CB-CG-CD1	9.46	126.68	121.00
1	A	392	LYS	CA-CB-CG	9.28	133.81	113.40
1	A	385	GLU	OE1-CD-OE2	-9.04	112.45	123.30
1	A	403	SER	N-CA-C	-8.85	87.09	111.00
1	A	403	SER	CA-CB-OG	8.68	134.63	111.20
1	A	399	ASP	N-CA-CB	8.62	126.12	110.60
1	A	350	LEU	CA-CB-CG	8.57	135.01	115.30
1	A	403	SER	O-C-N	-8.54	109.04	122.70
1	A	383	SER	N-CA-CB	8.52	123.28	110.50
1	A	344	ARG	CA-CB-CG	8.16	131.36	113.40
1	A	364	SER	N-CA-CB	8.11	122.67	110.50
1	A	400	THR	O-C-N	8.00	135.50	122.70
1	A	400	THR	CA-C-N	-8.00	99.61	117.20
1	A	424	THR	N-CA-C	8.00	132.59	111.00
1	A	427	VAL	CB-CA-C	-7.97	96.26	111.40
1	A	399	ASP	O-C-N	7.94	135.41	122.70
1	A	385	GLU	N-CA-C	7.91	132.36	111.00
1	A	418	ASN	N-CA-CB	-7.84	96.48	110.60
1	A	381	TRP	CB-CA-C	7.83	126.07	110.40
1	A	413	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	410	LEU	CA-CB-CG	7.80	133.25	115.30
1	A	424	THR	CA-CB-OG1	-7.79	92.64	109.00
1	A	446	GLY	N-CA-C	-7.57	94.19	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	349	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	A	415	ASP	N-CA-CB	7.47	124.04	110.60
1	A	349	TYR	N-CA-C	7.43	131.06	111.00
1	A	394	THR	N-CA-C	-7.36	91.14	111.00
1	A	344	ARG	CB-CG-CD	7.32	130.62	111.60
1	A	344	ARG	C-N-CA	7.31	139.98	121.70
1	A	361	LYS	CG-CD-CE	7.29	133.76	111.90
1	A	415	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	347	GLU	CG-CD-OE1	7.21	132.72	118.30
1	A	362	LYS	N-CA-CB	-7.18	97.68	110.60
1	A	433	PRO	O-C-N	7.13	134.10	122.70
1	A	403	SER	CB-CA-C	7.09	123.57	110.10
1	A	348	VAL	CB-CA-C	-7.04	98.02	111.40
1	A	413	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	341	GLY	N-CA-C	6.99	130.56	113.10
1	A	349	TYR	CA-CB-CG	-6.96	100.18	113.40
1	A	369	ILE	C-N-CA	-6.94	104.34	121.70
1	A	431	ALA	CA-C-N	-6.94	101.94	117.20
1	A	346	PRO	N-CA-C	6.90	130.04	112.10
1	A	422	SER	CA-C-N	6.86	132.29	117.20
1	A	390	ASP	N-CA-C	6.85	129.50	111.00
1	A	384	SER	CB-CA-C	6.83	123.07	110.10
1	A	379	VAL	CB-CA-C	-6.82	98.44	111.40
1	A	382	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	338	LYS	N-CA-C	6.79	129.34	111.00
1	A	391	TYR	CA-C-N	-6.72	102.41	117.20
1	A	365	LEU	CB-CA-C	6.71	122.96	110.20
1	A	351	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	391	TYR	O-C-N	6.58	133.24	122.70
1	A	370	THR	CA-CB-CG2	6.58	121.62	112.40
1	A	391	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	385	GLU	CG-CD-OE2	6.54	131.39	118.30
1	A	378	ASN	N-CA-CB	6.53	122.35	110.60
1	A	441	ILE	CB-CA-C	6.51	124.63	111.60
1	A	404	PHE	O-C-N	6.49	133.08	122.70
1	A	423	PHE	N-CA-C	6.46	128.43	111.00
1	A	418	ASN	CA-C-O	-6.45	106.56	120.10
1	A	335	THR	N-CA-CB	-6.43	98.08	110.30
1	A	422	SER	O-C-N	-6.42	112.42	122.70
1	A	361	LYS	N-CA-C	6.42	128.32	111.00
1	A	343	PRO	N-CA-C	6.41	128.77	112.10
1	A	372	PHE	CA-CB-CG	6.38	129.20	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	373	TYR	N-CA-CB	6.35	122.03	110.60
1	A	366	THR	N-CA-C	6.31	128.03	111.00
1	A	424	THR	N-CA-CB	-6.30	98.33	110.30
1	A	376	ASP	CA-CB-CG	6.27	127.19	113.40
1	A	434	ASN	O-C-N	6.23	132.67	122.70
