



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:10 AM UTC

PDB ID : 2OQI / pdb_00002oqi
Title : Human Dipeptidyl Peptidase IV (DPP4) with Piperidinone-constrained phenethylamine
Authors : Pei, Z.; Li, X.; von Geldern, T.W.; Longenecker, K.L.; Pireh, D.; Stewart, K.D.; Backes, B.J.; Lai, C.; Lubben, T.H.; Ballaron, S.J.; Beno, D.W.; Kempf-Grote, A.J.; Sham, H.L.; Trevillyan, J.M.
Deposited on : 2007-01-31
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

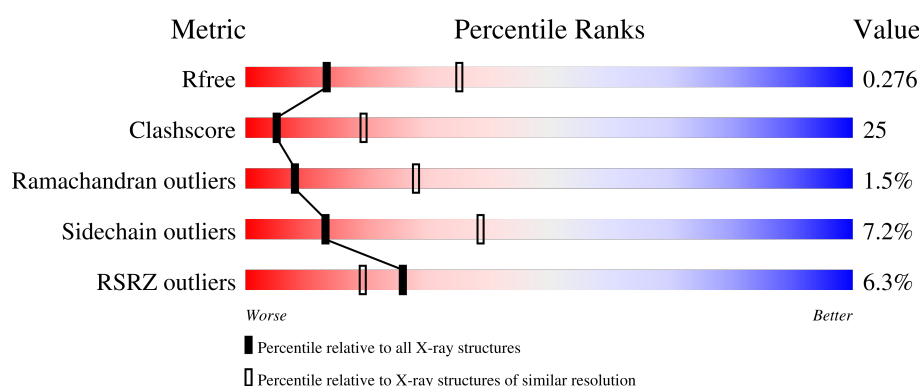
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	7% 56% 37% 6%
1	B	728	8% 57% 36% 6%
1	C	728	4% 52% 40% 6% •
1	D	728	6% 53% 39% 6% •

2 Entry composition [i](#)

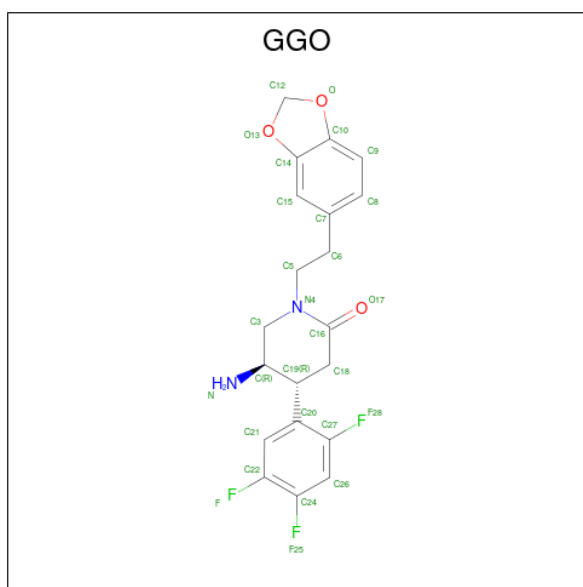
There are 2 unique types of molecules in this entry. The entry contains 23820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (AD-ABP).

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

- Molecule 2 is (4R,5R)-5-AMINO-1-[2-(1,3-BENZODIOXOL-5-YL)ETHYL]-4-(2,4,5-TRIFLUOROPHENYL)PIPERIDIN-2-ONE (CCD ID: GGO) (formula: C₂₀H₁₉F₃N₂O₃).

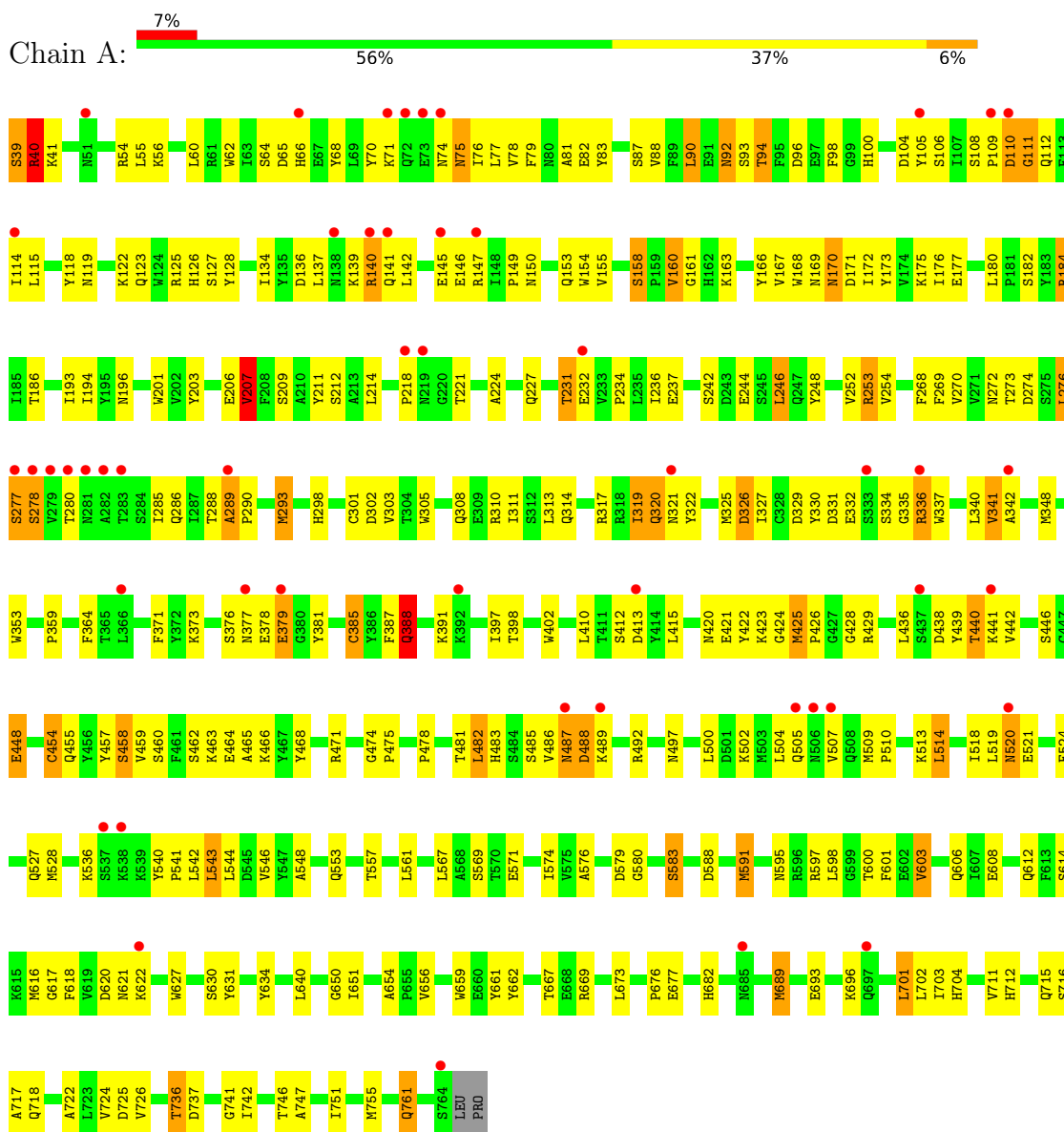


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

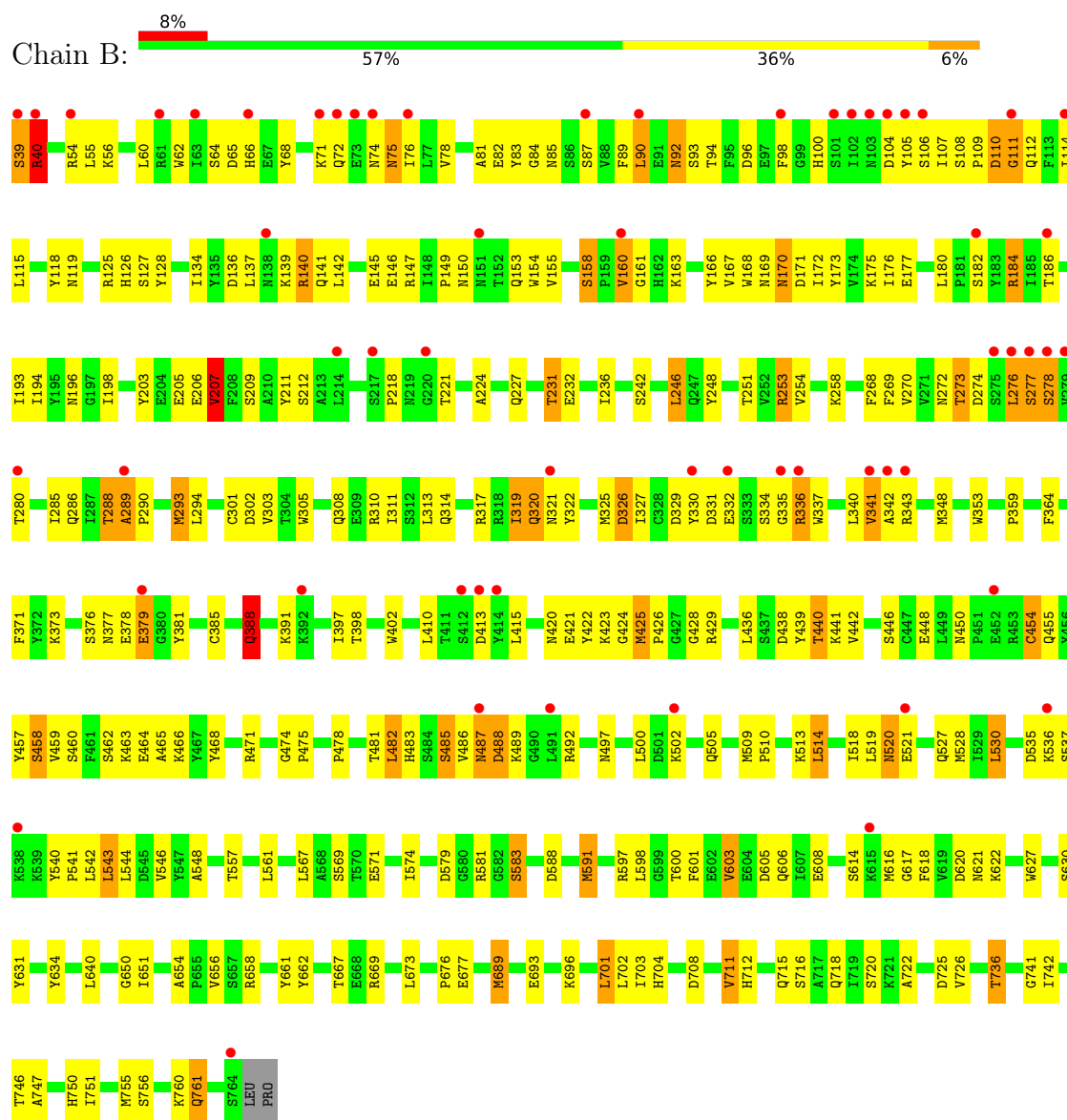
3 Residue-property plots

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.

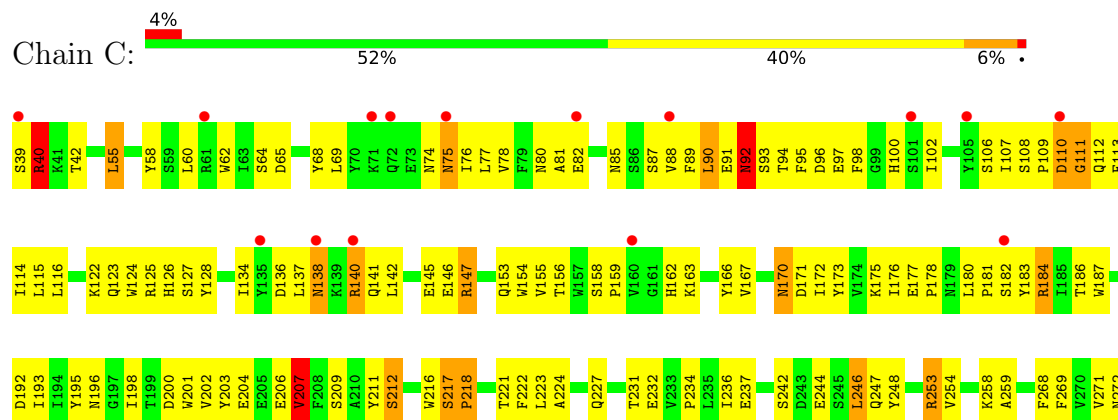
- Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)

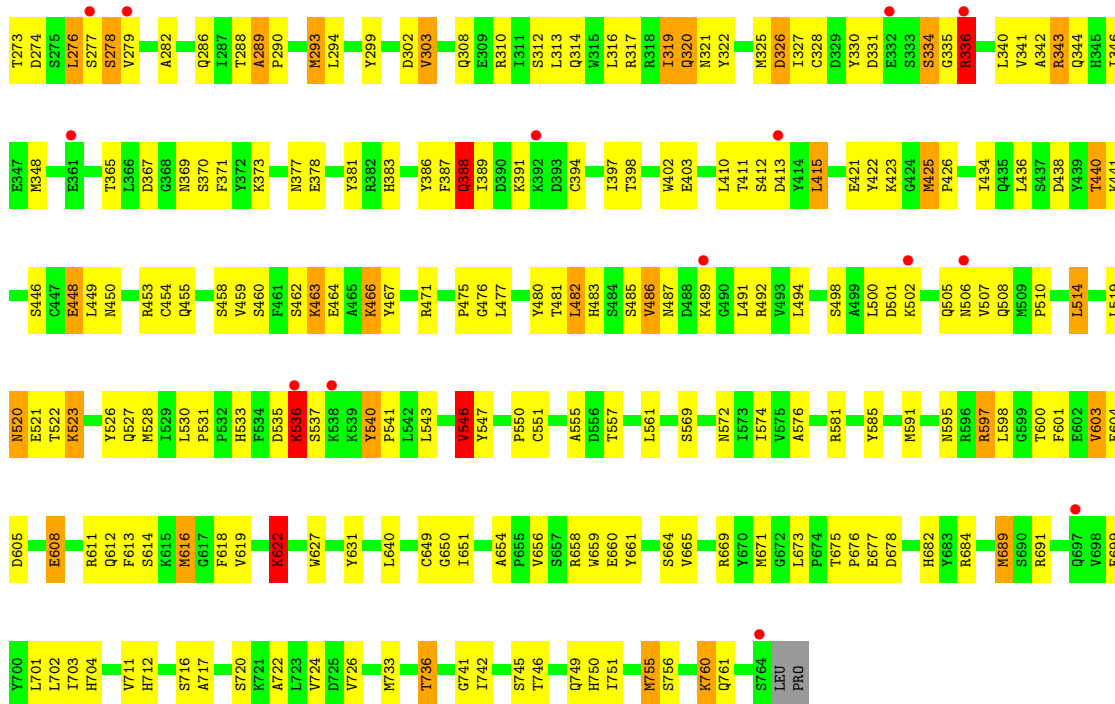


- Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)

