



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:14 AM UTC

PDB ID : 4QQV / pdb_00004qqv
Title : Extracellular domains of mouse IL-3 beta receptor
Authors : Jackson, C.J.; Young, I.G.; Murphy, J.M.; Carr, P.D.; Ewens, C.L.; Dai, J.;
Ollis, D.L.
Deposited on : 2014-06-30
Resolution : 3.45 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 ⓘ](#)) 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
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

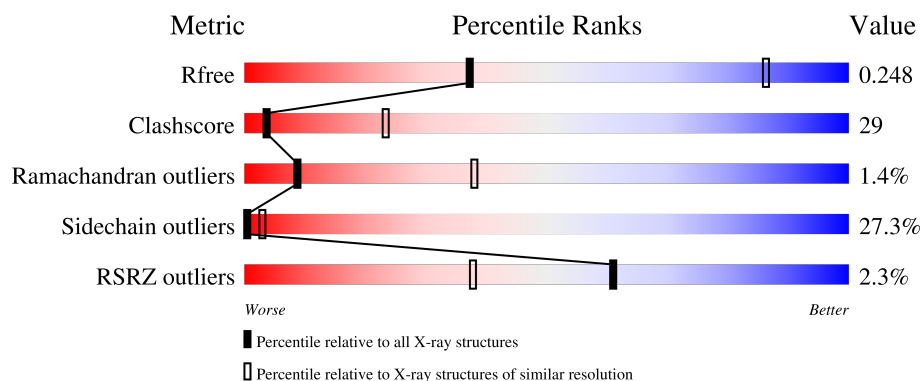
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	416	 3% 41% 38% 15% • •
1	B	416	 2% 37% 40% 17% • 5%
1	C	416	 3% 36% 41% 19% •
1	D	416	 % 31% 33% 11% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12274 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.

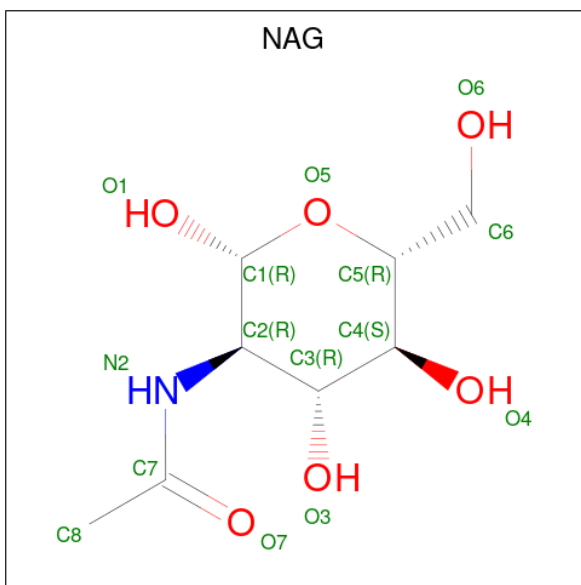
- Molecule 1 is a protein called Interleukin-3 receptor class 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3229	2045	548	619	17			
1	B	395	Total	C	N	O	S	0	0	0
			3195	2023	543	612	17			
1	C	402	Total	C	N	O	S	0	0	0
			3252	2058	552	625	17			
1	D	316	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	GLN	ASN	engineered mutation	UNP P26954
A	331	ALA	LYS	engineered mutation	UNP P26954
A	333	ALA	ARG	engineered mutation	UNP P26954
A	334	ALA	ASP	engineered mutation	UNP P26954
B	328	GLN	ASN	engineered mutation	UNP P26954
B	331	ALA	LYS	engineered mutation	UNP P26954
B	333	ALA	ARG	engineered mutation	UNP P26954
B	334	ALA	ASP	engineered mutation	UNP P26954
C	328	GLN	ASN	engineered mutation	UNP P26954
C	331	ALA	LYS	engineered mutation	UNP P26954
C	333	ALA	ARG	engineered mutation	UNP P26954
C	334	ALA	ASP	engineered mutation	UNP P26954
D	328	GLN	ASN	engineered mutation	UNP P26954
D	331	ALA	LYS	engineered mutation	UNP P26954
D	333	ALA	ARG	engineered mutation	UNP P26954
D	334	ALA	ASP	engineered mutation	UNP P26954