1	A	410	LEU	CA-C-N	-6.23	103.50	117.20
1	A	356	ASN	CA-CB-CG	6.21	127.05	113.40
1	A	373	TYR	CA-CB-CG	6.20	125.18	113.40
1	A	418	ASN	CA-CB-CG	6.16	126.96	113.40
1	A	358	LEU	CA-C-O	6.13	132.97	120.10
1	A	436	VAL	CA-C-N	-6.12	103.74	117.20
1	A	432	LEU	CB-CA-C	6.00	121.59	110.20
1	A	389	SER	C-N-CA	5.99	136.68	121.70
1	A	389	SER	CB-CA-C	5.95	121.39	110.10
1	A	419	ASN	CA-CB-CG	-5.94	100.33	113.40
1	A	391	TYR	N-CA-CB	5.93	121.28	110.60
1	A	378	ASN	CA-C-O	5.89	132.47	120.10
1	A	390	ASP	N-CA-CB	-5.80	100.17	110.60
1	A	436	VAL	CB-CA-C	-5.65	100.66	111.40
1	A	392	LYS	CB-CA-C	5.65	121.69	110.40
1	A	428	MET	CA-CB-CG	5.61	122.84	113.30
1	A	399	ASP	CA-C-N	-5.60	104.88	117.20
1	A	431	ALA	N-CA-C	-5.60	95.88	111.00
1	A	378	ASN	CA-C-N	-5.55	104.99	117.20
1	A	429	HIS	O-C-N	5.54	131.57	122.70
1	A	347	GLU	CB-CG-CD	5.54	129.15	114.20
1	A	397	VAL	N-CA-C	-5.53	96.06	111.00
1	A	425	CYS	CB-CA-C	-5.53	99.33	110.40
1	A	357	GLU	N-CA-CB	-5.53	100.65	110.60
1	A	363	VAL	N-CA-CB	-5.50	99.41	111.50
1	A	424	THR	OG1-CB-CG2	5.49	122.64	110.00
1	A	444	SER	CA-CB-OG	5.49	126.03	111.20
1	A	407	TYR	CA-C-O	-5.48	108.58	120.10
1	A	379	VAL	CA-C-N	-5.47	105.17	117.20
1	A	443	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	428	MET	CA-C-N	-5.45	105.22	117.20
1	A	361	LYS	CA-C-N	5.44	129.17	117.20
1	A	349	TYR	CB-CG-CD1	5.44	124.26	121.00
1	A	373	TYR	N-CA-C	-5.44	96.32	111.00
1	A	433	PRO	C-N-CA	-5.42	108.15	121.70
1	A	401	ASP	CA-C-N	-5.40	105.41	116.20
1	A	355	ARG	O-C-N	5.39	131.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	VAL	C-N-CA	5.39	135.17	121.70
1	A	401	ASP	OD1-CG-OD2	5.35	133.47	123.30
1	A	378	ASN	C-N-CA	5.35	135.07	121.70
1	A	399	ASP	CA-CB-CG	-5.35	101.64	113.40
1	A	338	LYS	CA-C-O	5.34	131.32	120.10
1	A	347	GLU	O-C-N	-5.34	114.16	122.70
1	A	416	ALA	CA-C-N	-5.30	105.54	117.20
1	A	411	LYS	C-N-CA	5.30	134.94	121.70
1	A	347	GLU	CB-CA-C	5.25	120.90	110.40
1	A	426	SER	CA-C-N	-5.25	105.66	117.20
1	A	415	ASP	O-C-N	5.23	131.07	122.70
1	A	406	LEU	CB-CG-CD1	5.21	119.86	111.00
1	A	365	LEU	CB-CG-CD1	5.19	119.83	111.00
1	A	436	VAL	CA-CB-CG1	5.18	118.67	110.90
1	A	381	TRP	CA-C-N	-5.15	105.88	117.20
1	A	350	LEU	O-C-N	5.14	130.93	122.70
1	A	370	THR	CA-CB-OG1	-5.14	98.21	109.00
1	A	372	PHE	CB-CG-CD1	5.14	124.40	120.80
1	A	338	LYS	CA-C-N	-5.12	105.93	117.20
1	A	438	GLN	N-CA-CB	5.12	119.82	110.60
1	A	431	ALA	CA-C-O	5.06	130.74	120.10
1	A	425	CYS	O-C-N	5.06	130.79	122.70
1	A	427	VAL	N-CA-CB	5.05	122.60	111.50
1	A	391	TYR	CA-CB-CG	5.03	122.95	113.40
1	A	336	ILE	CB-CA-C	5.02	121.65	111.60
1	A	422	SER	N-CA-CB	-5.01	102.98	110.50

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	THR	Mainchain,Peptide
1	A	392	LYS	Mainchain,Peptide
1	A	398	PHE	Mainchain
1	A	402	GLY	Mainchain,Peptide
1	A	403	SER	Mainchain,Peptide
1	A	418	ASN	Mainchain
1	A	422	SER	Peptide

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	878	0	845	328	5
All	All	878	0	845	328	5

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 190.