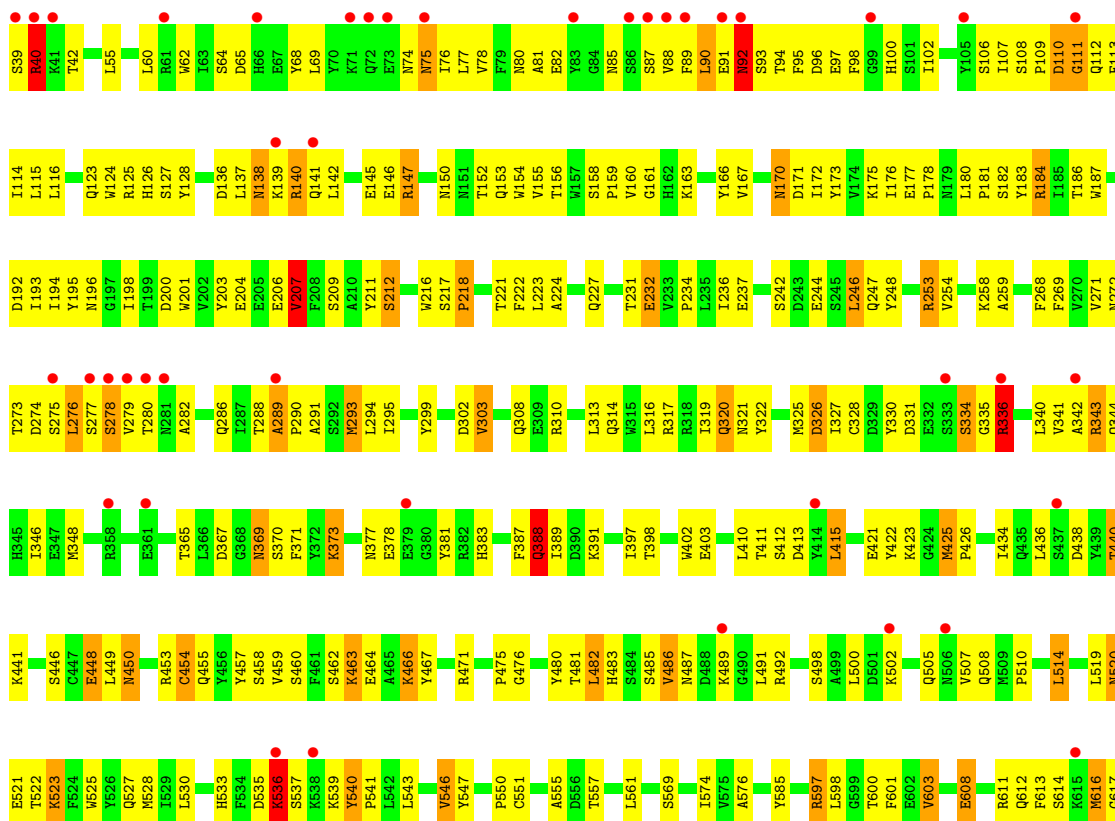


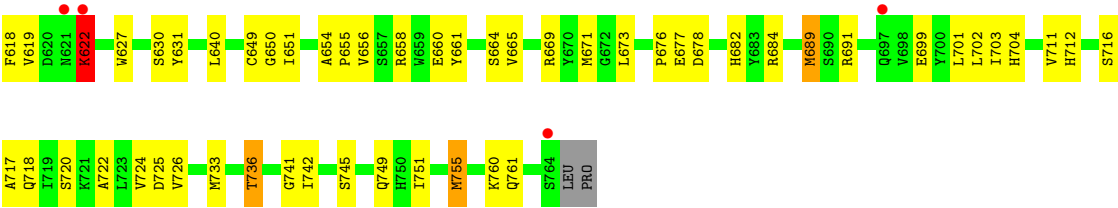
- Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP)





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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.29Å 127.30Å 126.80Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (50.00-2.80) 90.0 (50.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.284 0.230 , 0.276	Depositor DCC
R_{free} test set	4148 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23820	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GGO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	0/6119	1.04	36/8321 (0.4%)
1	B	0.55	0/6119	1.04	39/8321 (0.5%)
1	C	0.51	1/6119 (0.0%)	1.05	32/8321 (0.4%)
1	D	0.52	1/6119 (0.0%)	1.04	32/8321 (0.4%)
All	All	0.53	2/24476 (0.0%)	1.04	139/33284 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	755	MET	SD-CE	-5.35	1.66	1.79
1	D	755	MET	SD-CE	-5.14	1.66	1.79