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

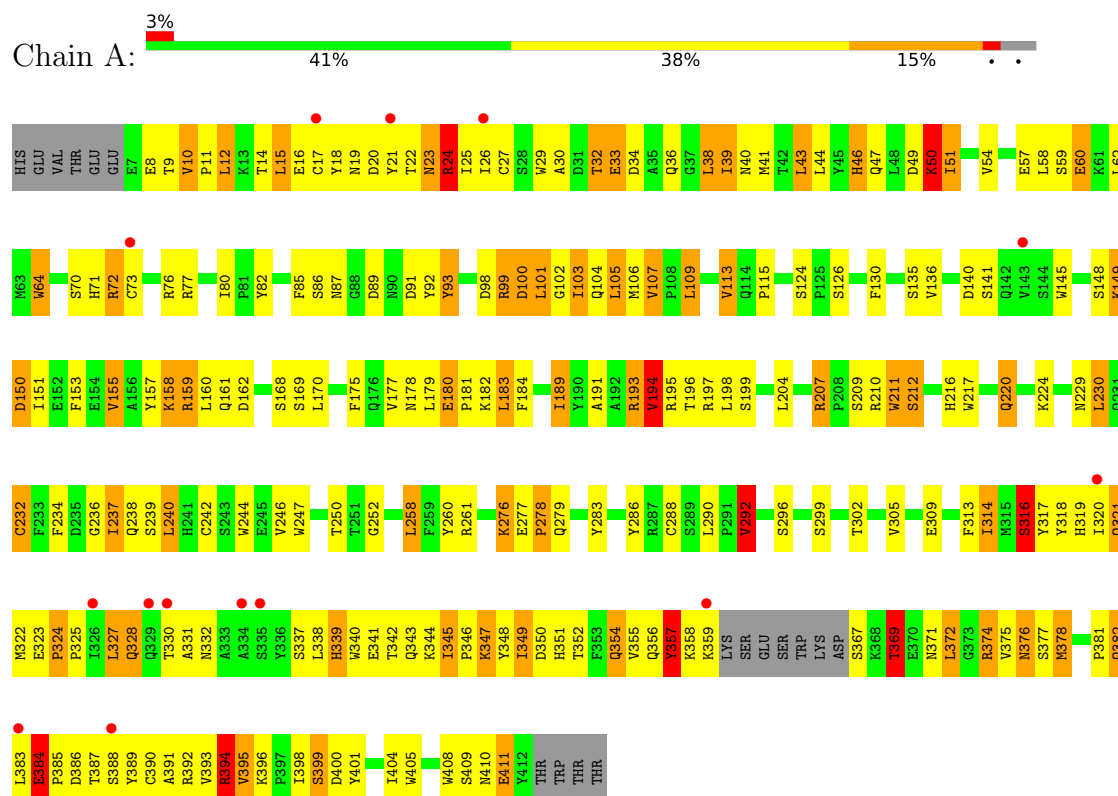


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

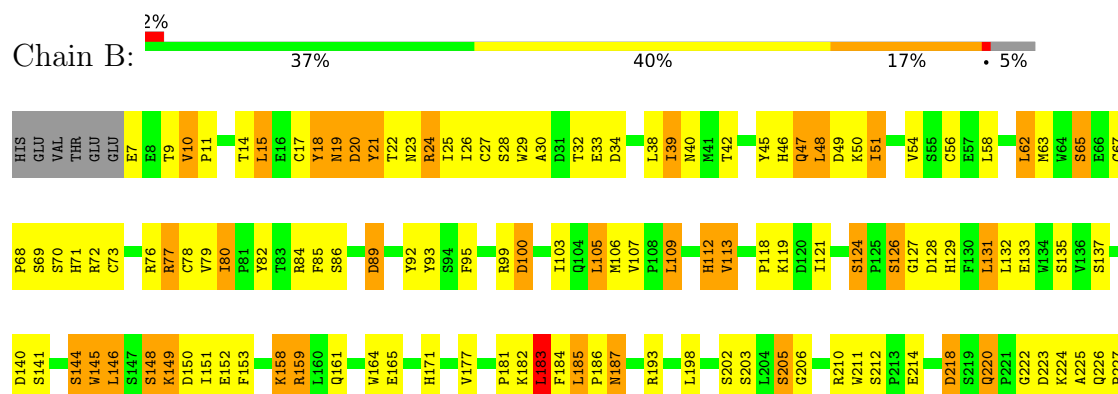
3 Residue-property plots

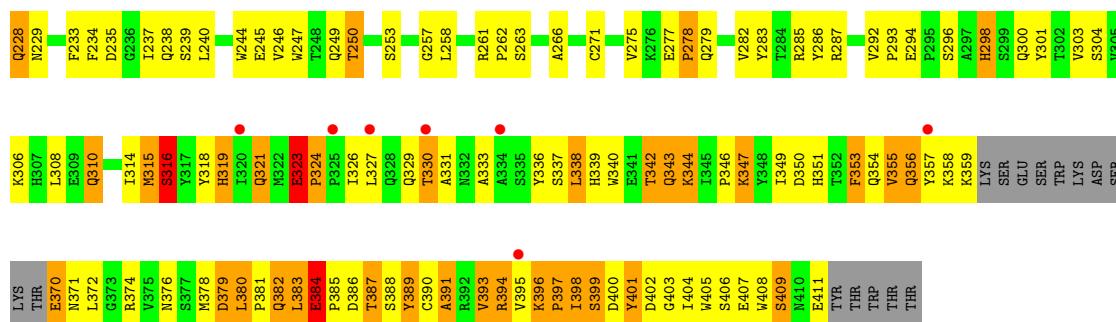
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Interleukin-3 receptor class 2 subunit beta