All (328) 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:361:LYS:N	1:A:414:THR:HG21	1.38	1.33
1:A:381:TRP:NE1	1:A:410:LEU:HB2	1.41	1.32
1:A:381:TRP:HE1	1:A:410:LEU:CB	1.44	1.31
1:A:444:SER:HB2	1:A:445:PRO:CD	1.66	1.24
1:A:372:PHE:N	1:A:404:PHE:H	1.36	1.23
1:A:377:ILE:CG2	1:A:429:HIS:HD2	1.52	1.20
1:A:377:ILE:HG21	1:A:429:HIS:HD2	1.06	1.20
1:A:344:ARG:NH1	1:A:344:ARG:H	1.38	1.20
1:A:373:TYR:HB3	1:A:374:PRO:CA	1.73	1.18
1:A:346:PRO:O	1:A:347:GLU:HG3	1.44	1.16
1:A:342:PRO:CA	1:A:373:TYR:HB2	1.74	1.16
1:A:443:ARG:O	1:A:444:SER:OG	1.63	1.13
1:A:427:VAL:HG12	1:A:436:VAL:HG22	1.14	1.11
1:A:381:TRP:CZ2	1:A:410:LEU:HB3	1.85	1.10
1:A:411:LYS:HD2	1:A:413:ASP:CA	1.80	1.10
1:A:370:THR:HG22	1:A:406:LEU:H	1.17	1.09
1:A:444:SER:HB2	1:A:445:PRO:HD2	1.22	1.09
1:A:377:ILE:CG2	1:A:429:HIS:CD2	2.35	1.08
1:A:349:TYR:CB	1:A:368:MET:HG3	1.85	1.07
1:A:342:PRO:HA	1:A:373:TYR:CB	1.84	1.07
1:A:379:VAL:HG12	1:A:379:VAL:O	1.54	1.06
1:A:361:LYS:H	1:A:414:THR:CG2	1.69	1.05
1:A:411:LYS:HD2	1:A:413:ASP:HA	1.11	1.05
1:A:404:PHE:HD1	1:A:405:PHE:N	1.53	1.04
1:A:342:PRO:HA	1:A:373:TYR:HB2	1.04	1.03
1:A:338:LYS:HB2	1:A:342:PRO:HG3	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:O	1:A:336:ILE:HG13	1.59	1.01
1:A:342:PRO:CG	1:A:343:PRO:HD2	1.89	1.01
1:A:439:LYS:O	1:A:440:SER:HB2	1.61	1.00
1:A:361:LYS:N	1:A:414:THR:CG2	2.24	0.99
1:A:370:THR:HB	1:A:405:PHE:HA	1.45	0.99
1:A:344:ARG:HH11	1:A:344:ARG:H	1.00	0.98
1:A:373:TYR:HB3	1:A:374:PRO:HA	0.99	0.98
1:A:421:GLU:O	1:A:422:SER:C	2.00	0.98
1:A:381:TRP:NE1	1:A:410:LEU:CB	2.13	0.97
1:A:372:PHE:H	1:A:404:PHE:N	1.61	0.96
1:A:394:THR:OG1	1:A:407:TYR:HB2	1.65	0.96
1:A:417:TRP:HE3	1:A:417:TRP:C	1.70	0.95
1:A:379:VAL:CG1	1:A:379:VAL:O	2.14	0.95
1:A:381:TRP:HZ2	1:A:410:LEU:HB3	1.28	0.94
1:A:427:VAL:CG1	1:A:436:VAL:HG22	1.96	0.94
1:A:349:TYR:HB2	1:A:368:MET:HG3	1.44	0.93
1:A:340:LYS:HD2	1:A:373:TYR:OH	1.68	0.93
1:A:370:THR:HG22	1:A:406:LEU:N	1.85	0.92
1:A:377:ILE:HG21	1:A:429:HIS:CD2	1.99	0.92
1:A:444:SER:CB	1:A:445:PRO:CD	2.47	0.92
1:A:421:GLU:HB3	1:A:423:PHE:CD2	2.04	0.92
1:A:373:TYR:CB	1:A:374:PRO:HA	1.95	0.91
1:A:344:ARG:NH1	1:A:344:ARG:N	2.18	0.91
1:A:404:PHE:CD1	1:A:405:PHE:N	2.38	0.91
1:A:406:LEU:C	1:A:407:TYR:HD2	1.73	0.90
1:A:380:GLU:HA	1:A:391:TYR:OH	1.70	0.90
1:A:339:ALA:HB1	1:A:340:LYS:HE2	1.54	0.90
1:A:372:PHE:H	1:A:404:PHE:H	0.91	0.88
1:A:434:ASN:HD21	1:A:436:VAL:HG13	1.37	0.88
1:A:342:PRO:HG2	1:A:343:PRO:HD2	1.55	0.88
1:A:402:GLY:O	1:A:405:PHE:CE1	2.26	0.88
1:A:406:LEU:O	1:A:407:TYR:CD2	2.26	0.87
1:A:364:SER:OG	1:A:365:LEU:N	2.02	0.87
1:A:372:PHE:N	1:A:404:PHE:N	2.19	0.86
1:A:381:TRP:NE1	1:A:410:LEU:HD22	1.90	0.86