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	VAL	N-CA-C	11.05	120.35	111.62
1	D	378	GLU	N-CA-C	-11.01	98.47	112.90
1	C	378	GLU	N-CA-C	-10.80	98.75	112.90
1	B	630	SER	CB-CA-C	-9.99	105.05	116.54
1	D	111	GLY	N-CA-C	-9.77	101.84	115.32
1	C	111	GLY	N-CA-C	-9.56	102.12	115.32
1	B	111	GLY	N-CA-C	-8.98	103.55	115.40
1	A	111	GLY	N-CA-C	-8.96	103.57	115.40
1	A	630	SER	CB-CA-C	-8.69	105.41	117.23
1	A	207	VAL	N-CA-C	8.16	118.83	111.81
1	B	378	GLU	N-CA-C	-8.09	103.39	113.18
1	A	378	GLU	N-CA-C	-7.84	103.70	113.18
1	B	207	VAL	N-CA-C	7.80	118.52	111.81
1	D	622	LYS	N-CA-C	-7.71	103.70	113.72
1	D	92	ASN	N-CA-C	-7.53	102.76	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	VAL	N-CA-C	-7.29	94.18	109.34
1	C	622	LYS	N-CA-C	-7.27	104.27	113.72
1	C	92	ASN	N-CA-C	-7.12	103.21	110.97
1	B	206	GLU	N-CA-C	7.09	122.11	112.68
1	A	206	GLU	N-CA-C	6.81	121.74	112.68
1	A	488	ASP	N-CA-C	-6.80	104.28	112.58
1	D	664	SER	N-CA-C	6.79	118.33	111.07
1	C	425	MET	CA-C-N	6.73	127.28	119.47
1	C	425	MET	C-N-CA	6.73	127.28	119.47
1	D	616	MET	N-CA-C	-6.72	104.78	114.12
1	B	341	VAL	N-CA-C	-6.71	95.39	109.34
1	C	664	SER	N-CA-C	6.63	118.17	111.07
1	A	425	MET	CA-C-N	6.46	126.15	119.82
1	A	425	MET	C-N-CA	6.46	126.15	119.82
1	C	616	MET	N-CA-C	-6.46	105.14	114.12
1	A	546	VAL	N-CA-C	6.42	118.03	108.46
1	D	425	MET	CA-C-N	6.35	126.83	119.47
1	D	425	MET	C-N-CA	6.35	126.83	119.47
1	B	546	VAL	N-CA-C	6.30	117.85	108.46
1	A	388	GLN	N-CA-C	-6.29	98.95	109.07
1	B	425	MET	CA-C-N	6.28	125.97	119.82
1	B	425	MET	C-N-CA	6.28	125.97	119.82
1	C	466	LYS	N-CA-C	-6.23	104.74	112.90
1	B	588	ASP	N-CA-C	6.20	118.83	111.71
1	D	466	LYS	N-CA-C	-6.18	104.80	112.90
1	D	388	GLN	N-CA-C	-6.17	98.46	108.52
1	C	206	GLU	N-CA-C	6.16	120.93	113.41
1	D	656	VAL	N-CA-C	-6.16	99.53	108.71
1	B	150	ASN	N-CA-C	-6.14	102.61	110.53
1	A	548	ALA	N-CA-C	6.13	120.07	112.47
1	C	343	ARG	N-CA-C	-6.12	105.46	113.17
1	D	540	TYR	N-CA-C	6.11	117.77	110.07
1	B	319	ILE	N-CA-C	-6.10	98.71	107.37
1	A	458	SER	N-CA-C	-6.08	99.80	109.23
1	C	388	GLN	N-CA-C	-6.06	98.65	108.52
1	B	488	ASP	N-CA-C	-5.96	104.62	112.24
1	B	454	CYS	N-CA-C	5.94	118.08	108.34
1	B	458	SER	N-CA-C	-5.94	100.03	109.23
1	B	288	THR	CB-CA-C	-5.90	107.02	114.40
1	A	319	ILE	N-CA-C	-5.89	99.00	107.37
1	B	548	ALA	N-CA-C	5.88	119.76	112.47
1	C	328	CYS	N-CA-C	5.86	118.79	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	TYR	N-CA-C	5.84	117.43	110.07
1	B	673	LEU	CA-C-N	5.84	127.14	119.84
1	B	673	LEU	C-N-CA	5.84	127.14	119.84
1	D	207	VAL	N-CA-C	5.83	116.57	111.56
1	D	206	GLU	N-CA-C	5.81	120.52	112.90
1	A	673	LEU	CA-C-N	5.81	127.10	119.84
1	A	673	LEU	C-N-CA	5.81	127.10	119.84
1	D	142	LEU	N-CA-C	-5.80	101.03	110.20
1	C	541	PRO	N-CA-C	-5.80	102.15	111.38
1	A	54	ARG	N-CA-C	5.79	118.17	108.96
1	D	212	SER	N-CA-C	5.76	118.06	109.59
1	A	541	PRO	N-CA-C	-5.75	102.07	111.68
1	B	485	SER	N-CA-C	5.75	118.32	111.71
1	C	656	VAL	N-CA-C	-5.73	100.17	108.71
1	A	454	CYS	N-CA-C	5.72	117.72	108.34
1	C	279	VAL	N-CA-C	-5.71	107.28	111.90
1	B	518	ILE	N-CA-C	5.69	116.33	107.28
1	B	541	PRO	N-CA-C	-5.65	102.24	111.68
1	D	343	ARG	N-CA-C	-5.65	106.05	113.17
1	A	591	MET	N-CA-C	5.59	117.05	111.07
1	B	388	GLN	N-CA-C	-5.58	99.43	108.52
1	A	518	ILE	N-CA-C	5.57	116.14	107.28
1	A	603	VAL	N-CA-C	-5.56	105.68	111.58
1	B	603	VAL	N-CA-C	-5.55	105.70	111.58
1	C	217	SER	N-CA-C	-5.55	102.64	110.29
1	C	365	THR	N-CA-C	-5.54	103.08	110.55
1	D	541	PRO	N-CA-C	-5.52	102.61	111.38
1	B	54	ARG	N-CA-C	5.49	117.69	108.96
1	B	466	LYS	N-CA-C	-5.47	106.74	113.41
1	B	104	ASP	N-CA-C	5.46	116.71	108.46
1	B	158	SER	N-CA-C	-5.46	102.10	110.07
1	D	458	SER	N-CA-C	-5.45	101.07	109.52
1	A	485	SER	N-CA-C	5.44	117.97	111.71
1	B	591	MET	N-CA-C	5.42	117.18	111.28
1	C	55	LEU	N-CA-C	-5.40	100.90	109.59
1	D	328	CYS	N-CA-C	5.39	118.03	109.24
1	A	150	ASN	N-CA-C	-5.38	103.28	110.55
1	B	711	VAL	N-CA-C	-5.38	99.21	106.85
1	C	202	VAL	N-CA-C	5.36	115.57	110.42
1	D	156	THR	N-CA-C	5.34	116.73	107.93
1	D	454	CYS	N-CA-C	5.34	117.11	108.41
1	A	448	GLU	N-CA-C	5.33	119.63	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	LYS	N-CA-C	-5.33	106.91	113.41
1	D	279	VAL	N-CA-C	-5.28	107.62	111.90
1	A	617	GLY	N-CA-C	5.27	122.54	115.59
1	D	630	SER	CB-CA-C	-5.27	110.48	116.54
1	C	397	ILE	N-CA-C	-5.26	107.85	112.90
1	A	201	TRP	N-CA-C	5.25	117.41	111.11
1	C	336	ARG	N-CA-C	5.25	118.49	110.36
1	D	369	ASN	N-CA-C	-5.25	106.78	114.39
1	C	454	CYS	N-CA-C	5.24	116.95	108.41
1	A	412	SER	N-CA-C	-5.23	106.86	113.18
1	C	458	SER	N-CA-C	-5.22	101.42	109.52
1	B	462	SER	N-CA-C	-5.22	103.80	110.53
1	A	158	SER	N-CA-C	-5.21	102.46	110.07
1	A	588	ASP	N-CA-C	5.21	118.74	112.38
1	C	212	SER	N-CA-C	5.19	117.75	109.96
1	D	336	ARG	N-CA-C	5.17	118.38	110.36
1	D	397	ILE	N-CA-C	-5.17	107.94	112.90
1	C	546	VAL	N-CA-C	5.16	117.18	108.81
1	B	72	GLN	N-CA-C	-5.16	102.52	109.95
1	B	530	LEU	N-CA-C	5.16	116.57	110.07
1	A	379	GLU	N-CA-C	-5.15	106.68	113.17
1	A	659	TRP	N-CA-C	5.14	118.65	112.38
1	D	206	GLU	CA-C-N	-5.14	117.89	123.08
1	D	206	GLU	C-N-CA	-5.14	117.89	123.08
1	A	104	ASP	N-CA-C	5.13	116.20	108.46
1	D	232	GLU	N-CA-C	5.12	119.02	112.26
1	C	142	LEU	N-CA-C	-5.09	102.16	110.20
1	B	617	GLY	N-CA-C	5.08	122.29	115.59
1	C	319	ILE	N-CA-C	-5.07	99.20	106.55
1	C	156	THR	N-CA-C	5.07	116.29	107.93
1	C	207	VAL	N-CA-C	5.07	115.92	111.56
1	D	365	THR	N-CA-C	-5.06	103.37	110.50
1	B	450	ASN	CA-C-N	5.05	126.16	119.84
1	B	450	ASN	C-N-CA	5.05	126.16	119.84
1	B	160	VAL	CB-CA-C	-5.05	106.55	111.05
1	A	711	VAL	N-CA-C	-5.04	99.69	106.85
1	D	150	ASN	N-CA-C	-5.04	103.28	110.59
1	A	160	VAL	N-CA-C	5.03	119.81	109.34
1	C	659	TRP	N-CA-C	5.03	118.52	112.38
1	B	379	GLU	N-CA-C	-5.03	106.83	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5948	0	5667	279	0
1	B	5948	0	5667	271	0
1	C	5948	0	5667	312	0
1	D	5948	0	5667	313	0
2	B	28	0	19	1	0
All	All	23820	0	22687	1147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:MET:HE2	1:D:317:ARG:HG3	1.22	1.20
1:C:293:MET:HE2	1:C:317:ARG:HG3	1.24	1.15
1:D:334:SER:HB3	1:D:336:ARG:NE	1.65	1.12
1:C:334:SER:HB3	1:C:336:ARG:NE	1.66	1.10
1:B:172:ILE:H	1:B:186:THR:HG22	1.18	1.09
1:B:39:SER:HB2	1:B:40:ARG:HE	1.18	1.08
1:D:334:SER:HB3	1:D:336:ARG:HE	0.95	1.06
1:C:334:SER:HB3	1:C:336:ARG:HE	0.95	1.06
1:A:172:ILE:H	1:A:186:THR:HG22	1.16	1.05
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.39	1.04
1:A:39:SER:HB2	1:A:40:ARG:HE	1.20	1.02
1:A:92:ASN:HD22	1:A:93:SER:N	1.57	1.02
1:B:92:ASN:HD22	1:B:93:SER:N	1.56	1.01
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.41	1.01
1:D:289:ALA:HB1	1:D:290:PRO:HA	1.44	0.98
1:A:293:MET:HE2	1:A:317:ARG:HG3	1.42	0.98
1:D:172:ILE:H	1:D:186:THR:HG22	1.27	0.97
1:B:293:MET:HE2	1:B:317:ARG:HG3	1.43	0.97
1:C:172:ILE:H	1:C:186:THR:HG22	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ALA:HB1	1:C:290:PRO:HA	1.48	0.95
1:A:172:ILE:H	1:A:186:THR:CG2	1.79	0.94
1:B:172:ILE:H	1:B:186:THR:CG2	1.80	0.94
1:A:253:ARG:HH22	1:B:253:ARG:HH22	0.98	0.92
1:D:528:MET:HE2	1:D:530:LEU:HD21	1.50	0.92
1:D:114:ILE:HD11	1:D:137:LEU:HD21	1.52	0.91
1:C:172:ILE:H	1:C:186:THR:CG2	1.84	0.89
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.54	0.89
1:C:253:ARG:HH22	1:D:253:ARG:NH2	1.71	0.88
1:C:253:ARG:NH2	1:D:253:ARG:HH22	1.71	0.88
1:C:334:SER:CB	1:C:336:ARG:HE	1.86	0.88
1:C:253:ARG:HH22	1:D:253:ARG:HH22	0.89	0.87
1:D:289:ALA:HB1	1:D:290:PRO:CA	2.03	0.86
1:D:172:ILE:H	1:D:186:THR:CG2	1.86	0.86
1:C:114:ILE:HD11	1:C:137:LEU:HD21	1.56	0.86
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.05	0.86
1:B:39:SER:CB	1:B:40:ARG:HE	1.89	0.85
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.59	0.84
1:C:289:ALA:HB1	1:C:290:PRO:CA	2.06	0.84
1:C:528:MET:HE2	1:C:530:LEU:HD21	1.57	0.84
1:D:528:MET:HE3	1:D:574:ILE:HG21	1.60	0.84
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.07	0.84
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.77	0.83
1:D:93:SER:HA	1:D:96:ASP:OD1	1.79	0.83
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.61	0.82
1:D:334:SER:CB	1:D:336:ARG:HE	1.86	0.82
1:A:341:VAL:O	1:A:342:ALA:HB3	1.78	0.82
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.62	0.82
1:B:76:ILE:HD12	1:B:90:LEU:HD11	1.59	0.82
1:B:114:ILE:HD11	1:B:137:LEU:HD21	1.62	0.82
1:B:341:VAL:O	1:B:342:ALA:HB3	1.81	0.81
1:D:276:LEU:CD2	1:D:276:LEU:H	1.94	0.81
1:D:614:SER:HA	1:D:619:VAL:HB	1.63	0.81
1:A:39:SER:CB	1:A:40:ARG:HE	1.93	0.80
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.79	0.80
1:C:528:MET:HE3	1:C:574:ILE:HG21	1.62	0.80
1:A:334:SER:HB3	1:A:336:ARG:NE	1.97	0.80
1:B:334:SER:HB3	1:B:336:ARG:NE	1.96	0.80
1:C:614:SER:HA	1:C:619:VAL:HB	1.64	0.79
1:D:76:ILE:HD12	1:D:90:LEU:HD11	1.63	0.79
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:H	1:C:276:LEU:CD2	1.96	0.78
1:A:293:MET:CE	1:A:317:ARG:HG3	2.12	0.78
1:C:93:SER:HA	1:C:96:ASP:OD1	1.82	0.78
1:D:114:ILE:CD1	1:D:137:LEU:HD21	2.12	0.78
1:A:334:SER:HB3	1:A:336:ARG:HE	1.49	0.77
1:C:114:ILE:CD1	1:C:137:LEU:HD21	2.15	0.77
1:B:487:ASN:HB3	1:B:489:LYS:HG3	1.66	0.77
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.50	0.76
1:C:110:ASP:HB3	1:C:112:GLN:HB2	1.64	0.76
1:B:293:MET:CE	1:B:317:ARG:HG3	2.16	0.76
1:A:114:ILE:HD11	1:A:137:LEU:HD21	1.66	0.76
1:C:147:ARG:HG2	1:C:147:ARG:HH11	1.50	0.76
1:A:76:ILE:HB	1:A:90:LEU:HD13	1.68	0.76
1:D:147:ARG:HH11	1:D:147:ARG:HG2	1.51	0.76
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.68	0.75
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.21	0.75
1:A:74:ASN:C	1:A:92:ASN:HB3	2.12	0.75
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.69	0.75
1:B:76:ILE:HB	1:B:90:LEU:HD13	1.69	0.75
1:D:486:VAL:HG13	1:D:487:ASN:N	2.01	0.75
1:A:487:ASN:HB3	1:A:489:LYS:HG3	1.68	0.75
1:D:77:LEU:HD23	1:D:88:VAL:HA	1.69	0.75
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.67	0.75
1:C:486:VAL:HG13	1:C:487:ASN:H	1.51	0.75
1:B:114:ILE:CD1	1:B:137:LEU:HD21	2.17	0.74
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.68	0.74
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.71	0.74
1:B:334:SER:HB3	1:B:336:ARG:HE	1.50	0.73
1:D:486:VAL:HG13	1:D:487:ASN:H	1.53	0.73
1:B:74:ASN:C	1:B:92:ASN:HB3	2.13	0.73
1:A:108:SER:C	1:A:110:ASP:H	1.96	0.73
1:A:597:ARG:HG3	1:A:600:THR:HG21	1.71	0.73
1:D:502:LYS:O	1:D:505:GLN:HG2	1.89	0.73
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.19	0.73
1:C:486:VAL:HG13	1:C:487:ASN:N	2.01	0.72
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.19	0.72
1:A:253:ARG:HH22	1:B:253:ARG:NH2	1.82	0.72
1:A:438:ASP:OD1	1:A:440:THR:HB	1.90	0.72
1:B:108:SER:C	1:B:110:ASP:H	1.96	0.72
1:A:455:GLN:HG3	1:A:475:PRO:CD	2.19	0.72
1:C:502:LYS:O	1:C:505:GLN:HG2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASN:HD22	1:D:274:ASP:H	1.38	0.72
1:C:528:MET:HG2	1:C:576:ALA:HB2	1.71	0.72
1:B:597:ARG:HG3	1:B:600:THR:HG21	1.72	0.71
1:C:77:LEU:HD23	1:C:88:VAL:HA	1.70	0.71
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.05	0.71
1:D:110:ASP:HB3	1:D:112:GLN:HB2	1.70	0.71
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.91	0.71
1:D:176:ILE:HD11	1:D:276:LEU:HD21	1.72	0.71
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.91	0.71
1:B:171:ASP:OD1	1:B:186:THR:HG23	1.90	0.71
1:B:455:GLN:HG3	1:B:475:PRO:CD	2.21	0.71
1:D:341:VAL:C	1:D:343:ARG:H	1.99	0.70
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.90	0.70
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.72	0.70
1:A:693:GLU:OE1	1:A:696:LYS:HE2	1.92	0.70
1:B:231:THR:HG22	1:B:232:GLU:HG3	1.72	0.70
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.73	0.70
1:B:693:GLU:OE1	1:B:696:LYS:HE2	1.92	0.70
1:D:471:ARG:HG2	1:D:480:TYR:CD2	2.26	0.70
1:C:276:LEU:H	1:C:276:LEU:HD22	1.57	0.70
1:D:276:LEU:H	1:D:276:LEU:HD22	1.56	0.70
1:A:231:THR:HG22	1:A:232:GLU:HG3	1.74	0.70
1:A:377:ASN:HB2	1:A:381:TYR:O	1.92	0.70
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.71	0.70
1:B:438:ASP:OD1	1:B:440:THR:HB	1.90	0.70
1:C:341:VAL:C	1:C:343:ARG:H	1.99	0.70
1:C:331:ASP:HB3	1:C:334:SER:HB2	1.74	0.69
1:D:528:MET:HG2	1:D:576:ALA:HB2	1.72	0.69
1:B:76:ILE:HB	1:B:90:LEU:CD1	2.21	0.69
1:C:176:ILE:HD11	1:C:276:LEU:HD21	1.72	0.69
1:B:455:GLN:HG3	1:B:475:PRO:HD2	1.73	0.69
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.07	0.69
1:D:438:ASP:OD2	1:D:440:THR:HG22	1.91	0.69
1:A:455:GLN:HG3	1:A:475:PRO:HD2	1.72	0.69
1:A:616:MET:HE2	1:A:618:PHE:CZ	2.27	0.69
1:C:183:TYR:HE1	1:C:277:SER:O	1.75	0.69
1:A:39:SER:HB2	1:A:40:ARG:NE	2.03	0.69
1:A:341:VAL:O	1:A:342:ALA:CB	2.41	0.69
1:B:314:GLN:HE22	1:B:373:LYS:HZ1	1.39	0.69
1:B:616:MET:HE2	1:B:618:PHE:CZ	2.27	0.68
1:C:277:SER:O	1:C:278:SER:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.75	0.68
1:B:377:ASN:HB2	1:B:381:TYR:O	1.93	0.68
1:D:289:ALA:CB	1:D:290:PRO:HA	2.22	0.68
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.24	0.68
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.92	0.68
1:D:415:LEU:HB3	1:D:434:ILE:HG22	1.76	0.68
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.74	0.67
1:B:273:THR:HA	1:B:276:LEU:HD13	1.75	0.67
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.74	0.67
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.91	0.67
1:D:272:ASN:ND2	1:D:274:ASP:H	1.92	0.67
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.59	0.67
1:D:334:SER:HB3	1:D:336:ARG:CD	2.25	0.67
1:B:173:TYR:CE2	1:B:184:ARG:HG2	2.30	0.67
1:D:627:TRP:CE3	1:D:755:MET:HE1	2.30	0.66
1:A:74:ASN:HB3	1:A:92:ASN:OD1	1.96	0.66
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.95	0.66
1:C:272:ASN:ND2	1:C:274:ASP:H	1.94	0.66
1:C:612:GLN:O	1:C:616:MET:HG3	1.95	0.66
1:D:612:GLN:O	1:D:616:MET:HG3	1.95	0.66
1:B:172:ILE:N	1:B:186:THR:HG22	2.01	0.66
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.77	0.66
1:C:415:LEU:HB3	1:C:434:ILE:HG22	1.78	0.66
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.78	0.66
1:C:272:ASN:HD22	1:C:274:ASP:H	1.41	0.66
1:D:76:ILE:HB	1:D:90:LEU:CD1	2.25	0.66
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.94	0.66
1:B:39:SER:HB2	1:B:40:ARG:NE	2.02	0.65
1:D:277:SER:O	1:D:278:SER:HB3	1.95	0.65
1:A:272:ASN:C	1:A:272:ASN:HD22	2.05	0.65
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.31	0.65
1:A:273:THR:HA	1:A:276:LEU:HD13	1.77	0.65
1:B:170:ASN:O	1:B:196:ASN:HB2	1.97	0.65
1:B:272:ASN:C	1:B:272:ASN:HD22	2.05	0.65
1:A:172:ILE:N	1:A:186:THR:HG22	2.01	0.65
1:A:289:ALA:CB	1:A:290:PRO:HA	2.22	0.65
1:A:528:MET:HE3	1:A:574:ILE:HG21	1.78	0.65
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.96	0.65
1:C:289:ALA:CB	1:C:290:PRO:HA	2.25	0.65
1:C:334:SER:HB3	1:C:336:ARG:CD	2.26	0.65
1:D:183:TYR:HE1	1:D:277:SER:O	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:HD22	1:B:92:ASN:C	2.05	0.64
1:D:704:HIS:HD2	1:D:716:SER:OG	1.80	0.64
1:C:627:TRP:CE3	1:C:755:MET:HE1	2.32	0.64
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.78	0.64
1:D:170:ASN:N	1:D:170:ASN:HD22	1.95	0.64
1:A:314:GLN:HE22	1:A:373:LYS:HZ1	1.44	0.64
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.80	0.64
1:B:92:ASN:ND2	1:B:93:SER:N	2.39	0.64
1:B:334:SER:HB3	1:B:336:ARG:CD	2.28	0.64
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.33	0.63
1:A:293:MET:HE2	1:A:317:ARG:CG	2.23	0.63
1:B:676:PRO:HG2	1:B:677:GLU:OE2	1.98	0.63
1:C:108:SER:C	1:C:110:ASP:H	2.04	0.63
1:D:410:LEU:HD13	1:D:415:LEU:HD23	1.80	0.63
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.83	0.63
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.29	0.63
1:D:613:PHE:O	1:D:616:MET:HB2	1.98	0.63
1:D:115:LEU:HD21	1:D:155:VAL:HG11	1.80	0.63
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.14	0.63
1:A:334:SER:HB3	1:A:336:ARG:CD	2.29	0.63
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.80	0.63
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.81	0.63
1:A:290:PRO:HG3	1:A:326:ASP:OD2	1.98	0.63
1:B:293:MET:HE2	1:B:317:ARG:CG	2.25	0.63
1:D:289:ALA:CB	1:D:290:PRO:CA	2.76	0.63
1:A:170:ASN:O	1:A:196:ASN:HB2	1.99	0.63
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.14	0.63
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.29	0.62
1:B:528:MET:HE1	1:B:618:PHE:CE1	2.33	0.62
1:C:341:VAL:HG22	1:C:342:ALA:N	2.13	0.62
1:C:438:ASP:OD2	1:C:440:THR:HG22	1.99	0.62
1:A:170:ASN:N	1:A:170:ASN:HD22	1.95	0.62
1:C:411:THR:C	1:C:413:ASP:H	2.06	0.62
1:B:90:LEU:HD22	1:B:90:LEU:O	2.00	0.62
1:C:651:ILE:HG21	1:C:755:MET:HE3	1.82	0.62
1:D:108:SER:C	1:D:110:ASP:H	2.07	0.62
1:D:676:PRO:HG2	1:D:677:GLU:OE2	2.00	0.62
1:B:160:VAL:HG23	1:B:161:GLY:N	2.14	0.61
1:B:170:ASN:N	1:B:170:ASN:HD22	1.96	0.61
1:D:276:LEU:CD2	1:D:276:LEU:N	2.63	0.61
1:C:276:LEU:CD2	1:C:276:LEU:N	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:GLN:HG3	1:C:475:PRO:HD2	1.82	0.61
1:A:92:ASN:HD22	1:A:92:ASN:C	2.08	0.61
1:B:289:ALA:CB	1:B:290:PRO:HA	2.24	0.61
1:D:74:ASN:O	1:D:92:ASN:HB3	2.00	0.61
1:D:388:GLN:CB	1:D:391:LYS:HB2	2.31	0.61
1:D:341:VAL:HG22	1:D:342:ALA:N	2.14	0.61
1:D:455:GLN:HG3	1:D:475:PRO:HD2	1.83	0.61
1:A:627:TRP:CE3	1:A:755:MET:HE1	2.35	0.61
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.00	0.61
1:C:346:ILE:HG21	1:C:348:MET:HE2	1.81	0.61
1:C:246:LEU:HD22	1:C:248:TYR:O	2.01	0.61
1:A:528:MET:HE1	1:A:618:PHE:CE1	2.35	0.61
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.35	0.61
1:D:411:THR:C	1:D:413:ASP:H	2.09	0.61
1:D:93:SER:HA	1:D:96:ASP:CG	2.25	0.61
1:B:92:ASN:HD22	1:B:93:SER:H	1.47	0.61
1:C:115:LEU:HD21	1:C:155:VAL:HG11	1.83	0.61
1:C:411:THR:C	1:C:413:ASP:N	2.58	0.61
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.31	0.60
1:B:341:VAL:O	1:B:342:ALA:CB	2.46	0.60
1:C:289:ALA:CB	1:C:290:PRO:CA	2.79	0.60
1:C:613:PHE:O	1:C:616:MET:HB2	2.01	0.60
1:D:192:ASP:O	1:D:193:ILE:HD13	2.00	0.60
1:A:111:GLY:O	1:A:137:LEU:HD12	2.02	0.60
1:B:290:PRO:HG3	1:B:326:ASP:OD2	2.00	0.60
1:B:81:ALA:O	1:B:492:ARG:NH2	2.33	0.60
1:C:272:ASN:HD22	1:C:272:ASN:C	2.08	0.60
1:B:528:MET:HE3	1:B:574:ILE:HG21	1.82	0.60
1:C:93:SER:HA	1:C:96:ASP:CG	2.26	0.60
1:C:340:LEU:O	1:C:343:ARG:HB3	2.01	0.60
1:C:388:GLN:CB	1:C:391:LYS:HB2	2.32	0.60
1:D:146:GLU:OE1	1:D:181:PRO:HA	2.02	0.60
1:D:325:MET:O	1:D:344:GLN:HB2	2.02	0.60
1:C:39:SER:O	1:C:40:ARG:HD2	2.02	0.60
1:B:520:ASN:O	1:B:521:GLU:HB2	2.01	0.60
1:D:39:SER:O	1:D:40:ARG:HD2	2.02	0.60
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.32	0.60
1:B:325:MET:CE	1:B:327:ILE:HD11	2.32	0.60
1:C:203:TYR:HA	1:C:207:VAL:HG13	1.83	0.60
1:A:579:ASP:HB3	1:A:583:SER:OG	2.01	0.59
1:B:334:SER:CB	1:B:336:ARG:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.17	0.59
1:C:704:HIS:HD2	1:C:716:SER:OG	1.85	0.59
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.84	0.59
1:D:272:ASN:HD22	1:D:272:ASN:C	2.08	0.59
1:D:340:LEU:O	1:D:343:ARG:HB3	2.02	0.59
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.84	0.59
1:A:334:SER:CB	1:A:336:ARG:HD2	2.32	0.59
1:C:377:ASN:HB2	1:C:381:TYR:O	2.01	0.59
1:A:325:MET:CE	1:A:327:ILE:HD11	2.31	0.59
1:B:111:GLY:O	1:B:137:LEU:HD12	2.03	0.59
1:C:192:ASP:O	1:C:193:ILE:HD13	2.02	0.59
1:A:60:LEU:HD12	1:A:60:LEU:C	2.27	0.59
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.84	0.59
1:D:346:ILE:HG21	1:D:348:MET:HE2	1.85	0.59
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.84	0.59
1:A:78:VAL:HG12	1:A:87:SER:O	2.03	0.58
1:A:90:LEU:O	1:A:90:LEU:HD22	2.02	0.58
1:A:520:ASN:O	1:A:521:GLU:HB2	2.03	0.58
1:C:325:MET:O	1:C:344:GLN:HB2	2.03	0.58
1:B:115:LEU:HD12	1:B:134:ILE:HG12	1.84	0.58
1:C:60:LEU:C	1:C:60:LEU:HD12	2.27	0.58
1:A:160:VAL:HG23	1:A:161:GLY:N	2.19	0.58
1:C:471:ARG:HG2	1:C:480:TYR:HD2	1.68	0.58
1:D:109:PRO:HG3	1:D:158:SER:O	2.03	0.58
1:D:39:SER:O	1:D:40:ARG:O	2.20	0.58