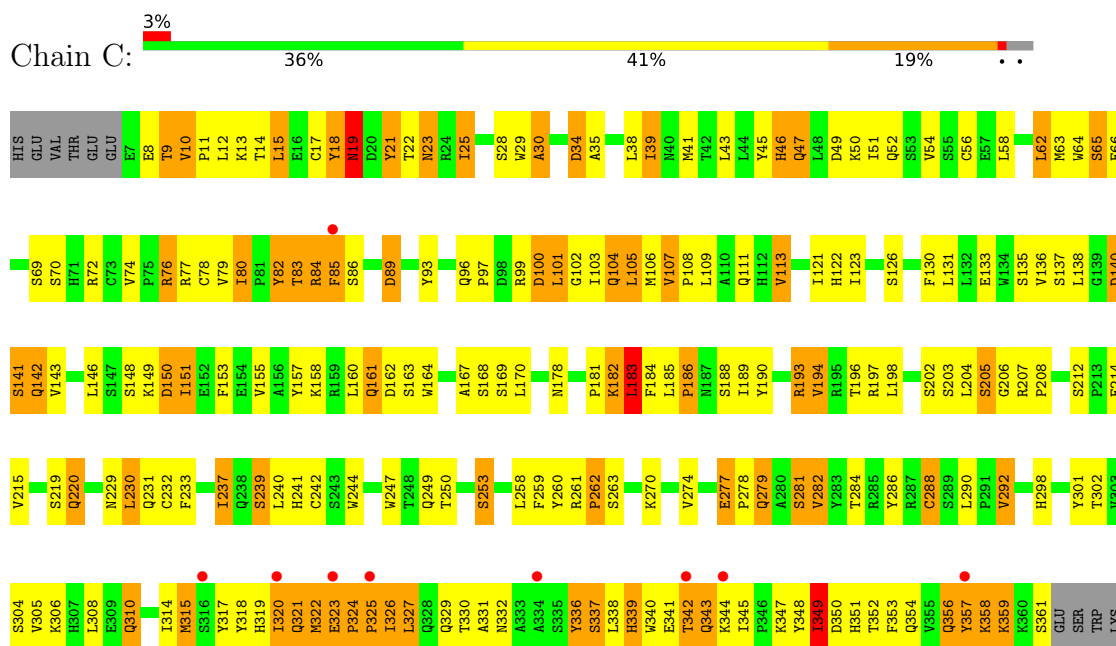


- Molecule 1: Interleukin-3 receptor class 2 subunit beta





• Molecule 1: Interleukin-3 receptor class 2 subunit beta



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.15Å 166.46Å 128.00Å 90.00° 122.77° 90.00°	Depositor
Resolution (Å)	19.91 – 3.45 19.91 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.91-3.45) 99.0 (19.91-3.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1558)	Depositor
R, R_{free}	0.203 , 0.248 0.209 , 0.248	Depositor DCC
R_{free} test set	2269 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

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

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	0.77	2/3327 (0.1%)	1.24	26/4535 (0.6%)
1	B	0.80	1/3292 (0.0%)	1.19	24/4488 (0.5%)
1	C	0.71	1/3350 (0.0%)	1.22	37/4565 (0.8%)
1	D	0.71	0/2620	1.11	17/3572 (0.5%)
All	All	0.75	4/12589 (0.0%)	1.20	104/17160 (0.6%)