1:A:360:LYS:O	1:A:361:LYS:HB2	1.75	0.86
1:A:421:GLU:O	1:A:423:PHE:N	2.09	0.85
1:A:381:TRP:NE1	1:A:410:LEU:CD2	2.40	0.85
1:A:352:PRO:O	1:A:354:PRO:HD3	1.77	0.84
1:A:434:ASN:ND2	1:A:436:VAL:HG13	1.93	0.84
1:A:377:ILE:HG22	1:A:429:HIS:CD2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TRP:CE3	1:A:417:TRP:C	2.51	0.83
1:A:351:LEU:HD11	1:A:366:THR:HG22	1.61	0.83
1:A:381:TRP:CE2	1:A:410:LEU:HB3	2.14	0.82
1:A:342:PRO:CD	1:A:343:PRO:HD2	2.08	0.82
1:A:353:PRO:HB2	1:A:444:SER:HA	1.61	0.82
1:A:366:THR:OG1	1:A:409:ARG:HG3	1.80	0.81
1:A:411:LYS:HD2	1:A:413:ASP:N	1.96	0.81
1:A:351:LEU:O	1:A:365:LEU:HG	1.82	0.80
1:A:377:ILE:HD13	1:A:404:PHE:CZ	2.16	0.80
1:A:353:PRO:O	1:A:443:ARG:HG3	1.83	0.78
1:A:381:TRP:HE1	1:A:410:LEU:HB2	0.62	0.78
1:A:372:PHE:O	1:A:404:PHE:CD2	2.35	0.78
1:A:336:ILE:HG22	1:A:337:SER:H	1.48	0.78
1:A:377:ILE:HG23	1:A:404:PHE:HE2	1.47	0.77
1:A:402:GLY:HA2	1:A:405:PHE:CZ	2.18	0.77
1:A:404:PHE:C	1:A:404:PHE:CD1	2.58	0.77
1:A:377:ILE:CD1	1:A:404:PHE:CZ	2.67	0.77
1:A:381:TRP:CE2	1:A:410:LEU:CB	2.67	0.77
1:A:364:SER:HB2	1:A:411:LYS:HB2	1.67	0.77
1:A:351:LEU:CD1	1:A:366:THR:HG22	2.14	0.77
1:A:439:LYS:O	1:A:440:SER:CB	2.33	0.77
1:A:349:TYR:HB3	1:A:368:MET:HG3	1.66	0.77
1:A:377:ILE:HD13	1:A:404:PHE:HZ	1.49	0.76
1:A:369:ILE:HG21	1:A:427:VAL:HG21	1.68	0.76
1:A:377:ILE:CD1	1:A:404:PHE:HZ	1.99	0.76
1:A:351:LEU:HD11	1:A:366:THR:CG2	2.16	0.76
1:A:342:PRO:CG	1:A:343:PRO:CD	2.65	0.75
1:A:360:LYS:CB	1:A:414:THR:HB	2.16	0.75
1:A:427:VAL:HG12	1:A:436:VAL:CG2	2.08	0.75
1:A:406:LEU:C	1:A:407:TYR:CD2	2.60	0.75
1:A:377:ILE:HB	1:A:429:HIS:CB	2.18	0.74
1:A:421:GLU:HB3	1:A:423:PHE:HD2	1.51	0.74
1:A:338:LYS:HB2	1:A:342:PRO:CG	2.18	0.74
1:A:342:PRO:HG2	1:A:343:PRO:CD	2.17	0.74
1:A:432:LEU:HD23	1:A:433:PRO:HD2	1.67	0.74
1:A:342:PRO:HA	1:A:373:TYR:CA	2.18	0.74
1:A:352:PRO:C	1:A:354:PRO:HD3	2.06	0.74
1:A:370:THR:HG21	1:A:405:PHE:HB3	1.69	0.74
1:A:402:GLY:HA2	1:A:405:PHE:HZ	1.51	0.73
1:A:344:ARG:N	1:A:344:ARG:HH11	1.83	0.73
1:A:351:LEU:CG	1:A:366:THR:HG22	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:O	1:A:365:LEU:CG	2.36	0.73
1:A:364:SER:OG	1:A:410:LEU:O	2.05	0.72
1:A:419:ASN:O	1:A:419:ASN:OD1	2.06	0.72
1:A:352:PRO:O	1:A:354:PRO:CD	2.36	0.72
1:A:342:PRO:CB	1:A:343:PRO:CD	2.67	0.72
1:A:421:GLU:CB	1:A:423:PHE:CE2	2.74	0.71
1:A:402:GLY:O	1:A:403:SER:C	2.28	0.71
1:A:345:ILE:HB	1:A:371:GLY:O	1.90	0.71
1:A:443:ARG:O	1:A:444:SER:CB	2.39	0.71
1:A:432:LEU:CD2	1:A:433:PRO:HD2	2.20	0.71
1:A:397:VAL:O	1:A:405:PHE:HB2	1.89	0.71
1:A:371:GLY:HA2	1:A:404:PHE:O	1.91	0.70
1:A:381:TRP:CD1	1:A:410:LEU:HD22	2.26	0.70
1:A:406:LEU:O	1:A:407:TYR:HD2	1.65	0.70