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.85	0.58
1:A:301:CYS:SG	1:A:359:PRO:HG2	2.44	0.58
1:A:459:VAL:HG22	1:A:460:SER:N	2.18	0.58
1:C:183:TYR:CE1	1:C:277:SER:O	2.56	0.58
1:C:411:THR:O	1:C:413:ASP:N	2.36	0.58
1:C:720:SER:O	1:C:724:VAL:HG23	2.04	0.58
1:A:81:ALA:O	1:A:492:ARG:NH2	2.37	0.58
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.28	0.58
1:B:78:VAL:HG12	1:B:87:SER:O	2.03	0.58
1:C:146:GLU:OE1	1:C:181:PRO:HA	2.03	0.58
1:B:74:ASN:HB3	1:B:92:ASN:OD1	2.03	0.58
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.38	0.58
1:A:487:ASN:CB	1:A:489:LYS:HG3	2.34	0.58
1:C:146:GLU:O	1:C:175:LYS:HE2	2.03	0.58
1:D:377:ASN:HB2	1:D:381:TYR:O	2.03	0.58
1:C:81:ALA:O	1:C:492:ARG:NH2	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASN:N	1:C:170:ASN:HD22	2.00	0.58
1:D:60:LEU:HD12	1:D:60:LEU:C	2.29	0.58
1:D:177:GLU:CG	1:D:180:LEU:HD22	2.34	0.58
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.03	0.57
1:A:289:ALA:CB	1:A:290:PRO:CA	2.79	0.57
1:B:314:GLN:HE22	1:B:373:LYS:NZ	2.01	0.57
1:A:82:GLU:HG2	1:A:83:TYR:CZ	2.39	0.57
1:A:353:TRP:CZ2	1:A:591:MET:HE3	2.40	0.57
1:B:108:SER:C	1:B:110:ASP:N	2.62	0.57
1:D:177:GLU:HB2	1:D:180:LEU:HD22	1.87	0.57
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.39	0.57
1:C:93:SER:HB2	1:C:96:ASP:OD2	2.05	0.57
1:A:172:ILE:N	1:A:186:THR:CG2	2.61	0.57
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.05	0.57
1:D:82:GLU:HB2	1:D:467:TYR:OH	2.03	0.57
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.29	0.57
1:A:237:GLU:OE1	1:B:251:THR:OG1	2.19	0.57
1:B:579:ASP:HB3	1:B:583:SER:OG	2.04	0.57
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.04	0.57
1:C:88:VAL:HG11	1:C:91:GLU:OE2	2.05	0.57
1:D:136:ASP:OD1	1:D:138:ASN:HB2	2.05	0.57
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.40	0.57
1:D:528:MET:HE3	1:D:574:ILE:CG2	2.34	0.57
1:A:92:ASN:HD22	1:A:93:SER:H	1.44	0.57
1:C:74:ASN:O	1:C:92:ASN:HB3	2.05	0.57
1:D:242:SER:HB3	1:D:246:LEU:HD12	1.86	0.57
1:D:246:LEU:HD22	1:D:248:TYR:O	2.04	0.57
1:C:600:THR:O	1:C:603:VAL:HG13	2.06	0.56
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.40	0.56
1:C:377:ASN:HB2	1:C:381:TYR:H	1.70	0.56
1:D:93:SER:HB2	1:D:96:ASP:OD2	2.06	0.56
1:D:651:ILE:HG21	1:D:755:MET:HE3	1.87	0.56
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.40	0.56
1:B:60:LEU:C	1:B:60:LEU:HD12	2.29	0.56
1:B:110:ASP:C	1:B:112:GLN:H	2.12	0.56
1:B:193:ILE:HG22	1:B:194:ILE:HG13	1.86	0.56
1:D:370:SER:HB3	1:D:388:GLN:NE2	2.20	0.56
1:A:110:ASP:C	1:A:112:GLN:H	2.14	0.56
1:D:146:GLU:O	1:D:175:LYS:HE2	2.05	0.56
1:A:65:ASP:HB3	1:A:66:HIS:CE1	2.40	0.56
1:C:341:VAL:HG22	1:C:342:ALA:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:THR:HG21	1:D:717:ALA:O	2.05	0.56
1:A:616:MET:HE2	1:A:618:PHE:HZ	1.71	0.56
1:B:272:ASN:HD22	1:B:274:ASP:H	1.53	0.56
1:C:153:GLN:HB3	1:C:211:TYR:CE2	2.41	0.56
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.56
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.88	0.56
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.88	0.56
1:B:172:ILE:N	1:B:186:THR:CG2	2.62	0.56
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.40	0.56
1:A:115:LEU:HD12	1:A:134:ILE:HG12	1.87	0.55
1:A:334:SER:HB3	1:A:336:ARG:HD2	1.88	0.55
1:C:370:SER:HB3	1:C:388:GLN:NE2	2.21	0.55
1:D:88:VAL:HG11	1:D:91:GLU:OE2	2.06	0.55
1:D:377:ASN:HB2	1:D:381:TYR:H	1.71	0.55
1:D:377:ASN:HB2	1:D:381:TYR:N	2.21	0.55
1:D:528:MET:HE1	1:D:618:PHE:CE1	2.41	0.55
1:D:528:MET:CE	1:D:530:LEU:HD21	2.30	0.55
1:A:544:LEU:HD21	1:A:606:GLN:HG3	1.89	0.55
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.07	0.55
1:C:64:SER:C	1:C:463:LYS:HG2	2.32	0.55
1:D:341:VAL:O	1:D:342:ALA:HB3	2.06	0.55
1:D:489:LYS:NZ	1:D:489:LYS:HB3	2.21	0.55
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.40	0.55
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.41	0.55
1:D:183:TYR:CE1	1:D:277:SER:O	2.59	0.55
1:B:487:ASN:CB	1:B:489:LYS:HG3	2.35	0.55
1:C:290:PRO:HG3	1:C:326:ASP:OD2	2.07	0.55
1:C:377:ASN:HB2	1:C:381:TYR:N	2.21	0.55
1:B:693:GLU:HA	1:B:726:VAL:HG11	1.87	0.55
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.41	0.55
1:C:102:ILE:HD13	1:C:116:LEU:HD22	1.89	0.55
1:C:109:PRO:HG3	1:C:158:SER:O	2.06	0.55
1:C:110:ASP:HB3	1:C:112:GLN:H	1.71	0.55
1:D:64:SER:C	1:D:463:LYS:HG2	2.31	0.55
1:B:305:TRP:CE3	1:B:311:ILE:HB	2.42	0.55
1:C:598:LEU:HD22	1:C:631:TYR:OH	2.06	0.55
1:D:598:LEU:HD22	1:D:631:TYR:OH	2.07	0.55
1:D:383:HIS:HB3	1:D:398:THR:OG1	2.07	0.55
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.89	0.55
1:C:528:MET:CE	1:C:530:LEU:HD21	2.32	0.55
1:D:486:VAL:CG1	1:D:487:ASN:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.88	0.55
1:B:528:MET:HE1	1:B:618:PHE:HE1	1.72	0.55
1:C:383:HIS:HB3	1:C:398:THR:OG1	2.06	0.55
1:C:536:LYS:CB	1:C:536:LYS:NZ	2.70	0.54
1:D:81:ALA:O	1:D:492:ARG:NH2	2.28	0.54
1:B:110:ASP:HB3	1:B:112:GLN:HB2	1.90	0.54
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.42	0.54
1:C:80:ASN:HB3	1:C:85:ASN:OD1	2.06	0.54
1:D:80:ASN:HB3	1:D:85:ASN:OD1	2.07	0.54
1:D:102:ILE:HD13	1:D:116:LEU:HD22	1.88	0.54
1:A:177:GLU:CG	1:A:180:LEU:HD22	2.36	0.54
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.72	0.54
1:B:622:LYS:HB2	1:B:622:LYS:NZ	2.23	0.54
1:C:65:ASP:OD2	1:C:466:LYS:HB2	2.07	0.54
1:C:486:VAL:CG1	1:C:487:ASN:H	2.19	0.54
1:D:341:VAL:HG22	1:D:342:ALA:H	1.71	0.54
1:D:411:THR:C	1:D:413:ASP:N	2.62	0.54
1:D:720:SER:O	1:D:724:VAL:HG23	2.06	0.54
1:B:56:LYS:HB2	1:B:497:ASN:OD1	2.07	0.54
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.42	0.54
1:C:741:GLY:O	1:C:742:ILE:C	2.50	0.54
1:A:168:TRP:O	1:A:169:ASN:HB2	2.07	0.54
1:A:489:LYS:NZ	1:A:489:LYS:HB3	2.22	0.54
1:D:388:GLN:HB2	1:D:391:LYS:HB2	1.90	0.54
1:D:704:HIS:HE1	1:D:711:VAL:O	1.91	0.54
1:B:128:TYR:CD1	1:B:128:TYR:C	2.85	0.54
1:C:415:LEU:C	1:C:415:LEU:HD13	2.33	0.54
1:B:140:ARG:HG2	1:B:140:ARG:NH1	2.23	0.54
1:B:459:VAL:HG22	1:B:460:SER:N	2.22	0.54
1:D:273:THR:O	1:D:276:LEU:HD21	2.07	0.54
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.42	0.54
1:B:177:GLU:CG	1:B:180:LEU:HD22	2.38	0.54
1:B:272:ASN:ND2	1:B:274:ASP:H	2.06	0.54
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.89	0.54
1:B:205:GLU:OE2	2:B:901:GGO:N	2.41	0.54
1:C:69:LEU:HD22	1:C:76:ILE:HG22	1.90	0.54
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.43	0.54
1:A:455:GLN:HG3	1:A:475:PRO:HD3	1.90	0.54
1:B:301:CYS:SG	1:B:359:PRO:HG2	2.48	0.54
1:C:39:SER:O	1:C:40:ARG:O	2.26	0.54
1:B:149:PRO:HB2	1:B:168:TRP:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.08	0.53
1:D:388:GLN:HB3	1:D:391:LYS:HB2	1.90	0.53
1:D:411:THR:O	1:D:413:ASP:N	2.41	0.53
1:A:39:SER:O	1:A:40:ARG:O	2.26	0.53
1:A:92:ASN:ND2	1:A:93:SER:N	2.41	0.53
1:C:269:PHE:CE2	1:C:286:GLN:HB2	2.44	0.53
1:A:726:VAL:HG12	1:A:726:VAL:O	2.08	0.53
1:C:177:GLU:CG	1:C:180:LEU:HD22	2.38	0.53
1:B:39:SER:O	1:B:40:ARG:O	2.26	0.53
1:B:167:VAL:HA	1:B:171:ASP:O	2.07	0.53
1:C:286:GLN:NE2	1:C:288:THR:HG22	2.24	0.53
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.90	0.53
1:B:176:ILE:HD11	1:B:276:LEU:HD21	1.91	0.53
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.89	0.53
1:D:153:GLN:HB3	1:D:211:TYR:CE2	2.44	0.53
1:B:353:TRP:CZ2	1:B:591:MET:HE3	2.43	0.53
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.74	0.53
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.44	0.53
1:B:489:LYS:NZ	1:B:489:LYS:HB3	2.22	0.53
1:C:388:GLN:HB3	1:C:391:LYS:HB2	1.91	0.53
1:D:110:ASP:HB3	1:D:112:GLN:H	1.74	0.53
1:A:167:VAL:HA	1:A:171:ASP:O	2.09	0.53
1:A:193:ILE:HG22	1:A:194:ILE:HG13	1.90	0.53
1:C:64:SER:O	1:C:463:LYS:HG2	2.09	0.53
1:D:341:VAL:C	1:D:343:ARG:N	2.67	0.53
1:B:616:MET:HE2	1:B:618:PHE:HZ	1.72	0.53
1:C:704:HIS:HE1	1:C:711:VAL:O	1.92	0.53
1:D:60:LEU:HD12	1:D:60:LEU:O	2.09	0.53
1:A:106:SER:HB3	1:A:115:LEU:HB3	1.91	0.52
1:C:341:VAL:O	1:C:342:ALA:HB3	2.10	0.52
1:C:528:MET:HE1	1:C:618:PHE:CE1	2.44	0.52
1:D:216:TRP:CZ3	1:D:273:THR:HG21	2.44	0.52
1:D:415:LEU:HD13	1:D:415:LEU:C	2.34	0.52
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.06	0.52
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.91	0.52
1:B:544:LEU:HD21	1:B:606:GLN:HG3	1.89	0.52
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.90	0.52
1:B:55:LEU:HD23	1:B:500:LEU:HD22	1.91	0.52
1:C:62:TRP:CE3	1:C:68:TYR:HB3	2.44	0.52
1:D:69:LEU:HD22	1:D:76:ILE:HG22	1.92	0.52
1:D:289:ALA:HB1	1:D:290:PRO:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:CB	1:A:180:LEU:HD22	2.40	0.52
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.45	0.52
1:C:60:LEU:HD12	1:C:60:LEU:O	2.09	0.52
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.35	0.52
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.45	0.52
1:A:62:TRP:CE3	1:A:68:TYR:HB3	2.45	0.52
1:C:489:LYS:NZ	1:C:489:LYS:HB3	2.25	0.52
1:C:717:ALA:O	1:D:736:THR:HG21	2.10	0.52
1:D:600:THR:O	1:D:603:VAL:HG13	2.10	0.52
1:B:168:TRP:O	1:B:169:ASN:HB2	2.09	0.52
1:D:745:SER:O	1:D:749:GLN:HG3	2.09	0.52
1:B:71:LYS:NZ	1:B:105:TYR:HB2	2.25	0.52
1:B:334:SER:HB3	1:B:336:ARG:HD2	1.89	0.52
1:D:341:VAL:O	1:D:343:ARG:N	2.43	0.52
1:D:486:VAL:CG1	1:D:487:ASN:H	2.21	0.52
1:D:726:VAL:HG12	1:D:726:VAL:O	2.08	0.51
1:C:273:THR:O	1:C:276:LEU:HD21	2.10	0.51
1:C:486:VAL:CG1	1:C:487:ASN:N	2.70	0.51
1:D:471:ARG:HG2	1:D:480:TYR:HD2	1.75	0.51
1:C:536:LYS:HB3	1:C:536:LYS:HZ3	1.76	0.51
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.45	0.51
1:A:125:ARG:HG2	1:A:126:HIS:CD2	2.45	0.51
1:A:305:TRP:CE3	1:A:311:ILE:HB	2.46	0.51
1:B:71:LYS:HZ3	1:B:105:TYR:HB2	1.76	0.51
1:C:673:LEU:O	1:C:678:ASP:HB3	2.11	0.51
1:D:62:TRP:CE3	1:D:68:TYR:HB3	2.46	0.51
1:D:600:THR:OG1	1:D:601:PHE:N	2.43	0.51
1:B:115:LEU:HD21	1:B:155:VAL:HG11	1.93	0.51
1:C:289:ALA:HB1	1:C:290:PRO:C	2.35	0.51
1:D:293:MET:CE	1:D:317:ARG:HG3	2.15	0.51
1:C:388:GLN:HB2	1:C:391:LYS:HB2	1.91	0.51
1:D:177:GLU:HG3	1:D:180:LEU:HD22	1.92	0.51
1:B:65:ASP:HB3	1:B:66:HIS:CE1	2.46	0.51
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.46	0.51
1:D:74:ASN:C	1:D:92:ASN:HB3	2.36	0.51
1:D:369:ASN:C	1:D:389:ILE:HG23	2.36	0.51
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.93	0.51
1:B:726:VAL:O	1:B:726:VAL:HG12	2.11	0.51
1:D:65:ASP:OD2	1:D:466:LYS:HB2	2.10	0.51
1:B:330:TYR:HE1	1:B:335:GLY:HA2	1.76	0.51
1:D:170:ASN:O	1:D:196:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:TYR:O	1:B:482:LEU:HD23	2.11	0.50
1:C:154:TRP:O	1:C:166:TYR:HA	2.11	0.50
1:C:341:VAL:O	1:C:343:ARG:N	2.42	0.50
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.26	0.50
1:A:137:LEU:O	1:A:140:ARG:NH1	2.44	0.50
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.75	0.50
1:A:248:TYR:CE1	1:B:258:LYS:HD2	2.47	0.50
1:D:491:LEU:O	1:D:492:ARG:HB3	2.12	0.50
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.47	0.50
1:A:231:THR:HG22	1:A:232:GLU:CG	2.41	0.50
1:A:244:GLU:CD	1:B:689:MET:HG3	2.37	0.50
1:A:272:ASN:HD22	1:A:274:ASP:H	1.60	0.50
1:A:622:LYS:HB2	1:A:622:LYS:NZ	2.26	0.50
1:C:277:SER:O	1:C:278:SER:CB	2.60	0.50
1:D:173:TYR:CE2	1:D:184:ARG:HG2	2.46	0.50
1:D:741:GLY:O	1:D:742:ILE:C	2.54	0.50
1:A:724:VAL:HG13	1:B:750:HIS:HB2	1.93	0.50
1:C:446:SER:HA	1:C:449:LEU:HG	1.93	0.50
1:A:110:ASP:HB3	1:A:112:GLN:HB2	1.93	0.50
1:C:597:ARG:NH1	1:C:682:HIS:HB2	2.27	0.50
1:B:147:ARG:HH11	1:B:147:ARG:HG2	1.77	0.50
1:B:377:ASN:CB	1:B:381:TYR:H	2.24	0.50
1:B:704:HIS:HD2	1:B:716:SER:OG	1.95	0.50
1:C:111:GLY:O	1:C:137:LEU:HD12	2.11	0.50
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.47	0.50
1:C:184:ARG:HD3	1:C:186:THR:O	2.11	0.50
1:C:276:LEU:N	1:C:276:LEU:HD23	2.27	0.50
1:D:154:TRP:O	1:D:166:TYR:HA	2.12	0.50
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.46	0.50
1:D:519:LEU:O	1:D:520:ASN:C	2.55	0.50
1:D:536:LYS:NZ	1:D:536:LYS:CB	2.75	0.50
1:D:550:PRO:O	1:D:551:CYS:HB3	2.12	0.50
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.93	0.49
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.47	0.49
1:D:65:ASP:CG	1:D:464:GLU:HB2	2.36	0.49
1:A:64:SER:O	1:A:463:LYS:HG2	2.12	0.49
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.47	0.49
1:B:455:GLN:HG3	1:B:475:PRO:HD3	1.93	0.49
1:D:111:GLY:O	1:D:137:LEU:HD12	2.12	0.49
1:D:269:PHE:CE2	1:D:286:GLN:HB2	2.47	0.49
1:A:128:TYR:C	1:A:128:TYR:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ASP:C	1:A:622:LYS:H	2.20	0.49
1:B:377:ASN:HB2	1:B:381:TYR:H	1.76	0.49
1:A:272:ASN:ND2	1:A:274:ASP:H	2.09	0.49
1:A:689:MET:HB3	1:A:722:ALA:HB2	1.95	0.49
1:C:113:PHE:CE2	1:C:178:PRO:HG2	2.48	0.49
1:D:90:LEU:HD22	1:D:90:LEU:C	2.38	0.49
1:D:113:PHE:CE2	1:D:178:PRO:HG2	2.48	0.49
1:D:446:SER:HA	1:D:449:LEU:HG	1.93	0.49
1:A:93:SER:HA	1:A:96:ASP:OD1	2.12	0.49
1:A:428:GLY:O	1:A:429:ARG:HD3	2.12	0.49
1:A:454:CYS:HA	1:A:474:GLY:O	2.12	0.49
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.94	0.49
1:C:608:GLU:O	1:C:611:ARG:HB3	2.13	0.49
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.76	0.49
1:D:276:LEU:N	1:D:276:LEU:HD23	2.26	0.49
1:D:485:SER:O	1:D:486:VAL:C	2.56	0.49
1:D:627:TRP:CZ3	1:D:755:MET:HE1	2.47	0.49
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.93	0.49
1:A:277:SER:OG	1:A:280:THR:HB	2.13	0.49
1:B:153:GLN:HB3	1:B:211:TYR:CE2	2.47	0.49
1:C:173:TYR:HB3	1:C:182:SER:OG	2.13	0.49
1:D:272:ASN:HD21	1:D:274:ASP:HB2	1.78	0.49
1:D:597:ARG:NH1	1:D:682:HIS:HB2	2.26	0.49
1:A:39:SER:CB	1:A:40:ARG:NE	2.70	0.49
1:A:487:ASN:O	1:A:488:ASP:HB2	2.13	0.49
1:B:125:ARG:HG2	1:B:126:HIS:CD2	2.47	0.49
1:B:171:ASP:HA	1:B:186:THR:CG2	2.43	0.49
1:C:171:ASP:OD1	1:C:186:THR:HG23	2.12	0.49
1:D:127:SER:O	1:D:128:TYR:HB3	2.11	0.49
1:D:654:ALA:HA	1:D:704:HIS:CD2	2.48	0.49
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.37	0.49
1:B:614:SER:HB2	1:B:621:ASN:HB3	1.95	0.49
1:C:745:SER:O	1:C:749:GLN:HG3	2.13	0.49
1:D:536:LYS:HZ3	1:D:536:LYS:HB3	1.78	0.49
1:C:90:LEU:C	1:C:90:LEU:HD22	2.37	0.48
1:C:519:LEU:O	1:C:520:ASN:C	2.55	0.48
1:D:608:GLU:O	1:D:611:ARG:HB3	2.12	0.48
1:D:459:VAL:HG22	1:D:460:SER:N	2.28	0.48
1:A:277:SER:O	1:A:278:SER:HB3	2.13	0.48
1:A:364:PHE:CD2	1:A:371:PHE:HB3	2.48	0.48
1:B:64:SER:O	1:B:463:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:THR:HG22	1:B:232:GLU:CG	2.40	0.48
1:B:747:ALA:O	1:B:751:ILE:HG22	2.13	0.48
1:B:137:LEU:O	1:B:140:ARG:NH1	2.47	0.48
1:C:223:LEU:O	1:C:271:VAL:HG12	2.14	0.48
1:D:171:ASP:OD1	1:D:186:THR:HG23	2.13	0.48
1:D:308:GLN:HA	1:D:308:GLN:OE1	2.13	0.48
1:A:149:PRO:HB2	1:A:168:TRP:CD1	2.48	0.48
1:A:310:ARG:NH1	1:A:329:ASP:OD2	2.47	0.48
1:A:704:HIS:HD2	1:A:716:SER:OG	1.96	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.48
1:B:701:LEU:HD22	1:B:703:ILE:HG13	1.94	0.48
1:B:109:PRO:HG2	1:B:161:GLY:O	2.12	0.48
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.42	0.48
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.28	0.48
1:C:110:ASP:C	1:C:112:GLN:H	2.22	0.48
1:C:147:ARG:HH11	1:C:147:ARG:CG	2.23	0.48
1:C:522:THR:HG22	1:C:523:LYS:N	2.29	0.48
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.44	0.48
1:D:614:SER:C	1:D:616:MET:H	2.22	0.48
1:A:153:GLN:HB3	1:A:211:TYR:CE2	2.48	0.48
1:A:171:ASP:HA	1:A:186:THR:CG2	2.44	0.48
1:A:747:ALA:O	1:A:751:ILE:HG22	2.14	0.48
1:B:428:GLY:O	1:B:429:ARG:HD3	2.14	0.48
1:C:170:ASN:O	1:C:196:ASN:HB2	2.14	0.48
1:C:346:ILE:CG2	1:C:348:MET:HE2	2.43	0.48
1:C:535:ASP:OD1	1:C:537:SER:HB3	2.14	0.48
1:D:673:LEU:O	1:D:678:ASP:HB3	2.13	0.48
1:A:276:LEU:CD2	1:A:276:LEU:H	2.26	0.48
1:A:330:TYR:HE1	1:A:335:GLY:HA2	1.79	0.48
1:A:528:MET:HE1	1:A:618:PHE:HE1	1.75	0.48
1:A:614:SER:HB2	1:A:621:ASN:HB3	1.96	0.48
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.96	0.48
1:C:122:LYS:HE2	1:C:124:TRP:O	2.14	0.48
1:C:244:GLU:CD	1:D:689:MET:HG3	2.38	0.48
1:C:491:LEU:O	1:C:492:ARG:HB3	2.13	0.48
1:D:316:LEU:HD21	1:D:320:GLN:CG	2.44	0.48
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.96	0.48
1:C:453:ARG:HG3	1:C:476:GLY:HA3	1.96	0.48
1:D:177:GLU:HB2	1:D:180:LEU:HB2	1.96	0.48
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.49	0.48
1:D:691:ARG:HG3	1:D:691:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.49	0.47
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.49	0.47
1:C:485:SER:O	1:C:486:VAL:C	2.56	0.47
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.94	0.47
1:D:449:LEU:O	1:D:450:ASN:HB2	2.12	0.47
1:A:377:ASN:CB	1:A:381:TYR:H	2.26	0.47
1:B:689:MET:HB3	1:B:722:ALA:HB2	1.95	0.47
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.49	0.47
1:D:114:ILE:CG1	1:D:137:LEU:HD21	2.44	0.47
1:A:108:SER:C	1:A:110:ASP:N	2.63	0.47
1:A:513:LYS:O	1:A:527:GLN:HA	2.15	0.47
1:B:277:SER:O	1:B:278:SER:HB3	2.14	0.47
1:C:95:PHE:O	1:C:96:ASP:C	2.56	0.47
1:A:509:MET:HE3	1:A:510:PRO:HD2	1.95	0.47
1:B:146:GLU:O	1:B:175:LYS:HE2	2.15	0.47
1:D:64:SER:O	1:D:463:LYS:HG2	2.15	0.47
1:D:217:SER:HB3	1:D:222:PHE:HB2	1.97	0.47
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.79	0.47
1:B:454:CYS:HA	1:B:474:GLY:O	2.15	0.47
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.97	0.47
1:A:415:LEU:C	1:A:415:LEU:HD13	2.39	0.47
1:A:425:MET:HA	1:A:426:PRO:HD2	1.77	0.47
1:A:701:LEU:HD22	1:A:703:ILE:HG13	1.96	0.47
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.96	0.47
1:C:627:TRP:CZ3	1:C:755:MET:HE1	2.50	0.47
1:D:539:LYS:NZ	1:D:617:GLY:O	2.47	0.47
1:A:726:VAL:O	1:A:726:VAL:CG1	2.62	0.47
1:C:75:ASN:ND2	1:C:92:ASN:OD1	2.48	0.47
1:C:172:ILE:N	1:C:186:THR:CG2	2.67	0.47
1:C:369:ASN:C	1:C:389:ILE:HG23	2.39	0.47
1:D:159:PRO:HB2	1:D:218:PRO:O	2.14	0.47
1:D:172:ILE:N	1:D:186:THR:HG22	2.11	0.47
1:D:319:ILE:O	1:D:321:ASN:N	2.43	0.47
1:D:453:ARG:HG3	1:D:476:GLY:HA3	1.96	0.47
1:D:522:THR:HG22	1:D:523:LYS:N	2.30	0.47
1:D:527:GLN:HG2	1:D:555:ALA:HA	1.97	0.47
1:A:71:LYS:HZ3	1:A:105:TYR:HB2	1.80	0.47
1:A:340:LEU:C	1:A:341:VAL:O	2.50	0.47
1:A:438:ASP:OD2	1:A:441:LYS:HG3	2.14	0.47
1:C:159:PRO:HB2	1:C:218:PRO:O	2.15	0.47
1:C:600:THR:OG1	1:C:601:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:LYS:HB2	1:C:622:LYS:NZ	2.30	0.47
1:D:39:SER:C	1:D:40:ARG:HD2	2.40	0.47
1:D:331:ASP:CB	1:D:334:SER:HB2	2.44	0.47
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.97	0.47
1:A:377:ASN:HB2	1:A:381:TYR:H	1.80	0.47
1:A:761:GLN:HE21	1:A:761:GLN:HB3	1.60	0.47
1:C:422:TYR:CE2	1:C:423:LYS:HD3	2.50	0.47
1:D:184:ARG:HD3	1:D:186:THR:O	2.15	0.47
1:C:236:ILE:HG12	1:C:712:HIS:CE1	2.49	0.47
1:D:177:GLU:CB	1:D:180:LEU:HD22	2.45	0.47
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.50	0.47
1:D:303:VAL:HG22	1:D:303:VAL:O	2.14	0.47
1:B:513:LYS:O	1:B:527:GLN:HA	2.15	0.46
1:C:114:ILE:CG1	1:C:137:LEU:HD21	2.44	0.46
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.50	0.46
1:D:520:ASN:O	1:D:521:GLU:HB2	2.15	0.46
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.40	0.46
1:C:308:GLN:OE1	1:C:308:GLN:HA	2.16	0.46
1:C:425:MET:HA	1:C:426:PRO:HD2	1.70	0.46
1:C:528:MET:HE3	1:C:574:ILE:CG2	2.38	0.46
1:C:614:SER:C	1:C:616:MET:H	2.23	0.46
1:D:286:GLN:NE2	1:D:288:THR:HG22	2.31	0.46
1:D:319:ILE:C	1:D:321:ASN:H	2.23	0.46
1:D:508:GLN:OE1	1:D:533:HIS:HE1	1.98	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.58	0.46
1:B:420:ASN:HB2	1:B:426:PRO:HA	1.97	0.46
1:C:108:SER:C	1:C:110:ASP:N	2.69	0.46
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.50	0.46
1:D:551:CYS:O	1:D:551:CYS:SG	2.73	0.46
1:D:614:SER:HA	1:D:619:VAL:CB	2.41	0.46
1:A:136:ASP:O	1:A:140:ARG:HA	2.16	0.46
1:B:125:ARG:O	1:B:125:ARG:HG3	2.15	0.46
1:C:153:GLN:HE22	1:C:170:ASN:HD21	1.60	0.46
1:C:299:TYR:CE1	1:C:665:VAL:HG22	2.50	0.46
1:C:536:LYS:NZ	1:C:536:LYS:HB3	2.30	0.46
1:C:247:GLN:HG2	1:D:258:LYS:HD2	1.98	0.46
1:C:314:GLN:HE22	1:C:373:LYS:HZ1	1.63	0.46
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.50	0.46
1:C:597:ARG:HD3	1:C:597:ARG:HA	1.74	0.46