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	4
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	THR	CA-CB	7.20	1.64	1.53
1	C	320	ILE	CA-CB	5.94	1.62	1.54
1	B	10	VAL	CA-C	5.92	1.57	1.52
1	A	352	THR	CA-CB	5.28	1.60	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	LYS	N-CA-C	12.74	126.36	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	THR	N-CA-C	-9.96	95.87	111.02
1	A	357	TYR	N-CA-C	8.95	119.73	108.45
1	B	50	LYS	N-CA-C	8.21	121.79	111.69
1	C	19	ASN	N-CA-C	8.15	121.78	108.26
1	A	345	ILE	CA-C-N	8.05	127.35	118.97
1	A	345	ILE	C-N-CA	8.05	127.35	118.97
1	C	321	GLN	N-CA-C	7.98	124.00	113.30
1	C	212	SER	CA-C-N	-7.60	112.50	120.03
1	C	212	SER	C-N-CA	-7.60	112.50	120.03
1	C	10	VAL	CB-CA-C	-7.53	106.36	114.35
1	C	349	ILE	N-CA-C	7.46	118.90	108.23
1	C	324	PRO	N-CA-C	7.37	119.69	110.70
1	D	50	LYS	N-CA-C	7.35	119.37	111.36
1	B	396	LYS	N-CA-C	7.27	116.50	108.14
1	A	49	ASP	N-CA-C	7.26	122.32	113.17
1	A	324	PRO	N-CA-C	7.23	119.52	110.70
1	C	46	HIS	N-CA-C	7.15	120.06	108.34
1	D	296	SER	N-CA-C	-7.00	100.08	110.23
1	C	343	GLN	CA-C-N	6.87	134.07	121.70
1	C	343	GLN	C-N-CA	6.87	134.07	121.70
1	B	38	LEU	N-CA-C	6.85	119.75	111.40
1	B	72	ARG	N-CA-C	-6.83	98.71	109.50
1	C	409	SER	N-CA-C	6.69	119.02	108.79
1	C	262	PRO	CA-C-O	-6.67	114.09	121.23
1	A	399	SER	CB-CA-C	-6.66	108.18	117.23
1	D	74	VAL	CA-C-N	6.58	126.55	120.03
1	D	74	VAL	C-N-CA	6.58	126.55	120.03
1	A	194	VAL	N-CA-C	6.37	118.20	108.71
1	C	277	GLU	CA-C-N	-6.33	112.39	118.97
1	C	277	GLU	C-N-CA	-6.33	112.39	118.97
1	C	369	THR	N-CA-C	6.25	119.65	110.59
1	D	294	GLU	CA-C-N	-6.24	112.74	119.98
1	D	294	GLU	C-N-CA	-6.24	112.74	119.98
1	B	395	VAL	N-CA-C	6.23	117.95	107.18
1	B	148	SER	N-CA-C	-6.23	103.80	111.40
1	A	395	VAL	N-CA-C	6.19	116.94	107.77
1	D	207	ARG	CA-C-N	6.19	126.22	119.90
1	D	207	ARG	C-N-CA	6.19	126.22	119.90
1	A	113	VAL	N-CA-C	6.18	116.99	108.84
1	A	337	SER	CB-CA-C	-6.14	107.78	115.89
1	B	399	SER	CB-CA-C	-6.10	109.55	116.63
1	B	324	PRO	N-CA-C	6.06	118.10	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ILE	CB-CA-C	-6.04	104.01	111.08
1	B	386	ASP	CB-CA-C	-6.01	107.93	116.34
1	A	24	ARG	N-CA-C	5.99	117.78	110.41
1	B	386	ASP	N-CA-C	5.99	116.86	108.00
1	D	226	GLN	CA-C-N	5.92	126.23	119.83
1	D	226	GLN	C-N-CA	5.92	126.23	119.83
1	C	324	PRO	C-N-CD	-5.90	100.83	125.00
1	A	102	GLY	N-CA-C	-5.85	102.60	110.56
1	C	384	GLU	N-CA-C	5.81	122.65	109.81
1	C	336	TYR	N-CA-C	5.73	115.85	108.34
1	C	384	GLU	C-N-CD	-5.71	101.58	125.00
1	C	74	VAL	CA-C-N	-5.70	114.73	120.31
1	C	74	VAL	C-N-CA	-5.70	114.73	120.31
1	B	183	LEU	N-CA-C	-5.67	106.40	113.38
1	D	281	SER	N-CA-C	-5.67	100.11	108.79
1	A	369	THR	N-CA-C	5.62	117.52	109.14
1	C	206	GLY	N-CA-C	5.61	118.35	110.38
1	C	30	ALA	N-CA-C	5.59	115.93	108.38
1	C	331	ALA	CB-CA-C	-5.53	110.18	116.54
1	B	384	GLU	N-CA-C	5.53	122.03	109.81
1	B	19	ASN	N-CA-C	5.50	118.20	109.50
1	B	171	HIS	N-CA-C	5.48	117.62	108.02
1	A	64	TRP	N-CA-C	5.48	120.07	113.17
1	C	186	PRO	CA-C-N	-5.46	113.17	122.56
1	C	186	PRO	C-N-CA	-5.46	113.17	122.56
1	B	303	VAL	N-CA-C	5.45	115.74	108.11
1	C	332	ASN	CB-CA-C	-5.43	110.33	116.63
1	A	384	GLU	CA-C-N	5.37	126.56	119.84
1	A	384	GLU	C-N-CA	5.37	126.56	119.84
1	D	306	LYS	CA-C-N	-5.36	115.54	123.05
1	D	306	LYS	C-N-CA	-5.36	115.54	123.05
1	B	225	ALA	N-CA-C	-5.34	105.51	112.23
1	A	292	VAL	CA-C-N	5.33	124.94	119.56
1	A	292	VAL	C-N-CA	5.33	124.94	119.56
1	B	343	GLN	CA-C-N	5.33	131.29	121.70
1	B	343	GLN	C-N-CA	5.33	131.29	121.70
1	B	409	SER	N-CA-C	5.30	118.09	109.24
1	A	189	ILE	N-CA-C	5.29	116.36	108.54
1	B	391	ALA	N-CA-C	5.28	117.51	108.90
1	B	296	SER	N-CA-C	-5.25	103.21	110.35
1	C	384	GLU	CA-C-N	5.25	126.41	119.84
1	C	384	GLU	C-N-CA	5.25	126.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	SER	N-CA-C	5.24	117.82	109.02
1	C	237	ILE	N-CA-C	5.24	115.05	106.72
1	B	323	GLU	N-CA-C	5.21	117.42	108.82
1	A	46	HIS	N-CA-C	5.18	117.16	107.99
1	C	380	LEU	CA-C-N	5.17	126.31	119.84
1	C	380	LEU	C-N-CA	5.17	126.31	119.84
1	C	39	ILE	N-CA-C	5.15	115.69	108.17
1	B	185	LEU	CA-C-N	5.15	126.27	119.84
1	B	185	LEU	C-N-CA	5.15	126.27	119.84
1	C	10	VAL	CA-C-N	-5.13	113.36	119.05
1	C	10	VAL	C-N-CA	-5.13	113.36	119.05
1	D	20	ASP	N-CA-C	-5.12	107.01	113.20
1	D	315	MET	CB-CA-C	-5.06	109.77	115.79
1	D	173	SER	N-CA-C	-5.03	106.92	113.16
1	C	183	LEU	N-CA-C	-5.03	107.15	113.28
1	A	10	VAL	CB-CA-C	-5.01	107.44	114.00
1	D	10	VAL	CB-CA-C	-5.01	109.04	114.35
1	C	231	GLN	N-CA-C	5.01	116.46	107.80
1	A	394	ARG	N-CA-C	5.00	116.42	108.96

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	GLU	Peptide
1	A	278	PRO	Peptide
1	A	316	SER	Peptide
1	A	384	GLU	Peptide
1	B	278	PRO	Peptide
1	B	316	SER	Peptide
1	B	384	GLU	Peptide
1	C	384	GLU	Peptide
1	C	49	ASP	Peptide
1	D	49	ASP	Peptide

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	3229	0	3067	180	0
1	B	3195	0	3035	219	0
1	C	3252	0	3089	217	0
1	D	2542	0	2413	140	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
All	All	12274	0	11656	695	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 29.