1:A:377:ILE:HB	1:A:429:HIS:HB2	1.72	0.70
1:A:370:THR:CG2	1:A:405:PHE:HA	2.22	0.69
1:A:402:GLY:O	1:A:403:SER:O	2.10	0.69
1:A:417:TRP:O	1:A:417:TRP:HE3	1.75	0.69
1:A:430:GLU:O	1:A:431:ALA:CB	2.40	0.69
1:A:337:SER:O	1:A:338:LYS:CB	2.40	0.69
1:A:411:LYS:CD	1:A:413:ASP:H	2.05	0.69
1:A:349:TYR:HD1	1:A:368:MET:O	1.75	0.69
1:A:360:LYS:O	1:A:361:LYS:CB	2.41	0.69
1:A:404:PHE:C	1:A:405:PHE:HD1	1.96	0.68
1:A:342:PRO:CB	1:A:373:TYR:HB2	2.23	0.68
1:A:444:SER:C	1:A:446:GLY:H	1.97	0.68
1:A:404:PHE:O	1:A:405:PHE:HD1	1.76	0.68
1:A:430:GLU:O	1:A:431:ALA:HB2	1.94	0.67
1:A:360:LYS:HB2	1:A:414:THR:HB	1.75	0.67
1:A:381:TRP:HE1	1:A:410:LEU:CG	2.08	0.67
1:A:396:PRO:CB	1:A:398:PHE:HE2	2.07	0.67
1:A:417:TRP:CH2	1:A:441:ILE:HG23	2.30	0.66
1:A:404:PHE:HD1	1:A:405:PHE:CA	2.09	0.66
1:A:404:PHE:C	1:A:405:PHE:CD1	2.70	0.66
1:A:411:LYS:CD	1:A:413:ASP:N	2.59	0.66
1:A:402:GLY:CA	1:A:405:PHE:CZ	2.79	0.66
1:A:404:PHE:CE1	1:A:406:LEU:HB2	2.31	0.65
1:A:401:ASP:O	1:A:402:GLY:C	2.35	0.65
1:A:370:THR:HG21	1:A:407:TYR:HE2	1.62	0.65
1:A:372:PHE:O	1:A:404:PHE:HD2	1.79	0.65
1:A:413:ASP:O	1:A:414:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:THR:CB	1:A:405:PHE:HA	2.23	0.65
1:A:380:GLU:OE2	1:A:383:SER:OG	2.14	0.64
1:A:399:ASP:O	1:A:402:GLY:N	2.30	0.64
1:A:382:ASP:HA	1:A:424:THR:HG22	1.79	0.64
1:A:410:LEU:HD12	1:A:411:LYS:O	1.97	0.64
1:A:341:GLY:O	1:A:344:ARG:NH2	2.31	0.64
1:A:361:LYS:O	1:A:361:LYS:CD	2.46	0.63
1:A:421:GLU:HB3	1:A:423:PHE:CE2	2.32	0.63
1:A:345:ILE:N	1:A:372:PHE:CE1	2.67	0.63
1:A:360:LYS:CA	1:A:414:THR:HB	2.28	0.63
1:A:417:TRP:O	1:A:418:ASN:O	2.17	0.63
1:A:370:THR:HB	1:A:405:PHE:CA	2.26	0.63
1:A:341:GLY:HA3	1:A:344:ARG:CZ	2.29	0.63
1:A:337:SER:O	1:A:338:LYS:HB2	1.97	0.63
1:A:351:LEU:HG	1:A:366:THR:HG22	1.81	0.63
1:A:427:VAL:CG1	1:A:427:VAL:O	2.38	0.62
1:A:396:PRO:HB2	1:A:398:PHE:HE2	1.64	0.62
1:A:374:PRO:CG	1:A:431:ALA:HB1	2.30	0.62
1:A:399:ASP:O	1:A:402:GLY:CA	2.47	0.62
1:A:358:LEU:HD12	1:A:363:VAL:HB	1.80	0.62
1:A:421:GLU:HB2	1:A:423:PHE:HE2	1.64	0.62
1:A:444:SER:CB	1:A:445:PRO:HD3	2.29	0.62
1:A:421:GLU:O	1:A:423:PHE:CD2	2.53	0.61
1:A:390:ASP:O	1:A:390:ASP:CG	2.39	0.61
1:A:404:PHE:HE1	1:A:406:LEU:N	1.97	0.61
1:A:361:LYS:HD2	1:A:361:LYS:O	1.98	0.61
1:A:366:THR:CB	1:A:409:ARG:HG3	2.30	0.61
1:A:337:SER:O	1:A:338:LYS:CG	2.49	0.61
1:A:374:PRO:CD	1:A:431:ALA:HB1	2.31	0.61
1:A:349:TYR:CD1	1:A:368:MET:O	2.53	0.61
1:A:345:ILE:N	1:A:372:PHE:HE1	1.99	0.61
1:A:372:PHE:O	1:A:404:PHE:HB3	1.99	0.61
1:A:345:ILE:H	1:A:372:PHE:HE1	1.49	0.60
1:A:417:TRP:HE1	1:A:444:SER:HB3	1.67	0.60
1:A:338:LYS:HD2	1:A:339:ALA:HB2	1.82	0.60
1:A:424:THR:OG1	1:A:439:LYS:HB3	2.01	0.60
1:A:335:THR:C	1:A:336:ILE:HG13	2.23	0.59