1:D:346:ILE:CG2	1:D:348:MET:HE2	2.45	0.46
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LEU:HD13	1:B:415:LEU:C	2.39	0.46
1:A:60:LEU:HD12	1:A:60:LEU:O	2.16	0.46
1:A:125:ARG:HG2	1:A:126:HIS:NE2	2.31	0.46
1:A:468:TYR:O	1:A:482:LEU:HD23	2.15	0.46
1:A:542:LEU:HD23	1:A:542:LEU:C	2.40	0.46
1:B:364:PHE:CD2	1:B:371:PHE:HB3	2.50	0.46
1:B:761:GLN:HE21	1:B:761:GLN:HB3	1.60	0.46
1:C:310:ARG:HD3	1:C:327:ILE:HG23	1.97	0.46
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.31	0.46
1:A:269:PHE:CE2	1:A:286:GLN:HB2	2.50	0.46
1:A:276:LEU:HD23	1:A:276:LEU:O	2.16	0.46
1:A:502:LYS:O	1:A:505:GLN:HG2	2.16	0.46
1:B:170:ASN:ND2	1:B:170:ASN:N	2.64	0.46
1:B:285:ILE:HD12	1:B:285:ILE:N	2.31	0.46
1:C:173:TYR:CE2	1:C:184:ARG:HG2	2.51	0.46
1:D:55:LEU:HD23	1:D:500:LEU:HD22	1.98	0.46
1:D:310:ARG:HD3	1:D:327:ILE:HG23	1.97	0.46
1:B:39:SER:O	1:B:40:ARG:C	2.59	0.46
1:B:93:SER:HA	1:B:96:ASP:OD1	2.15	0.46
1:B:422:TYR:C	1:B:424:GLY:N	2.72	0.46
1:C:127:SER:O	1:C:128:TYR:HB3	2.15	0.46
1:C:671:MET:HE1	1:C:682:HIS:CD2	2.51	0.46
1:D:110:ASP:C	1:D:112:GLN:H	2.21	0.46
1:D:535:ASP:C	1:D:537:SER:H	2.23	0.46
1:A:236:ILE:O	1:A:253:ARG:HA	2.16	0.46
1:A:746:THR:HG21	1:B:725:ASP:HA	1.98	0.46
1:B:340:LEU:C	1:B:341:VAL:O	2.54	0.46
1:B:446:SER:HB2	1:B:457:TYR:CD1	2.51	0.46
1:C:74:ASN:C	1:C:92:ASN:HB3	2.39	0.46
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.98	0.46
1:D:75:ASN:ND2	1:D:92:ASN:OD1	2.49	0.46
1:D:153:GLN:HE22	1:D:170:ASN:HD21	1.56	0.46
1:A:422:TYR:C	1:A:424:GLY:N	2.72	0.45
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.96	0.45
1:C:65:ASP:HB2	1:C:463:LYS:HB2	1.98	0.45
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.76	0.45
1:C:272:ASN:HD21	1:C:274:ASP:HB2	1.81	0.45
1:C:314:GLN:HE22	1:C:373:LYS:NZ	2.13	0.45
1:D:173:TYR:HB3	1:D:182:SER:OG	2.15	0.45
1:D:370:SER:HB2	1:D:387:PHE:O	2.16	0.45
1:B:110:ASP:C	1:B:112:GLN:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.99	0.45
1:C:167:VAL:HG21	1:C:198:ILE:HG23	1.98	0.45
1:C:172:ILE:N	1:C:186:THR:HG22	2.11	0.45
1:C:258:LYS:HD2	1:D:247:GLN:HG2	1.97	0.45
1:C:535:ASP:C	1:C:537:SER:H	2.23	0.45
1:D:195:TYR:O	1:D:227:GLN:HA	2.16	0.45
1:C:217:SER:HB3	1:C:222:PHE:HB2	1.98	0.45
1:C:527:GLN:HG2	1:C:555:ALA:HA	1.98	0.45
1:D:39:SER:HB2	1:D:40:ARG:NE	2.30	0.45
1:A:110:ASP:HB3	1:A:112:GLN:H	1.81	0.45
1:B:276:LEU:HD23	1:B:276:LEU:O	2.16	0.45
1:C:39:SER:C	1:C:40:ARG:HD2	2.41	0.45
1:C:195:TYR:O	1:C:227:GLN:HA	2.15	0.45
1:C:449:LEU:O	1:C:450:ASN:HB2	2.16	0.45
1:C:459:VAL:HG22	1:C:460:SER:N	2.32	0.45
1:C:508:GLN:OE1	1:C:533:HIS:HE1	2.00	0.45
1:D:95:PHE:O	1:D:96:ASP:C	2.59	0.45
1:D:425:MET:HA	1:D:426:PRO:HD2	1.73	0.45
1:A:286:GLN:NE2	1:A:288:THR:HG22	2.31	0.45
1:A:724:VAL:HG13	1:B:750:HIS:CB	2.47	0.45
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.51	0.45
1:B:422:TYR:C	1:B:424:GLY:H	2.25	0.45
1:C:597:ARG:HG3	1:C:600:THR:HG21	1.99	0.45
1:D:74:ASN:O	1:D:92:ASN:HA	2.16	0.45
1:D:200:ASP:O	1:D:201:TRP:C	2.57	0.45
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.98	0.45
1:D:658:ARG:HD2	1:D:661:TYR:CE1	2.51	0.45
1:A:519:LEU:O	1:A:520:ASN:C	2.60	0.45
1:A:717:ALA:O	1:B:736:THR:HG21	2.16	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.59	0.45
1:C:78:VAL:HG12	1:C:87:SER:O	2.16	0.45
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.60	0.45
1:D:170:ASN:ND2	1:D:170:ASN:N	2.64	0.45
1:A:661:TYR:CD2	1:A:715:GLN:HG2	2.52	0.45
1:C:123:GLN:HG2	1:C:124:TRP:CD2	2.52	0.45
1:C:136:ASP:OD1	1:C:138:ASN:HB2	2.17	0.45
1:C:237:GLU:HG2	1:C:253:ARG:HB3	1.98	0.45
1:C:289:ALA:HA	1:C:294:LEU:HG	1.99	0.45
1:C:341:VAL:C	1:C:343:ARG:N	2.67	0.45
1:C:614:SER:HA	1:C:619:VAL:CB	2.42	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLN:HA	1:B:308:GLN:OE1	2.17	0.45
1:B:319:ILE:C	1:B:321:ASN:H	2.24	0.45
1:B:322:TYR:CE2	1:B:348:MET:HE2	2.52	0.45
1:D:39:SER:HB2	1:D:40:ARG:HE	1.82	0.45
1:D:108:SER:C	1:D:110:ASP:N	2.71	0.45
1:D:223:LEU:O	1:D:271:VAL:HG12	2.17	0.45
1:D:299:TYR:CE1	1:D:665:VAL:HG22	2.52	0.45
1:D:322:TYR:OH	1:D:346:ILE:HD13	2.15	0.45
1:B:110:ASP:HB3	1:B:112:GLN:H	1.82	0.45
1:B:377:ASN:HB3	1:B:379:GLU:H	1.82	0.45
1:C:325:MET:HE1	1:C:371:PHE:CE2	2.51	0.45
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.15	0.44
1:A:661:TYR:HD2	1:A:715:GLN:HG2	1.82	0.44
1:B:92:ASN:ND2	1:B:93:SER:H	2.11	0.44
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.63	0.44
1:B:478:PRO:HB2	1:B:497:ASN:ND2	2.32	0.44
1:C:370:SER:HB2	1:C:387:PHE:O	2.16	0.44
1:C:550:PRO:O	1:C:551:CYS:HB3	2.17	0.44
1:C:746:THR:HG21	1:D:725:ASP:HA	1.98	0.44
1:D:316:LEU:HD21	1:D:320:GLN:HG2	1.98	0.44
1:D:325:MET:HE1	1:D:371:PHE:CE2	2.53	0.44
1:A:41:LYS:O	1:A:507:VAL:HG23	2.16	0.44
1:A:154:TRP:O	1:A:166:TYR:HA	2.17	0.44
1:A:620:ASP:OD1	1:A:622:LYS:HB2	2.17	0.44
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.46	0.44
1:D:481:THR:OG1	1:D:483:HIS:HE1	2.00	0.44
1:A:285:ILE:N	1:A:285:ILE:HD12	2.31	0.44
1:B:154:TRP:O	1:B:166:TYR:HA	2.17	0.44
1:B:310:ARG:NH1	1:B:329:ASP:OD2	2.51	0.44
1:B:425:MET:HA	1:B:426:PRO:HD2	1.80	0.44
1:B:543:LEU:HD12	1:B:567:LEU:HD13	1.99	0.44
1:B:627:TRP:CZ3	1:B:755:MET:HE1	2.53	0.44
1:C:200:ASP:O	1:C:201:TRP:C	2.60	0.44
1:C:327:ILE:HB	1:C:343:ARG:HG2	1.98	0.44
1:A:446:SER:HB2	1:A:457:TYR:CD1	2.53	0.44
1:A:627:TRP:CZ3	1:A:755:MET:HE1	2.52	0.44
1:B:39:SER:CB	1:B:40:ARG:NE	2.68	0.44
1:B:620:ASP:C	1:B:622:LYS:H	2.25	0.44
1:C:689:MET:HG3	1:D:244:GLU:CD	2.42	0.44
1:D:65:ASP:HB2	1:D:463:LYS:HB2	1.99	0.44
1:D:123:GLN:HG2	1:D:124:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:ASN:N	1:D:381:TYR:O	2.51	0.44
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.48	0.44
1:B:634:TYR:HD1	1:B:656:VAL:O	2.00	0.44
1:C:367:ASP:OD2	1:C:369:ASN:OD1	2.35	0.44
1:D:124:TRP:HB2	1:D:204:GLU:OE2	2.18	0.44
1:D:171:ASP:HA	1:D:186:THR:CG2	2.48	0.44
1:D:327:ILE:HB	1:D:343:ARG:HG2	1.98	0.44
1:D:535:ASP:OD1	1:D:537:SER:HB3	2.17	0.44
1:A:458:SER:OG	1:A:471:ARG:HB2	2.17	0.44
1:B:286:GLN:NE2	1:B:288:THR:HG22	2.32	0.44
1:B:289:ALA:HA	1:B:294:LEU:HD11	1.99	0.44
1:B:334:SER:C	1:B:336:ARG:H	2.26	0.44
1:B:726:VAL:O	1:B:726:VAL:CG1	2.65	0.44
1:D:259:ALA:HB3	1:D:660:GLU:HA	1.98	0.44
1:D:448:GLU:O	1:D:449:LEU:C	2.61	0.44
1:A:66:HIS:ND1	1:A:66:HIS:N	2.65	0.44
1:A:74:ASN:C	1:A:92:ASN:CB	2.88	0.44
1:A:420:ASN:HB2	1:A:426:PRO:HA	1.98	0.44
1:B:74:ASN:C	1:B:92:ASN:CB	2.88	0.44
1:B:272:ASN:C	1:B:274:ASP:H	2.26	0.44
1:B:458:SER:OG	1:B:471:ARG:HB2	2.17	0.44
1:C:482:LEU:C	1:C:483:HIS:ND1	2.75	0.44
1:C:691:ARG:HG3	1:C:691:ARG:HH11	1.81	0.44
1:C:726:VAL:HG12	1:C:726:VAL:O	2.16	0.44
1:D:314:GLN:HE22	1:D:373:LYS:HZ1	1.65	0.44
1:D:514:LEU:HD12	1:D:557:THR:CG2	2.47	0.44
1:D:703:ILE:HG12	1:D:733:MET:HB3	2.00	0.44
1:A:146:GLU:O	1:A:175:LYS:HE2	2.18	0.44
1:A:332:GLU:OE1	1:A:332:GLU:HA	2.18	0.44
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.53	0.44
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.99	0.44
1:B:127:SER:HB3	1:B:211:TYR:CG	2.53	0.44
1:B:519:LEU:O	1:B:520:ASN:C	2.60	0.44
1:C:177:GLU:HG3	1:C:180:LEU:HD22	1.98	0.44
1:A:39:SER:O	1:A:40:ARG:C	2.61	0.44
1:C:90:LEU:HD22	1:C:90:LEU:O	2.18	0.44
1:C:448:GLU:O	1:C:449:LEU:C	2.59	0.44
1:D:671:MET:HE1	1:D:682:HIS:CD2	2.53	0.44
1:A:464:GLU:O	1:A:465:ALA:HB3	2.17	0.43
1:B:276:LEU:CD2	1:B:276:LEU:H	2.30	0.43
1:B:708:ASP:CG	1:B:711:VAL:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:THR:HB	1:C:569:SER:OG	2.18	0.43
1:C:303:VAL:O	1:C:303:VAL:HG22	2.18	0.43
1:D:310:ARG:HD3	1:D:327:ILE:CG2	2.48	0.43
1:B:136:ASP:O	1:B:140:ARG:HA	2.18	0.43
1:C:40:ARG:NH1	1:C:505:GLN:O	2.51	0.43
1:C:217:SER:O	1:C:218:PRO:C	2.61	0.43
1:C:481:THR:OG1	1:C:483:HIS:HE1	2.01	0.43
1:D:40:ARG:NH1	1:D:505:GLN:O	2.51	0.43
1:D:597:ARG:HA	1:D:597:ARG:HD3	1.74	0.43
1:A:175:LYS:NZ	1:A:182:SER:HB2	2.33	0.43
1:A:234:PRO:HB2	1:B:248:TYR:CE2	2.54	0.43
1:A:322:TYR:CE2	1:A:348:MET:HE2	2.53	0.43
1:A:528:MET:HG2	1:A:576:ALA:HB2	2.00	0.43
1:A:612:GLN:HE21	1:A:612:GLN:HB3	1.66	0.43
1:B:314:GLN:NE2	1:B:373:LYS:NZ	2.65	0.43
1:B:464:GLU:O	1:B:465:ALA:HB3	2.18	0.43
1:B:542:LEU:C	1:B:542:LEU:HD23	2.43	0.43
1:C:68:TYR:CD1	1:C:68:TYR:C	2.95	0.43
1:D:277:SER:O	1:D:278:SER:CB	2.60	0.43
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.99	0.43
1:A:319:ILE:C	1:A:321:ASN:H	2.24	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.83	0.43
1:B:84:GLY:O	1:B:85:ASN:C	2.61	0.43
1:B:446:SER:HB2	1:B:457:TYR:CE1	2.52	0.43
1:C:39:SER:HB2	1:C:40:ARG:NE	2.33	0.43
1:C:58:TYR:CD2	1:C:494:LEU:HB3	2.53	0.43
1:C:535:ASP:O	1:C:537:SER:N	2.51	0.43
1:D:381:TYR:N	1:D:381:TYR:CD1	2.86	0.43
1:D:622:LYS:HB2	1:D:622:LYS:NZ	2.32	0.43
1:A:76:ILE:CD1	1:A:90:LEU:HD11	2.37	0.43
1:A:422:TYR:C	1:A:424:GLY:H	2.25	0.43
1:B:438:ASP:OD2	1:B:441:LYS:HG3	2.17	0.43
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.41	0.43
1:C:751:ILE:O	1:C:755:MET:HG3	2.18	0.43
1:D:78:VAL:HG12	1:D:87:SER:O	2.17	0.43
1:D:88:VAL:HG11	1:D:91:GLU:CD	2.44	0.43
1:D:147:ARG:HH11	1:D:147:ARG:CG	2.24	0.43
1:D:334:SER:HB3	1:D:336:ARG:HD2	1.99	0.43
1:A:109:PRO:HG2	1:A:161:GLY:O	2.18	0.43
1:B:90:LEU:HD22	1:B:90:LEU:C	2.44	0.43
1:C:40:ARG:HB2	1:C:506:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:VAL:HG22	1:C:272:ASN:N	2.33	0.43
1:D:535:ASP:O	1:D:537:SER:N	2.51	0.43
1:A:90:LEU:HD22	1:A:90:LEU:C	2.44	0.43
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.54	0.43
1:A:634:TYR:HD1	1:A:656:VAL:O	2.02	0.43
1:A:651:ILE:CG2	1:A:755:MET:HE3	2.41	0.43
1:B:388:GLN:CB	1:B:391:LYS:HB2	2.48	0.43
1:B:567:LEU:O	1:B:571:GLU:HB2	2.18	0.43
1:B:600:THR:OG1	1:B:601:PHE:N	2.50	0.43
1:C:65:ASP:HA	1:C:462:SER:HB2	2.01	0.43
1:C:110:ASP:OD2	1:C:162:HIS:HB3	2.18	0.43
1:C:310:ARG:HD3	1:C:327:ILE:CG2	2.49	0.43
1:C:319:ILE:C	1:C:321:ASN:H	2.24	0.43
1:D:93:SER:O	1:D:94:THR:C	2.62	0.43
1:D:163:LYS:NZ	1:D:273:THR:OG1	2.50	0.43
1:D:703:ILE:HA	1:D:733:MET:O	2.19	0.43
1:A:277:SER:OG	1:A:280:THR:CB	2.66	0.43
1:C:93:SER:O	1:C:94:THR:C	2.62	0.43
1:C:322:TYR:OH	1:C:346:ILE:HD13	2.18	0.43
1:D:482:LEU:C	1:D:483:HIS:ND1	2.76	0.43
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.19	0.43
1:A:478:PRO:HB2	1:A:497:ASN:ND2	2.34	0.43
1:A:524:PHE:CD2	1:A:580:GLY:HA2	2.53	0.43
1:B:661:TYR:CD2	1:B:715:GLN:HG2	2.53	0.43
1:C:153:GLN:HE22	1:C:170:ASN:HD22	1.60	0.43
1:C:520:ASN:O	1:C:521:GLU:HB2	2.19	0.43
1:C:546:VAL:CG2	1:C:547:TYR:N	2.81	0.43
1:A:540:TYR:CD1	1:A:540:TYR:N	2.86	0.43
1:C:203:TYR:HA	1:C:207:VAL:CG1	2.48	0.43
1:C:316:LEU:HD21	1:C:320:GLN:CG	2.49	0.43
1:C:658:ARG:HD2	1:C:661:TYR:CE1	2.53	0.43
1:A:276:LEU:CD2	1:A:276:LEU:N	2.81	0.42
1:A:334:SER:C	1:A:336:ARG:H	2.27	0.42
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.19	0.42
1:B:661:TYR:HD2	1:B:715:GLN:HG2	1.84	0.42
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.86	0.42
1:C:703:ILE:HG12	1:C:733:MET:HB3	2.01	0.42
1:D:597:ARG:HG3	1:D:600:THR:HG21	2.01	0.42
1:D:704:HIS:CE1	1:D:711:VAL:O	2.69	0.42
1:A:75:ASN:N	1:A:92:ASN:HB3	2.34	0.42
1:A:270:VAL:HG11	1:A:337:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PRO:O	1:A:553:GLN:NE2	2.50	0.42
1:B:171:ASP:HA	1:B:186:THR:HG21	2.01	0.42
1:B:221:THR:HG23	1:B:274:ASP:OD2	2.19	0.42
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.01	0.42
1:C:177:GLU:HB2	1:C:180:LEU:HB2	2.00	0.42
1:C:244:GLU:HG3	1:D:689:MET:HE3	2.00	0.42
1:C:386:TYR:O	1:C:394:CYS:HB2	2.19	0.42
1:C:514:LEU:HD12	1:C:557:THR:CG2	2.48	0.42
1:D:115:LEU:HD12	1:D:115:LEU:HA	1.89	0.42
1:D:217:SER:O	1:D:218:PRO:C	2.62	0.42
1:D:367:ASP:OD2	1:D:369:ASN:OD1	2.37	0.42
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.84	0.42
1:B:486:VAL:HG13	1:B:487:ASN:N	2.35	0.42
1:C:89:PHE:CE1	1:C:107:ILE:HD13	2.54	0.42
1:C:171:ASP:HA	1:C:186:THR:CG2	2.49	0.42
1:C:331:ASP:CB	1:C:334:SER:HB2	2.44	0.42
1:D:68:TYR:CD1	1:D:68:TYR:C	2.97	0.42
1:D:90:LEU:HD22	1:D:90:LEU:O	2.19	0.42
1:D:289:ALA:HA	1:D:294:LEU:HG	2.02	0.42
1:B:160:VAL:CG2	1:B:161:GLY:N	2.82	0.42
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.44	0.42
1:D:314:GLN:HE22	1:D:373:LYS:NZ	2.17	0.42
1:D:341:VAL:CG2	1:D:342:ALA:N	2.82	0.42
1:D:684:ARG:HA	1:D:684:ARG:HD3	1.85	0.42
1:A:600:THR:OG1	1:A:601:PHE:N	2.52	0.42
1:B:270:VAL:HG11	1:B:337:TRP:CZ2	2.54	0.42
1:C:421:GLU:O	1:C:422:TYR:C	2.63	0.42
1:C:551:CYS:HB2	1:C:591:MET:SD	2.60	0.42
1:C:689:MET:HB3	1:C:722:ALA:HB2	2.01	0.42
1:D:540:TYR:N	1:D:540:TYR:CD1	2.87	0.42
1:D:689:MET:HB3	1:D:722:ALA:HB2	2.00	0.42
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.34	0.42
1:A:736:THR:CG2	1:B:720:SER:OG	2.67	0.42
1:B:535:ASP:OD1	1:B:537:SER:HB3	2.19	0.42
1:C:177:GLU:CB	1:C:180:LEU:HD22	2.49	0.42
1:C:675:THR:HB	1:C:676:PRO:HD2	2.02	0.42
1:D:277:SER:OG	1:D:280:THR:HB	2.20	0.42
1:A:272:ASN:C	1:A:272:ASN:ND2	2.74	0.42
1:C:259:ALA:HB3	1:C:660:GLU:HA	2.01	0.42
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.45	0.42
1:D:42:THR:HB	1:D:569:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:VAL:CG2	1:D:547:TYR:N	2.82	0.42
1:A:627:TRP:HB2	1:A:651:ILE:HB	2.01	0.42
1:B:540:TYR:CD1	1:B:540:TYR:N	2.87	0.42
1:C:74:ASN:O	1:C:92:ASN:HA	2.19	0.42
1:C:231:THR:HG22	1:C:232:GLU:HG3	2.00	0.42
1:C:603:VAL:HG22	1:C:604:GLU:N	2.35	0.42
1:C:704:HIS:CE1	1:C:711:VAL:O	2.72	0.42
1:D:147:ARG:HG2	1:D:147:ARG:NH1	2.27	0.42
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.19	0.42
1:A:322:TYR:CD2	1:A:348:MET:HE2	2.55	0.42
1:A:331:ASP:OD1	1:A:331:ASP:C	2.63	0.42
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.35	0.42
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.45	0.42
1:B:331:ASP:OD1	1:B:331:ASP:C	2.63	0.42
1:B:332:GLU:HA	1:B:332:GLU:OE1	2.19	0.42
1:B:620:ASP:OD1	1:B:622:LYS:HB2	2.20	0.42
1:C:341:VAL:CG2	1:C:342:ALA:N	2.81	0.42
1:C:438:ASP:OD2	1:C:441:LYS:HG3	2.19	0.42
1:C:684:ARG:HA	1:C:684:ARG:HD3	1.85	0.42
1:C:703:ILE:HA	1:C:733:MET:O	2.19	0.42
1:D:186:THR:HG21	1:D:196:ASN:CB	2.50	0.42
1:D:276:LEU:H	1:D:276:LEU:HD23	1.77	0.42
1:D:438:ASP:OD2	1:D:441:LYS:HG3	2.20	0.42
1:A:486:VAL:HG13	1:A:487:ASN:N	2.34	0.41
1:A:567:LEU:O	1:A:571:GLU:HB2	2.20	0.41
1:B:285:ILE:N	1:B:285:ILE:CD1	2.83	0.41
1:C:312:SER:HA	1:C:326:ASP:O	2.20	0.41
1:C:381:TYR:N	1:C:381:TYR:CD1	2.87	0.41
1:C:595:ASN:C	1:C:597:ARG:N	2.76	0.41
1:D:535:ASP:C	1:D:537:SER:N	2.78	0.41
1:A:77:LEU:HD23	1:A:88:VAL:HA	2.01	0.41
1:B:60:LEU:HD12	1:B:60:LEU:O	2.18	0.41
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.55	0.41
1:B:242:SER:CB	1:B:246:LEU:HD12	2.44	0.41
1:B:502:LYS:O	1:B:505:GLN:HG2	2.20	0.41
1:C:415:LEU:C	1:C:415:LEU:CD1	2.93	0.41
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.82	0.41
1:D:726:VAL:O	1:D:726:VAL:CG1	2.67	0.41
1:A:285:ILE:N	1:A:285:ILE:CD1	2.83	0.41
1:B:175:LYS:NZ	1:B:182:SER:HB2	2.35	0.41
1:B:598:LEU:HD22	1:B:631:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:TYR:HE1	1:C:335:GLY:O	2.03	0.41
1:D:422:TYR:CE2	1:D:423:LYS:HD3	2.55	0.41
1:A:725:ASP:HA	1:B:746:THR:HG21	2.03	0.41
1:B:76:ILE:CD1	1:B:90:LEU:HD11	2.42	0.41
1:C:124:TRP:HB2	1:C:204:GLU:OE2	2.19	0.41
1:C:551:CYS:O	1:C:551:CYS:SG	2.78	0.41
1:B:75:ASN:N	1:B:92:ASN:HB3	2.35	0.41
1:C:88:VAL:HG11	1:C:91:GLU:CD	2.45	0.41
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.20	0.41
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.86	0.41
1:D:751:ILE:O	1:D:755:MET:HG3	2.19	0.41
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.41
1:A:242:SER:CB	1:A:246:LEU:HD12	2.44	0.41
1:C:136:ASP:O	1:C:140:ARG:N	2.54	0.41
1:D:39:SER:CB	1:D:40:ARG:HE	2.33	0.41
1:D:523:LYS:H	1:D:523:LYS:HG2	1.69	0.41
1:A:92:ASN:ND2	1:A:93:SER:H	2.11	0.41
1:A:118:TYR:CD2	1:A:119:ASN:ND2	2.88	0.41
1:B:66:HIS:ND1	1:B:66:HIS:N	2.69	0.41
1:C:377:ASN:N	1:C:381:TYR:O	2.52	0.41
1:C:540:TYR:CD1	1:C:540:TYR:N	2.88	0.41
1:D:92:ASN:ND2	1:D:93:SER:H	2.18	0.41
1:D:454:CYS:HB3	1:D:457:TYR:CZ	2.56	0.41
1:A:293:MET:HG3	1:A:298:HIS:HB3	2.03	0.41
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.85	0.41
1:C:756:SER:O	1:C:760:LYS:CG	2.69	0.41
1:D:170:ASN:HD22	1:D:170:ASN:H	1.67	0.41
1:D:291:ALA:O	1:D:295:ILE:HG23	2.21	0.41
1:A:118:TYR:CE2	1:A:119:ASN:ND2	2.88	0.41
1:A:122:LYS:CG	1:A:123:GLN:N	2.84	0.41
1:A:487:ASN:HD22	1:A:487:ASN:HA	1.64	0.41
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.36	0.41
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.55	0.41
1:B:140:ARG:NH1	1:B:140:ARG:CG	2.84	0.41
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.81	0.41
1:B:289:ALA:HA	1:B:294:LEU:CD1	2.51	0.41
1:B:528:MET:HE2	1:B:530:LEU:HD21	2.02	0.41
1:C:336:ARG:HH11	1:C:336:ARG:HG2	1.86	0.41
1:C:581:ARG:HE	1:C:605:ASP:CG	2.29	0.41
1:D:65:ASP:HA	1:D:462:SER:HB2	2.03	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:LEU:HD22	1:D:525:TRP:HE3	1.85	0.41
1:A:272:ASN:C	1:A:274:ASP:H	2.28	0.41
1:A:662:TYR:HB3	1:A:667:THR:OG1	2.21	0.41
1:A:736:THR:O	1:A:737:ASP:HB2	2.21	0.41
1:B:68:TYR:CD1	1:B:68:TYR:C	2.98	0.41
1:B:167:VAL:HG21	1:B:198:ILE:HG23	2.02	0.41
1:B:277:SER:OG	1:B:280:THR:HB	2.21	0.41
1:B:310:ARG:HH12	1:B:343:ARG:NH1	2.18	0.41
1:B:487:ASN:O	1:B:488:ASP:HB2	2.21	0.41
1:D:89:PHE:HD1	1:D:90:LEU:HD12	1.85	0.41
1:D:128:TYR:CD1	1:D:128:TYR:C	2.99	0.41
1:D:193:ILE:HG22	1:D:194:ILE:HG13	2.03	0.41
1:D:612:GLN:HE21	1:D:612:GLN:HB3	1.65	0.41
1:D:654:ALA:N	1:D:655:PRO:CD	2.84	0.41
1:A:62:TRP:CG	1:A:462:SER:HA	2.56	0.40
1:A:127:SER:HB3	1:A:211:TYR:CG	2.56	0.40
1:A:171:ASP:HA	1:A:186:THR:HG21	2.04	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.93	0.40
1:A:595:ASN:C	1:A:597:ARG:N	2.79	0.40
1:B:118:TYR:CD2	1:B:119:ASN:ND2	2.90	0.40
1:C:92:ASN:ND2	1:C:93:SER:H	2.18	0.40
1:C:319:ILE:O	1:C:321:ASN:N	2.47	0.40
1:C:334:SER:HB3	1:C:336:ARG:HD2	2.00	0.40
1:D:152:THR:HG23	1:D:167:VAL:O	2.21	0.40
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.86	0.40
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.81	0.40
1:B:236:ILE:O	1:B:253:ARG:HA	2.22	0.40
1:B:301:CYS:O	1:B:302:ASP:HB2	2.21	0.40
1:C:115:LEU:HD12	1:C:134:ILE:HG12	2.02	0.40
1:D:231:THR:HG22	1:D:232:GLU:HG3	2.03	0.40
1:A:301:CYS:O	1:A:302:ASP:HB2	2.20	0.40
1:B:662:TYR:HB3	1:B:667:THR:OG1	2.21	0.40
1:B:756:SER:O	1:B:760:LYS:HG2	2.21	0.40
1:C:39:SER:HB2	1:C:40:ARG:HE	1.86	0.40
1:C:74:ASN:HB3	1:C:92:ASN:HB3	2.04	0.40
1:C:477:LEU:HD12	1:C:501:ASP:HB2	2.02	0.40
1:C:522:THR:CG2	1:C:523:LYS:N	2.85	0.40
1:D:125:ARG:HG2	1:D:126:HIS:CE1	2.55	0.40
1:A:70:TYR:HB3	1:A:79:PHE:CE2	2.57	0.40
1:A:93:SER:O	1:A:94:THR:C	2.63	0.40
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HD12	1:A:557:THR:CG2	2.48	0.40
1:B:509:MET:HE3	1:B:510:PRO:HD2	2.03	0.40
1:B:581:ARG:NE	1:B:605:ASP:OD2	2.47	0.40
1:C:286:GLN:HE21	1:C:288:THR:HG22	1.86	0.40
1:C:316:LEU:HD21	1:C:320:GLN:HG2	2.04	0.40
1:C:750:HIS:CD2	1:D:724:VAL:HA	2.56	0.40
1:D:69:LEU:CD1	1:D:107:ILE:HD12	2.52	0.40
1:D:160:VAL:HG23	1:D:161:GLY:N	2.36	0.40
1:D:183:TYR:CD2	1:D:276:LEU:HG	2.56	0.40
1:A:334:SER:HB2	1:A:336:ARG:HD2	2.04	0.40
1:A:459:VAL:CG2	1:A:460:SER:N	2.82	0.40
1:A:598:LEU:HD22	1:A:631:TYR:OH	2.21	0.40
1:A:620:ASP:C	1:A:622:LYS:N	2.78	0.40
1:B:92:ASN:C	1:B:92:ASN:ND2	2.77	0.40
1:B:336:ARG:HD2	1:B:336:ARG:H	1.86	0.40
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.57	0.40
1:C:55:LEU:HD23	1:C:500:LEU:HD22	2.04	0.40
1:C:514:LEU:HD23	1:C:526:TYR:O	2.22	0.40
1:D:95:PHE:HB3	1:D:98:PHE:HB2	2.02	0.40
1:D:330:TYR:HE1	1:D:335:GLY:O	2.04	0.40
1:D:522:THR:CG2	1:D:523:LYS:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	724/728 (100%)	647 (89%)	69 (10%)	8 (1%)	11	36
1	B	724/728 (100%)	650 (90%)	65 (9%)	9 (1%)	10	34
1	C	724/728 (100%)	643 (89%)	68 (9%)	13 (2%)	6	23
1	D	724/728 (100%)	643 (89%)	67 (9%)	14 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2896/2912 (100%)	2583 (89%)	269 (9%)	44 (2%)	8	28