All (695) 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:B:357:TYR:HE1	1:B:391:ALA:CB	1.40	1.35
1:B:357:TYR:CE1	1:B:391:ALA:CB	2.16	1.27
1:B:357:TYR:CE1	1:B:391:ALA:HB2	1.79	1.18
1:C:169:SER:C	1:C:170:LEU:HD12	1.70	1.16
1:C:14:THR:HG23	1:C:62:LEU:HD11	1.19	1.12
1:C:14:THR:CG2	1:C:62:LEU:HD11	1.77	1.11
1:C:169:SER:O	1:C:170:LEU:HD12	1.59	1.01
1:B:357:TYR:HE1	1:B:391:ALA:CA	1.74	1.00
1:B:357:TYR:CE1	1:B:391:ALA:HB1	2.02	0.93
1:B:45:TYR:CE2	1:B:47:GLN:NE2	2.35	0.93
1:C:356:GLN:NE2	1:C:368:LYS:O	2.01	0.93
1:C:14:THR:HG22	1:C:29:TRP:HA	1.51	0.92
1:C:325:PRO:O	1:C:410:ASN:ND2	2.07	0.88
1:C:47:GLN:HB2	1:C:50:LYS:HB2	1.59	0.84
1:B:15:LEU:HD23	1:B:29:TRP:HB3	1.61	0.82
1:B:394:ARG:HD2	1:B:408:TRP:HE1	1.45	0.82
1:C:14:THR:HG23	1:C:62:LEU:CD1	2.06	0.81
1:B:357:TYR:CZ	1:B:391:ALA:CB	2.65	0.80
1:B:45:TYR:HE2	1:B:47:GLN:NE2	1.81	0.79
1:A:50:LYS:HE2	1:A:51:ILE:H	1.48	0.79
1:C:352:THR:HA	1:C:373:GLY:HA2	1.65	0.79
1:C:342:THR:HA	1:C:343:GLN:HB2	1.64	0.78
1:C:390:CYS:HB3	1:C:411:GLU:HB3	1.65	0.78
1:D:129:HIS:HA	1:D:181:PRO:HD3	1.66	0.77
1:A:100:ASP:N	1:A:100:ASP:OD1	2.13	0.77
1:C:361:SER:HB3	1:C:367:SER:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ILE:HG22	1:A:347:LYS:HG2	1.67	0.76
1:C:84:ARG:HH11	1:C:84:ARG:HB3	1.50	0.76
1:C:383:LEU:C	1:C:385:PRO:HD2	2.11	0.76
1:C:15:LEU:HA	1:C:29:TRP:HB3	1.68	0.75
1:C:169:SER:C	1:C:170:LEU:CD1	2.55	0.74
1:D:207:ARG:HB2	1:D:207:ARG:CZ	2.17	0.74
1:D:230:LEU:HD23	1:D:244:TRP:HB3	1.70	0.74
1:C:54:VAL:HG13	1:C:80:ILE:HG12	1.70	0.74
1:B:357:TYR:CZ	1:B:391:ALA:HB2	2.23	0.73
1:C:302:THR:HG22	1:D:106:MET:HE3	1.70	0.73
1:B:227:PRO:HB3	1:B:246:VAL:HG12	1.70	0.73
1:C:108:PRO:HB2	1:C:111:GLN:HG2	1.70	0.73
1:B:331:ALA:HB2	1:B:387:THR:HG23	1.71	0.73
1:D:132:LEU:HB3	1:D:177:VAL:HG12	1.71	0.73
1:A:323:GLU:OE2	1:A:323:GLU:N	2.20	0.72
1:B:351:HIS:HB2	1:B:374:ARG:HG3	1.70	0.72
1:B:10:VAL:HG23	1:B:68:PRO:HG2	1.70	0.72
1:A:46:HIS:HA	1:A:50:LYS:HD3	1.71	0.72
1:A:155:VAL:HG13	1:A:170:LEU:HB2	1.72	0.71
1:C:350:ASP:OD1	1:C:398:ILE:N	2.21	0.71
1:A:305:VAL:HB	1:B:103:ILE:HG22	1.73	0.71
1:B:357:TYR:CZ	1:B:391:ALA:HB1	2.24	0.71
1:B:229:ASN:ND2	1:B:245:GLU:OE2	2.23	0.71
1:B:218:ASP:OD1	1:B:218:ASP:N	2.24	0.71
1:C:310:GLN:HE21	1:D:8:GLU:HA	1.56	0.71
1:B:327:LEU:HD21	1:B:389:TYR:CZ	2.26	0.71
1:B:338:LEU:HD21	1:B:357:TYR:OH	1.91	0.71
1:C:259:PHE:HE2	1:C:270:LYS:HD2	1.55	0.71
1:B:357:TYR:HE2	1:B:380:LEU:CD2	2.03	0.70
1:C:149:LYS:HD2	1:C:150:ASP:HA	1.72	0.70
1:D:224:LYS:HG3	1:D:247:TRP:CG	2.26	0.70
1:D:121:ILE:HD12	1:D:134:TRP:HB3	1.71	0.70
1:B:238:GLN:HA	1:B:292:VAL:HG22	1.73	0.70