1:A:427:VAL:HG12	1:A:427:VAL:O	2.01	0.59
1:A:366:THR:HG23	1:A:367:CYS:N	2.16	0.59
1:A:394:THR:HG1	1:A:407:TYR:HB2	1.65	0.59
1:A:370:THR:HG22	1:A:405:PHE:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:HD3	1:A:413:ASP:H	1.67	0.59
1:A:411:LYS:HD3	1:A:412:VAL:H	1.67	0.58
1:A:367:CYS:HB2	1:A:381:TRP:CZ3	2.39	0.58
1:A:341:GLY:O	1:A:344:ARG:NH1	2.37	0.57
1:A:444:SER:C	1:A:446:GLY:N	2.57	0.57
1:A:372:PHE:H	1:A:404:PHE:CA	2.17	0.57
1:A:363:VAL:O	1:A:363:VAL:HG13	2.02	0.57
1:A:399:ASP:HB2	1:A:405:PHE:CE2	2.39	0.57
1:A:344:ARG:O	1:A:345:ILE:HG13	2.05	0.57
1:A:421:GLU:HB2	1:A:423:PHE:CE2	2.39	0.57
1:A:377:ILE:CG2	1:A:404:PHE:HE2	2.18	0.56
1:A:444:SER:O	1:A:446:GLY:N	2.39	0.56
1:A:385:GLU:O	1:A:387:PRO:C	2.44	0.56
1:A:385:GLU:O	1:A:387:PRO:O	2.24	0.56
1:A:424:THR:OG1	1:A:439:LYS:CB	2.53	0.56
1:A:377:ILE:HG23	1:A:404:PHE:CE2	2.37	0.56
1:A:364:SER:O	1:A:365:LEU:HD13	2.05	0.55
1:A:337:SER:O	1:A:338:LYS:HG2	2.06	0.55
1:A:343:PRO:O	1:A:372:PHE:CE1	2.60	0.55
1:A:434:ASN:CG	1:A:434:ASN:O	2.44	0.55
1:A:417:TRP:HZ2	1:A:441:ILE:HG12	1.72	0.55
1:A:342:PRO:HB2	1:A:343:PRO:CD	2.37	0.55
1:A:346:PRO:C	1:A:347:GLU:HG3	2.23	0.55
1:A:371:GLY:CA	1:A:404:PHE:O	2.55	0.55
1:A:399:ASP:HB2	1:A:405:PHE:HE2	1.72	0.55
1:A:361:LYS:H	1:A:414:THR:HG21	0.73	0.55
1:A:374:PRO:CD	1:A:431:ALA:CB	2.85	0.54
1:A:417:TRP:HH2	1:A:441:ILE:HG23	1.72	0.54
1:A:341:GLY:C	1:A:344:ARG:NH1	2.61	0.54
1:A:377:ILE:HD11	1:A:406:LEU:HD12	1.90	0.54
1:A:431:ALA:O	1:A:432:LEU:HB2	2.07	0.54
1:A:438:GLN:HG2	1:A:439:LYS:N	2.22	0.54
1:A:381:TRP:CE2	1:A:410:LEU:CD2	2.90	0.54
1:A:361:LYS:N	1:A:414:THR:CB	2.71	0.53
1:A:396:PRO:HB3	1:A:398:PHE:HE2	1.73	0.53
1:A:404:PHE:HE1	1:A:406:LEU:HB2	1.72	0.53
1:A:354:PRO:HB2	1:A:356:ASN:ND2	2.24	0.53
1:A:351:LEU:O	1:A:365:LEU:CD2	2.57	0.53
1:A:397:VAL:O	1:A:405:PHE:CB	2.57	0.53
1:A:417:TRP:CE3	1:A:418:ASN:N	2.77	0.53
1:A:431:ALA:O	1:A:432:LEU:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TRP:CH2	1:A:441:ILE:CG2	2.91	0.53
1:A:365:LEU:O	1:A:409:ARG:HG2	2.09	0.52
1:A:381:TRP:NE1	1:A:410:LEU:CG	2.69	0.52
1:A:377:ILE:HB	1:A:429:HIS:HA	1.90	0.52
1:A:341:GLY:O	1:A:344:ARG:CZ	2.57	0.52
1:A:381:TRP:CE2	1:A:410:LEU:HD23	2.45	0.52
1:A:349:TYR:HB2	1:A:368:MET:CG	2.30	0.52
1:A:404:PHE:CE1	1:A:406:LEU:N	2.78	0.52
1:A:344:ARG:HA	1:A:372:PHE:HE1	1.75	0.52
1:A:354:PRO:O	1:A:356:ASN:N	2.42	0.52
1:A:361:LYS:HA	1:A:414:THR:OG1	2.10	0.52
1:A:361:LYS:O	1:A:361:LYS:HD3	2.09	0.52
1:A:434:ASN:ND2	1:A:434:ASN:C	2.63	0.51
1:A:344:ARG:CZ	1:A:344:ARG:O	2.58	0.51
1:A:351:LEU:HD12	1:A:365:LEU:HG	1.91	0.51
1:A:396:PRO:HA	1:A:405:PHE:O	2.09	0.51
1:A:428:MET:HB2	1:A:435:HIS:CD2	2.45	0.51