All (44) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	D	334	SER
1	D	463	LYS
1	B	94	THR
1	B	273	THR
1	C	218	PRO
1	D	450	ASN
1	D	218	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/653 (100%)	606 (93%)	45 (7%)	14	41
1	B	651/653 (100%)	606 (93%)	45 (7%)	14	41
1	C	651/653 (100%)	603 (93%)	48 (7%)	13	37
1	D	651/653 (100%)	601 (92%)	50 (8%)	12	36
All	All	2604/2612 (100%)	2416 (93%)	188 (7%)	13	39

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	75	ASN
1	A	90	LEU
1	A	92	ASN
1	A	110	ASP
1	A	140	ARG
1	A	141	GLN
1	A	145	GLU
1	A	170	ASN
1	A	184	ARG
1	A	207	VAL
1	A	209	SER
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	231	THR
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	276	LEU
1	A	293	MET
1	A	303	VAL
1	A	313	LEU
1	A	326	ASP
1	A	336	ARG
1	A	376	SER
1	A	385	CYS
1	A	388	GLN
1	A	413	ASP
1	A	436	LEU
1	A	440	THR
1	A	442	VAL
1	A	448	GLU
1	A	482	LEU
1	A	487	ASN
1	A	514	LEU
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	603	VAL
1	A	608	GLU
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	736	THR
1	A	761	GLN
1	B	39	SER
1	B	40	ARG
1	B	75	ASN
1	B	90	LEU
1	B	92	ASN
1	B	110	ASP
1	B	140	ARG
1	B	141	GLN
1	B	145	GLU
1	B	170	ASN
1	B	184	ARG