1:C:89:ASP:OD1	1:C:89:ASP:N	2.21	0.70
1:A:399:SER:OG	1:A:400:ASP:N	2.22	0.70
1:B:126:SER:OG	1:B:127:GLY:N	2.24	0.69
1:A:320:ILE:O	1:A:321:GLN:HG2	1.92	0.69
1:B:357:TYR:CE2	1:B:380:LEU:CD2	2.75	0.69
1:C:319:HIS:H	1:C:403:GLY:HA2	1.56	0.69
1:A:230:LEU:HD23	1:A:244:TRP:HB3	1.74	0.69
1:C:400:ASP:N	1:C:400:ASP:OD1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASP:HB3	1:B:202:SER:HB2	1.74	0.68
1:C:230:LEU:HD23	1:C:244:TRP:HB3	1.75	0.68
1:A:384:GLU:HB3	1:A:385:PRO:HD3	1.74	0.68
1:A:30:ALA:HB2	1:A:62:LEU:HD21	1.75	0.68
1:B:357:TYR:HE1	1:B:391:ALA:HA	1.57	0.68
1:B:187:ASN:OD1	1:B:222:GLY:N	2.27	0.68
1:D:229:ASN:O	1:D:244:TRP:HA	1.94	0.68
1:B:398:ILE:HG22	1:B:399:SER:H	1.59	0.67
1:A:328:GLN:H	1:A:328:GLN:HE21	1.41	0.67
1:B:357:TYR:CE2	1:B:380:LEU:HD23	2.29	0.67
1:C:258:LEU:HD23	1:C:288:CYS:SG	2.35	0.67
1:A:19:ASN:N	1:A:19:ASN:OD1	2.27	0.67
1:D:181:PRO:HB3	1:D:220:GLN:HG2	1.75	0.67
1:B:350:ASP:OD2	1:B:398:ILE:N	2.20	0.67
1:C:150:ASP:OD1	1:C:150:ASP:N	2.26	0.67
1:B:357:TYR:OH	1:B:391:ALA:HB1	1.95	0.67
1:B:390:CYS:HB2	1:B:411:GLU:HG3	1.77	0.67
1:D:150:ASP:OD1	1:D:150:ASP:N	2.28	0.67
1:A:194:VAL:O	1:A:212:SER:HB3	1.95	0.67
1:C:385:PRO:O	1:C:386:ASP:HB2	1.93	0.66
1:D:179:LEU:HB3	1:D:184:PHE:HZ	1.59	0.66
1:B:357:TYR:OH	1:B:391:ALA:CB	2.44	0.66
1:C:8:GLU:HA	1:D:310:GLN:NE2	2.09	0.66
1:C:202:SER:OG	1:C:204:LEU:HB2	1.96	0.66
1:A:328:GLN:OE1	1:A:339:HIS:NE2	2.26	0.66
1:B:118:PRO:HB2	1:B:212:SER:HB3	1.78	0.66
1:C:140:ASP:N	1:C:140:ASP:OD1	2.28	0.66
1:D:155:VAL:HG13	1:D:170:LEU:HB2	1.77	0.66
1:C:319:HIS:H	1:C:403:GLY:CA	2.09	0.66
1:B:342:THR:HG23	1:B:344:LYS:HD3	1.78	0.65
1:B:358:LYS:HZ3	1:B:370:GLU:N	1.92	0.65
1:A:325:PRO:HA	1:A:339:HIS:O	1.97	0.65
1:A:392:ARG:HB2	1:A:408:TRP:CE3	2.31	0.65
1:B:319:HIS:CD2	1:B:397:PRO:HG3	2.31	0.65
1:B:357:TYR:CE1	1:B:391:ALA:HA	2.32	0.65
1:B:357:TYR:CE1	1:B:391:ALA:CA	2.65	0.65
1:C:185:LEU:HD21	1:C:229:ASN:HB2	1.79	0.64
1:A:58:LEU:HA	1:A:76:ARG:HA	1.78	0.64
1:D:149:LYS:HE2	1:D:150:ASP:HA	1.79	0.64
1:C:21:TYR:CZ	1:C:85:PHE:HB3	2.32	0.64
1:A:105:LEU:HD22	1:A:106:MET:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HG22	1:A:238:GLN:HG2	1.78	0.64
1:D:141:SER:O	1:D:144:SER:HB3	1.98	0.64
1:A:372:LEU:HD21	1:A:378:MET:HB2	1.80	0.64
1:B:342:THR:C	1:B:344:LYS:HB2	2.23	0.64
1:C:19:ASN:OD1	1:C:25:ILE:HG22	1.97	0.64
1:A:43:LEU:HD12	1:A:44:LEU:H	1.63	0.63
1:A:278:PRO:HB2	1:A:279:GLN:HA	1.79	0.63
1:C:398:ILE:HG12	1:C:399:SER:N	2.10	0.63
1:A:349:ILE:HG21	1:A:401:TYR:CD2	2.33	0.63
1:C:83:THR:OG1	1:C:84:ARG:NH1	2.28	0.63
1:D:62:LEU:HD12	1:D:62:LEU:H	1.63	0.63
1:C:102:GLY:O	1:D:226:GLN:NE2	2.32	0.63