1:A:377:ILE:CB	1:A:429:HIS:CD2	2.95	0.50
1:A:404:PHE:CD1	1:A:405:PHE:CA	2.92	0.50
1:A:444:SER:C	1:A:446:GLY:O	2.49	0.50
1:A:370:THR:CG2	1:A:405:PHE:CA	2.89	0.50
1:A:361:LYS:HA	1:A:414:THR:HG1	1.76	0.50
1:A:373:TYR:CB	1:A:374:PRO:CA	2.59	0.50
1:A:342:PRO:HB3	1:A:373:TYR:HB2	1.93	0.49
1:A:443:ARG:C	1:A:444:SER:HG	1.92	0.49
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.95	0.49
1:A:341:GLY:O	1:A:403:SER:OG	2.31	0.49
1:A:373:TYR:HA	1:A:374:PRO:O	2.12	0.49
1:A:394:THR:O	1:A:406:LEU:CD2	2.60	0.49
1:A:413:ASP:O	1:A:414:THR:CB	2.60	0.49
1:A:427:VAL:CG1	1:A:436:VAL:CG2	2.82	0.49
1:A:381:TRP:CD1	1:A:391:TYR:CD1	3.01	0.49
1:A:365:LEU:C	1:A:409:ARG:HG2	2.33	0.48
1:A:399:ASP:O	1:A:402:GLY:HA3	2.14	0.48
1:A:413:ASP:O	1:A:414:THR:CG2	2.61	0.48
1:A:421:GLU:C	1:A:423:PHE:CD2	2.87	0.47
1:A:368:MET:C	1:A:369:ILE:HG13	2.35	0.47
1:A:377:ILE:HD13	1:A:404:PHE:CE2	2.49	0.47
1:A:395:PRO:O	1:A:396:PRO:C	2.53	0.47
1:A:417:TRP:CE3	1:A:418:ASN:CA	2.98	0.47
1:A:394:THR:O	1:A:406:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLU:CB	1:A:423:PHE:CD2	2.85	0.47
1:A:428:MET:CB	1:A:435:HIS:CD2	2.98	0.47
1:A:377:ILE:HB	1:A:429:HIS:CA	2.44	0.47
1:A:370:THR:HG22	1:A:405:PHE:CA	2.45	0.47
1:A:342:PRO:HB3	1:A:373:TYR:CB	2.45	0.47
1:A:404:PHE:HE1	1:A:406:LEU:CB	2.28	0.46
1:A:351:LEU:O	1:A:365:LEU:HD23	2.14	0.46
1:A:380:GLU:HA	1:A:391:TYR:CZ	2.51	0.46
1:A:412:VAL:O	1:A:413:ASP:HB2	2.16	0.46
1:A:336:ILE:CG2	1:A:337:SER:H	2.24	0.46
1:A:404:PHE:HE1	1:A:406:LEU:CA	2.29	0.46
1:A:370:THR:C	1:A:404:PHE:O	2.54	0.46
1:A:417:TRP:CE3	1:A:418:ASN:HA	2.51	0.46
1:A:444:SER:O	1:A:446:GLY:O	2.34	0.45
1:A:404:PHE:CD1	1:A:405:PHE:C	2.90	0.45
1:A:401:ASP:O	1:A:403:SER:N	2.49	0.45
1:A:440:SER:O	1:A:441:ILE:HB	2.17	0.45
1:A:342:PRO:HB2	1:A:343:PRO:HD3	1.99	0.45
1:A:369:ILE:HD13	1:A:427:VAL:HG23	1.97	0.45
1:A:342:PRO:HB3	1:A:374:PRO:CA	2.47	0.45
1:A:342:PRO:HA	1:A:373:TYR:N	2.32	0.45
1:A:381:TRP:CD1	1:A:391:TYR:HD1	2.35	0.45
1:A:338:LYS:HB3	1:A:339:ALA:H	1.31	0.45
1:A:381:TRP:HB3	1:A:391:TYR:CE1	2.52	0.44
1:A:353:PRO:CB	1:A:444:SER:HA	2.40	0.44
1:A:391:TYR:CD2	1:A:391:TYR:O	2.70	0.44
1:A:366:THR:OG1	1:A:408:SER:O	2.29	0.44
1:A:364:SER:CB	1:A:411:LYS:HB2	2.43	0.44
1:A:370:THR:HG21	1:A:407:TYR:CE2	2.48	0.44
1:A:432:LEU:HD22	1:A:433:PRO:HD2	1.98	0.44
1:A:342:PRO:C	1:A:344:ARG:HH12	2.21	0.44
1:A:417:TRP:O	1:A:418:ASN:C	2.56	0.44
1:A:396:PRO:HB3	1:A:398:PHE:CE2	2.52	0.43
1:A:440:SER:C	1:A:441:ILE:HG22	2.38	0.43
1:A:407:TYR:CD2	1:A:407:TYR:N	2.85	0.43
1:A:413:ASP:O	1:A:414:THR:OG1	2.29	0.43
1:A:377:ILE:HB	1:A:429:HIS:CG	2.53	0.43
1:A:423:PHE:HD1	1:A:441:ILE:HG21	1.84	0.43