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Mol	Chain	Res	Type
1	B	207	VAL
1	B	209	SER
1	B	231	THR
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	276	LEU
1	B	293	MET
1	B	303	VAL
1	B	313	LEU
1	B	326	ASP
1	B	336	ARG
1	B	376	SER
1	B	385	CYS
1	B	388	GLN
1	B	413	ASP
1	B	436	LEU
1	B	440	THR
1	B	442	VAL
1	B	448	GLU
1	B	482	LEU
1	B	485	SER
1	B	487	ASN
1	B	514	LEU
1	B	536	LYS
1	B	543	LEU
1	B	561	LEU
1	B	603	VAL
1	B	608	GLU
1	B	689	MET
1	B	701	LEU
1	B	702	LEU
1	B	736	THR
1	B	761	GLN
1	C	40	ARG
1	C	75	ASN
1	C	90	LEU
1	C	92	ASN
1	C	97	GLU
1	C	110	ASP
1	C	140	ARG
1	C	141	GLN

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Mol	Chain	Res	Type
1	C	145	GLU
1	C	147	ARG
1	C	170	ASN
1	C	184	ARG
1	C	207	VAL
1	C	209	SER
1	C	221	THR
1	C	246	LEU
1	C	253	ARG
1	C	254	VAL
1	C	276	LEU
1	C	293	MET
1	C	303	VAL
1	C	313	LEU
1	C	326	ASP
1	C	336	ARG
1	C	388	GLN
1	C	415	LEU
1	C	436	LEU
1	C	440	THR
1	C	448	GLU
1	C	482	LEU
1	C	498	SER
1	C	507	VAL
1	C	514	LEU
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU
1	C	546	VAL
1	C	561	LEU
1	C	597	ARG
1	C	603	VAL
1	C	608	GLU
1	C	622	LYS
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	736	THR
1	C	760	LYS
1	C	761	GLN
1	D	40	ARG
1	D	75	ASN