1:C:9:THR:HB	1:C:11:PRO:HD2	1.81	0.63
1:A:234:PHE:O	1:B:113:VAL:HG23	1.99	0.62
1:C:14:THR:HG21	1:C:30:ALA:N	2.14	0.62
1:B:10:VAL:HG13	1:B:11:PRO:HD3	1.80	0.62
1:C:113:VAL:HG13	1:C:198:LEU:HD11	1.82	0.62
1:A:47:GLN:H	1:A:50:LYS:CD	2.12	0.62
1:A:99:ARG:NH2	1:B:223:ASP:OD1	2.26	0.62
1:C:327:LEU:H	1:C:327:LEU:HD22	1.64	0.62
1:B:181:PRO:HB3	1:B:220:GLN:HE21	1.64	0.62
1:D:61:LYS:HG3	1:D:62:LEU:N	2.15	0.62
1:A:391:ALA:O	1:A:411:GLU:HG3	1.98	0.62
1:A:89:ASP:OD1	1:A:89:ASP:N	2.33	0.62
1:C:305:VAL:HB	1:D:103:ILE:HG22	1.82	0.61
1:A:276:LYS:HD3	1:A:286:TYR:HE1	1.65	0.61
1:A:86:SER:OG	1:A:89:ASP:N	2.33	0.61
1:D:292:VAL:HG12	1:D:301:TYR:CZ	2.36	0.61
1:D:26:ILE:HG12	1:D:79:VAL:HG12	1.81	0.61
1:C:358:LYS:HE2	1:C:359:LYS:HE2	1.80	0.61
1:B:67:CYS:CB	1:B:73:CYS:SG	2.88	0.61
1:A:314:ILE:HG23	1:A:318:TYR:HD2	1.66	0.61
1:A:330:THR:HB	1:A:387:THR:HB	1.83	0.61
1:B:292:VAL:HG23	1:B:293:PRO:O	2.00	0.61
1:A:351:HIS:HB2	1:A:374:ARG:HG3	1.82	0.61
1:B:330:THR:HG22	1:B:388:SER:H	1.66	0.61
1:C:247:TRP:CD1	1:C:249:GLN:HB2	2.36	0.60
1:A:318:TYR:O	1:B:19:ASN:HB3	2.01	0.60
1:B:357:TYR:HE2	1:B:380:LEU:HD21	1.67	0.60
1:B:402:ASP:OD1	1:B:403:GLY:N	2.34	0.60
1:B:124:SER:HB2	1:B:131:LEU:CD1	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:GLU:HA	1:D:310:GLN:HE21	1.66	0.60
1:C:323:GLU:OE1	1:C:395:VAL:CG2	2.50	0.60
1:A:18:TYR:CD1	1:B:318:TYR:HB3	2.37	0.60
1:A:50:LYS:HE2	1:A:51:ILE:N	2.16	0.60
1:A:314:ILE:HB	1:B:93:TYR:CE1	2.37	0.60
1:C:357:TYR:CE2	1:C:391:ALA:HB2	2.37	0.60
1:B:124:SER:O	1:B:131:LEU:N	2.34	0.59
1:B:132:LEU:HB3	1:B:177:VAL:HG12	1.83	0.59
1:B:229:ASN:HB3	1:B:245:GLU:HG3	1.83	0.59
1:D:10:VAL:O	1:D:14:THR:OG1	2.20	0.59
1:D:47:GLN:HG3	1:D:50:LYS:HD2	1.82	0.59
1:C:375:VAL:HG12	1:C:377:SER:H	1.67	0.59
1:C:399:SER:OG	1:C:400:ASP:OD1	2.20	0.59
1:A:324:PRO:HD2	1:A:342:THR:H	1.67	0.59
1:A:103:ILE:HG22	1:B:227:PRO:HG2	1.83	0.59
1:C:38:LEU:O	1:C:99:ARG:NH2	2.33	0.59
1:C:47:GLN:CB	1:C:50:LYS:HB2	2.31	0.59
1:C:390:CYS:HB2	1:C:412:TYR:HB2	1.83	0.59
1:D:277:GLU:OE2	1:D:285:ARG:NH1	2.36	0.59
1:B:124:SER:HB2	1:B:131:LEU:HD13	1.84	0.58
1:C:358:LYS:NZ	1:C:359:LYS:O	2.26	0.58
1:A:47:GLN:H	1:A:50:LYS:HD3	1.68	0.58
1:C:324:PRO:HD2	1:C:342:THR:HG23	1.85	0.58
1:C:322:MET:N	1:C:406:SER:OG	2.36	0.58
1:D:240:LEU:HD23	1:D:290:LEU:HD11	1.85	0.58
1:D:23:ASN:O	1:D:82:TYR:N	2.25	0.58
1:A:324:PRO:HG2	1:A:341:GLU:HB3	1.85	0.58
1:C:323:GLU:OE1	1:C:395:VAL:HG23	2.03	0.58
1:B:164:TRP:CH2	1:B:193:ARG:HG3	2.38	0.58
1:B:228:GLN:NE2	1:B:283:TYR:OH	2.37	0.58
1:A:327:LEU:HD22	1:A:411:GLU:CD	2.28	0.57
1:A:386:ASP:OD1	1:A:387:THR:N	2.36	0.57