1:A:417:TRP:CZ2	1:A:441:ILE:HD13	2.53	0.42
1:A:338:LYS:HB3	1:A:342:PRO:HD3	2.02	0.42
1:A:344:ARG:CA	1:A:372:PHE:HE1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HG2	1:A:340:LYS:H	1.64	0.42
1:A:342:PRO:HB3	1:A:374:PRO:CB	2.50	0.42
1:A:360:LYS:C	1:A:414:THR:CB	2.89	0.41
1:A:340:LYS:HG3	1:A:373:TYR:CE1	2.55	0.41
1:A:417:TRP:CZ3	1:A:423:PHE:CE1	3.08	0.41
1:A:342:PRO:HD2	1:A:343:PRO:HD2	1.98	0.41
1:A:346:PRO:O	1:A:347:GLU:CG	2.38	0.41
1:A:405:PHE:N	1:A:405:PHE:CD1	2.89	0.41
1:A:417:TRP:CZ2	1:A:441:ILE:HG23	2.55	0.41
1:A:423:PHE:CD1	1:A:441:ILE:HG21	2.55	0.41
1:A:360:LYS:HA	1:A:414:THR:CG2	2.51	0.41
1:A:342:PRO:N	1:A:343:PRO:HD2	2.30	0.40
1:A:382:ASP:OD2	1:A:382:ASP:C	2.59	0.40
1:A:407:TYR:HD2	1:A:407:TYR:N	2.16	0.40
1:A:420:GLY:O	1:A:421:GLU:HG2	2.21	0.40

All (5) 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:350:LEU:CD1	1:A:356:ASN:OD1[2_655]	1.23	0.97
1:A:350:LEU:CD1	1:A:356:ASN:CG[2_655]	1.62	0.58
1:A:344:ARG:CB	1:A:435:HIS:NE2[3_645]	1.82	0.38
1:A:407:TYR:OH	1:A:409:ARG:CZ[2_655]	1.90	0.30
1:A:407:TYR:OH	1:A:409:ARG:NH2[2_655]	2.13	0.07

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	109/113 (96%)	66 (61%)	13 (12%)	30 (28%)	0 0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	PRO
1	A	355	ARG
1	A	361	LYS
1	A	374	PRO
1	A	382	ASP
1	A	383	SER
1	A	387	PRO
1	A	400	THR
1	A	402	GLY
1	A	403	SER
1	A	414	THR
1	A	418	ASN
1	A	432	LEU
1	A	440	SER
1	A	443	ARG
1	A	444	SER
1	A	336	ILE
1	A	389	SER
1	A	413	ASP
1	A	431	ALA
1	A	338	LYS
1	A	345	ILE
1	A	357	GLU
1	A	422	SER
1	A	445	PRO
1	A	337	SER
1	A	342	PRO
1	A	354	PRO
1	A	441	ILE
1	A	396	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	102/104 (98%)	60 (59%)	42 (41%)	0 0

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	LYS
1	A	344	ARG
1	A	348	VAL
1	A	350	LEU
1	A	351	LEU
1	A	356	ASN
1	A	359	SER
1	A	360	LYS
1	A	365	LEU
1	A	366	THR
1	A	372	PHE
1	A	377	ILE
1	A	378	ASN
1	A	379	VAL
1	A	381	TRP
1	A	383	SER
1	A	385	GLU
1	A	387	PRO
1	A	391	TYR
1	A	393	ASN
1	A	399	ASP
1	A	404	PHE
1	A	406	LEU
1	A	407	TYR
1	A	411	LYS
1	A	412	VAL
1	A	413	ASP
1	A	417	TRP
1	A	423	PHE
1	A	424	THR
1	A	427	VAL
1	A	428	MET
1	A	429	HIS
1	A	430	GLU
1	A	434	ASN

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Mol	Chain	Res	Type
1	A	435	HIS
1	A	437	ILE
1	A	438	GLN
1	A	439	LYS
1	A	440	SER
1	A	442	SER
1	A	444	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	378	ASN
1	A	429	HIS
1	A	434	ASN
1	A	435	HIS

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	370:THR	C	371:GLY	N	1.19
1	A	392:LYS	C	393:ASN	N	1.16
1	A	398:PHE	C	399:ASP	N	1.10
1	A	402:GLY	C	403:SER	N	1.10

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.