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Mol	Chain	Res	Type
1	D	90	LEU
1	D	92	ASN
1	D	97	GLU
1	D	110	ASP
1	D	140	ARG
1	D	141	GLN
1	D	145	GLU
1	D	147	ARG
1	D	170	ASN
1	D	184	ARG
1	D	207	VAL
1	D	209	SER
1	D	221	THR
1	D	246	LEU
1	D	253	ARG
1	D	254	VAL
1	D	275	SER
1	D	276	LEU
1	D	293	MET
1	D	303	VAL
1	D	313	LEU
1	D	326	ASP
1	D	336	ARG
1	D	373	LYS
1	D	388	GLN
1	D	415	LEU
1	D	436	LEU
1	D	440	THR
1	D	448	GLU
1	D	482	LEU
1	D	498	SER
1	D	507	VAL
1	D	514	LEU
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	546	VAL
1	D	561	LEU
1	D	597	ARG
1	D	603	VAL
1	D	608	GLU
1	D	622	LYS

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Mol	Chain	Res	Type
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	736	THR
1	D	760	LYS
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	92	ASN
1	A	119	ASN
1	A	138	ASN
1	A	150	ASN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	286	GLN
1	A	314	GLN
1	A	338	ASN
1	A	344	GLN
1	A	369	ASN
1	A	388	GLN
1	A	455	GLN
1	A	483	HIS
1	A	487	ASN
1	A	612	GLN
1	A	679	ASN
1	A	685	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	748	HIS
1	A	761	GLN
1	B	72	GLN
1	B	92	ASN
1	B	119	ASN
1	B	138	ASN
1	B	150	ASN
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	286	GLN
1	B	314	GLN
1	B	338	ASN
1	B	344	GLN
1	B	388	GLN
1	B	455	GLN
1	B	483	HIS
1	B	487	ASN
1	B	612	GLN
1	B	679	ASN
1	B	685	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	748	HIS
1	B	761	GLN
1	C	72	GLN
1	C	75	ASN
1	C	123	GLN
1	C	169	ASN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	286	GLN
1	C	314	GLN
1	C	338	ASN
1	C	369	ASN
1	C	388	GLN
1	C	483	HIS
1	C	487	ASN
1	C	505	GLN
1	C	520	ASN
1	C	533	HIS
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	685	ASN
1	C	694	ASN
1	C	704	HIS

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Mol	Chain	Res	Type
1	C	718	GLN
1	C	761	GLN
1	D	72	GLN
1	D	75	ASN
1	D	123	GLN
1	D	169	ASN
1	D	170	ASN
1	D	247	GLN
1	D	272	ASN
1	D	286	GLN
1	D	314	GLN
1	D	338	ASN
1	D	369	ASN
1	D	388	GLN
1	D	430	ASN
1	D	483	HIS
1	D	487	ASN
1	D	505	GLN
1	D	520	ASN
1	D	533	HIS
1	D	572	ASN
1	D	612	GLN
1	D	679	ASN
1	D	685	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	731	GLN
1	D	761	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GGO	B	901	-	31,31,31	1.81	5 (16%)	41,45,45	1.16	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GGO	B	901	-	-	0/9/31/31	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	GGO	C16-N4	4.83	1.40	1.34
2	B	901	GGO	C18-C16	4.24	1.57	1.51
2	B	901	GGO	C8-C7	4.14	1.47	1.38
2	B	901	GGO	C20-C27	3.22	1.43	1.38
2	B	901	GGO	C5-C6	2.25	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	GGO	C-C3-N4	2.91	113.74	110.43
2	B	901	GGO	O13-C12-O	2.47	111.98	108.09
2	B	901	GGO	C12-O13-C14	-2.31	102.22	105.32
2	B	901	GGO	C12-O-C10	-2.30	102.24	105.32

There are no chirality outliers.

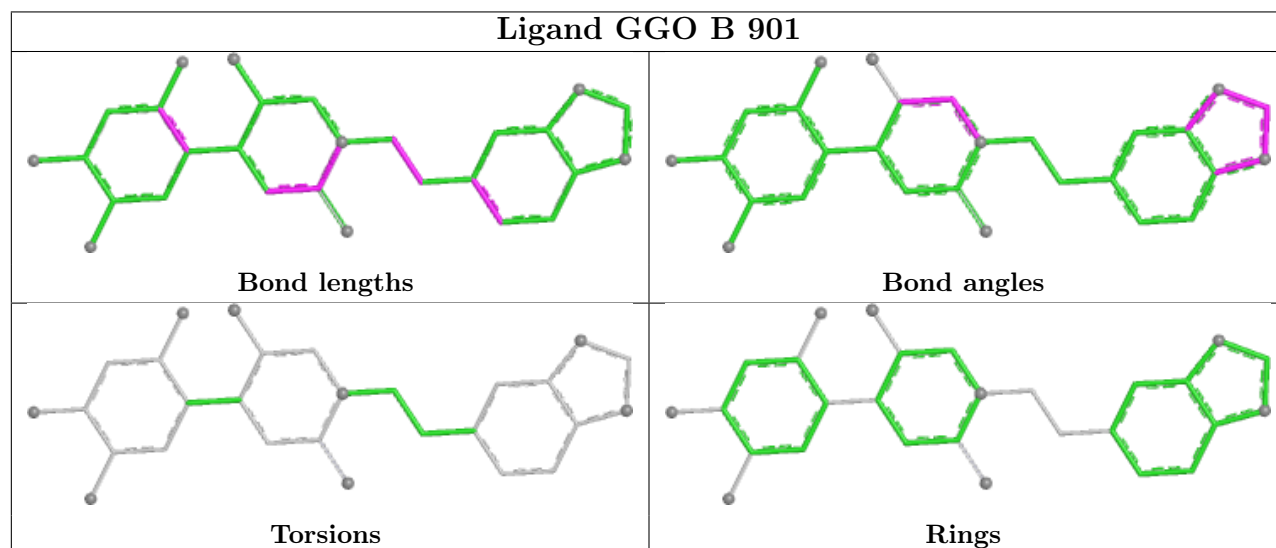
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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, 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	726/728 (99%)	0.41	49 (6%)	24	17	3, 27, 62, 153	0
1	B	726/728 (99%)	0.47	59 (8%)	18	13	6, 28, 68, 116	0
1	C	726/728 (99%)	0.31	29 (3%)	42	33	5, 33, 69, 111	0
1	D	726/728 (99%)	0.33	46 (6%)	26	19	10, 31, 66, 146	0
All	All	2904/2912 (99%)	0.38	183 (6%)	26	19	3, 29, 67, 153	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	LYS	8.0
1	A	278	SER	7.7
1	A	280	THR	6.8
1	A	282	ALA	6.4
1	D	71	LYS	6.2
1	A	281	ASN	6.2
1	A	279	VAL	5.9
1	B	105	TYR	5.5
1	B	280	THR	5.2
1	C	71	LYS	5.1
1	A	487	ASN	5.1
1	A	277	SER	4.9
1	B	61	ARG	4.8
1	A	333	SER	4.7
1	C	105	TYR	4.7
1	D	621	ASN	4.6
1	B	764	SER	4.6
1	D	111	GLY	4.5
1	D	91	GLU	4.4
1	D	361	GLU	4.3
1	A	71	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	332	GLU	4.3
1	B	289	ALA	4.0
1	C	277	SER	4.0
1	D	764	SER	4.0
1	A	489	LYS	3.9
1	A	764	SER	3.9
1	B	278	SER	3.7
1	D	39	SER	3.7
1	C	39	SER	3.7
1	A	138	ASN	3.7
1	C	392	LYS	3.6
1	D	61	ARG	3.6
1	D	278	SER	3.6
1	B	413	ASP	3.6
1	A	342	ALA	3.6
1	B	615	LYS	3.5
1	B	336	ARG	3.5
1	D	66	HIS	3.5
1	B	39	SER	3.5
1	D	40	ARG	3.5
1	B	342	ALA	3.5
1	B	66	HIS	3.4
1	A	72	GLN	3.4
1	D	141	GLN	3.4
1	D	281	ASN	3.4
1	A	366	LEU	3.4
1	A	392	LYS	3.4
1	B	72	GLN	3.4
1	A	73	GLU	3.3
1	A	437	SER	3.3
1	C	764	SER	3.3
1	B	341	VAL	3.3
1	A	74	ASN	3.3
1	A	140	ARG	3.3
1	C	361	GLU	3.3
1	C	538	LYS	3.3
1	B	114	ILE	3.3
1	D	277	SER	3.2
1	A	114	ILE	3.2
1	D	289	ALA	3.2
1	B	487	ASN	3.2
1	D	697	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	111	GLY	3.2
1	C	82	GLU	3.2
1	D	105	TYR	3.1
1	D	89	PHE	3.1
1	D	139	LYS	3.1
1	B	63	ILE	3.1
1	B	343	ARG	3.1
1	A	141	GLN	3.1
1	D	489	LYS	3.1
1	C	138	ASN	3.0
1	C	140	ARG	3.0
1	D	536	LYS	3.0
1	A	109	PRO	3.0
1	C	61	ARG	3.0
1	A	219	ASN	3.0
1	D	538	LYS	3.0
1	A	105	TYR	2.9
1	B	90	LEU	2.9
1	B	277	SER	2.9
1	B	138	ASN	2.9
1	D	88	VAL	2.9
1	D	333	SER	2.9
1	A	218	PRO	2.8
1	B	392	LYS	2.8
1	C	489	LYS	2.8
1	C	502	LYS	2.8
1	B	220	GLY	2.8
1	C	72	GLN	2.8
1	B	73	GLU	2.7
1	B	76	ILE	2.7
1	B	414	TYR	2.7
1	A	66	HIS	2.7
1	C	536	LYS	2.6
1	D	280	THR	2.6
1	B	74	ASN	2.6
1	A	622	LYS	2.6
1	A	289	ALA	2.6
1	D	83	TYR	2.6
1	A	441	LYS	2.6
1	B	151	ASN	2.6
1	D	506	ASN	2.6
1	C	413	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	182	SER	2.6
1	D	41	LYS	2.6
1	B	379	GLU	2.6
1	B	40	ARG	2.5
1	B	412	SER	2.5
1	D	99	GLY	2.5
1	D	279	VAL	2.5
1	D	72	GLN	2.5
1	A	377	ASN	2.5
1	A	110	ASP	2.5
1	B	104	ASP	2.5
1	D	87	SER	2.5
1	C	697	GLN	2.5
1	B	321	ASN	2.5
1	C	75	ASN	2.5
1	A	283	THR	2.5
1	B	538	LYS	2.5
1	A	520	ASN	2.5
1	D	358	ARG	2.4
1	A	505	GLN	2.4
1	D	342	ALA	2.4
1	A	506	ASN	2.4
1	B	103	ASN	2.4
1	B	102	ILE	2.4
1	B	182	SER	2.4
1	A	336	ARG	2.4
1	C	336	ARG	2.4
1	B	160	VAL	2.3
1	B	98	PHE	2.3
1	C	110	ASP	2.3
1	C	332	GLU	2.3
1	D	379	GLU	2.3
1	D	502	LYS	2.3
1	A	145	GLU	2.3
1	B	101	SER	2.3
1	B	275	SER	2.3
1	A	685	ASN	2.3
1	D	75	ASN	2.3
1	B	276	LEU	2.3
1	B	87	SER	2.3
1	A	51	ASN	2.2
1	A	537	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	2.2
1	D	437	SER	2.2
1	D	275	SER	2.2
1	A	321	ASN	2.2
1	A	413	ASP	2.2
1	D	615	LYS	2.2
1	A	232	GLU	2.2
1	C	160	VAL	2.2
1	A	538	LYS	2.2
1	C	135	TYR	2.2
1	B	452	GLU	2.2
1	C	506	ASN	2.1
1	D	92	ASN	2.1
1	B	491	LEU	2.1
1	A	697	GLN	2.1
1	B	502	LYS	2.1
1	B	186	THR	2.1
1	B	335	GLY	2.1
1	B	217	SER	2.1
1	B	54	ARG	2.1
1	B	330	TYR	2.1
1	C	101	SER	2.1
1	A	507	VAL	2.1
1	B	214	LEU	2.1
1	B	106	SER	2.0
1	D	86	SER	2.0
1	B	279	VAL	2.0
1	A	147	ARG	2.0
1	D	336	ARG	2.0
1	A	379	GLU	2.0
1	D	414	TYR	2.0
1	C	279	VAL	2.0
1	B	521	GLU	2.0
1	B	536	LYS	2.0
1	D	73	GLU	2.0
1	D	622	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

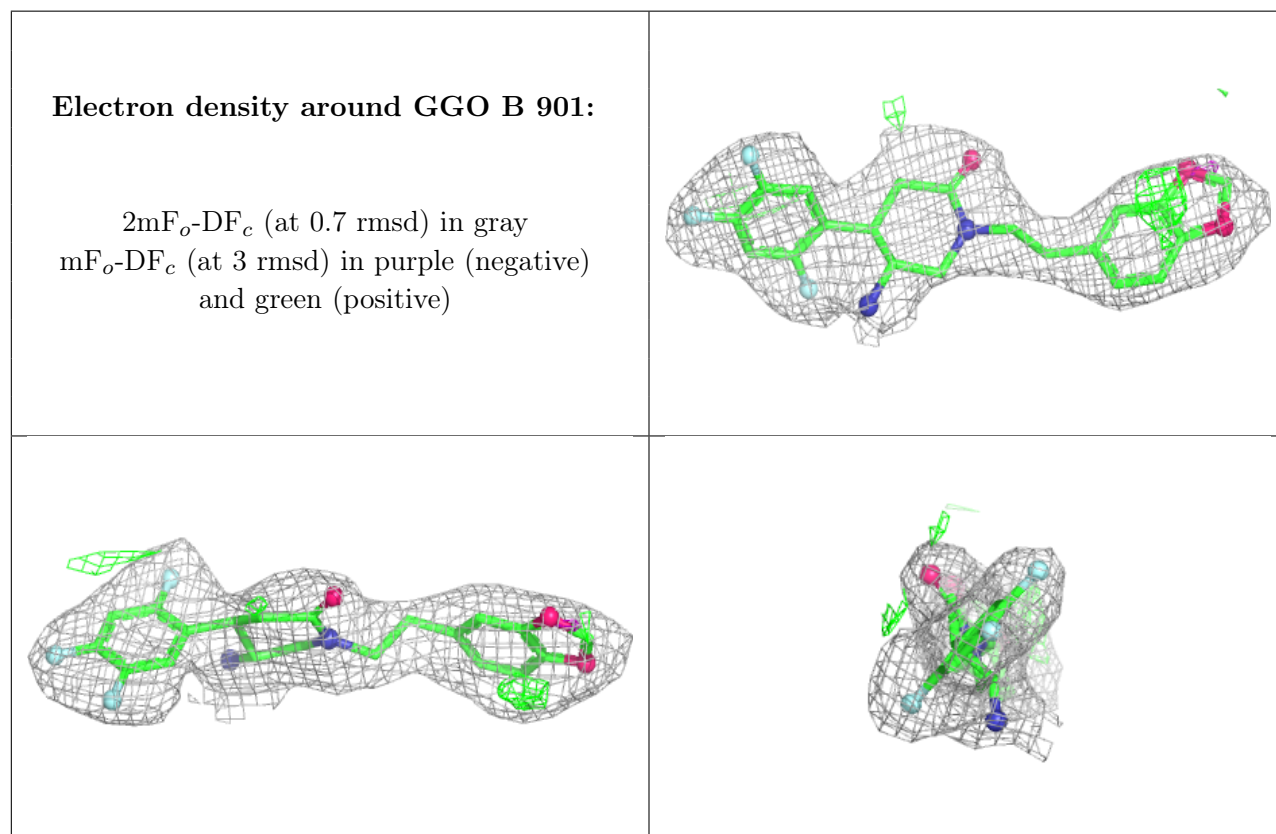
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GGO	B	901	28/28	0.90	0.13	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.