1:D:17:CYS:SG	1:D:93:TYR:HE2	2.27	0.57
1:C:326:ILE:HG13	1:C:339:HIS:HB3	1.86	0.57
1:C:356:GLN:NE2	1:C:357:TYR:H	2.02	0.57
1:C:23:ASN:O	1:C:82:TYR:N	2.27	0.57
1:C:158:LYS:HE3	1:C:164:TRP:CE2	2.40	0.57
1:C:350:ASP:C	1:C:351:HIS:HD1	2.13	0.57
1:A:193:ARG:NH2	1:A:211:TRP:NE1	2.53	0.57
1:B:67:CYS:CB	1:B:73:CYS:HG	2.17	0.57
1:C:323:GLU:OE2	1:C:340:TRP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LYS:HB3	1:B:405:TRP:CE3	2.39	0.57
1:D:119:LYS:HG2	1:D:120:ASP:H	1.69	0.56
1:A:43:LEU:HD12	1:A:44:LEU:N	2.20	0.56
1:C:302:THR:CG2	1:D:106:MET:HE3	2.36	0.56
1:D:181:PRO:HA	1:D:220:GLN:HE21	1.69	0.56
1:B:126:SER:HB3	1:B:129:HIS:CD2	2.41	0.56
1:B:316:SER:HA	1:B:318:TYR:H	1.71	0.56
1:B:394:ARG:HD2	1:B:408:TRP:NE1	2.19	0.56
1:A:159:ARG:NH2	1:A:161:GLN:HE21	2.04	0.56
1:B:82:TYR:OH	1:B:89:ASP:OD2	2.18	0.56
1:A:247:TRP:HE3	1:A:283:TYR:CE1	2.23	0.56
1:A:342:THR:HA	1:A:343:GLN:HB2	1.86	0.56
1:B:314:ILE:C	1:B:315:MET:HG2	2.31	0.56
1:B:357:TYR:CE2	1:B:380:LEU:HD21	2.41	0.56
1:D:187:ASN:ND2	1:D:222:GLY:O	2.39	0.56
1:A:149:LYS:HD2	1:A:150:ASP:HA	1.88	0.55
1:C:249:GLN:NE2	1:D:38:LEU:HD21	2.21	0.55
1:A:47:GLN:O	1:A:50:LYS:HG3	2.06	0.55
1:A:170:LEU:HD23	1:A:177:VAL:HG21	1.88	0.55
1:B:329:GLN:CD	1:B:333:ALA:HB3	2.31	0.55
1:C:160:LEU:HD13	1:C:189:ILE:HG22	1.88	0.55
1:D:15:LEU:HD23	1:D:29:TRP:HB3	1.87	0.55
1:D:151:ILE:HG12	1:D:152:GLU:N	2.21	0.55
1:A:319:HIS:HA	1:B:19:ASN:O	2.06	0.55
1:B:330:THR:HG23	1:B:388:SER:HB3	1.87	0.55
1:C:321:GLN:HE21	1:C:397:PRO:HD3	1.72	0.55
1:A:196:THR:N	1:A:209:SER:OG	2.29	0.55
1:C:233:PHE:CD2	1:D:207:ARG:NH2	2.74	0.55
1:C:10:VAL:HG23	1:D:252:GLY:O	2.07	0.55
1:C:21:TYR:OH	1:C:85:PHE:HB3	2.07	0.55
1:B:100:ASP:OD1	1:B:100:ASP:N	2.38	0.55
1:B:314:ILE:HG22	1:B:315:MET:O	2.07	0.55
1:B:355:VAL:O	1:B:370:GLU:N	2.40	0.54
1:C:373:GLY:O	1:C:375:VAL:HG23	2.06	0.54
1:D:47:GLN:HB2	1:D:50:LYS:HB2	1.89	0.54
1:A:150:ASP:N	1:A:150:ASP:OD1	2.40	0.54
1:A:342:THR:OG1	1:A:344:LYS:HG2	2.07	0.54
1:B:63:MET:HE1	1:B:77:ARG:NH1	2.23	0.54
1:B:344:LYS:N	1:B:344:LYS:HD2	2.22	0.54
1:B:346:PRO:HG2	1:B:351:HIS:CE1	2.42	0.54
1:C:340:TRP:CD1	1:C:393:VAL:HG21	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:PHE:CE2	1:C:270:LYS:HD2	2.41	0.54
1:A:160:LEU:HD13	1:A:189:ILE:HB	1.88	0.54
1:B:15:LEU:HG	1:B:95:PHE:CZ	2.42	0.54
1:A:91:ASP:H	1:B:315:MET:HE2	1.73	0.54
1:B:181:PRO:O	1:B:182:LYS:HB2	2.08	0.54
1:C:321:GLN:NE2	1:C:397:PRO:HD3	2.22	0.54
1:B:257:GLY:HA3	1:B:308:LEU:HD21	1.90	0.54
1:C:244:TRP:NE1	1:C:286:TYR:HD2	2.06	0.54
1:C:383:LEU:HD12	1:C:383:LEU:H	1.73	0.54
1:B:396:LYS:HD3	1:B:405:TRP:CE2	2.43	0.54
1:A:313:PHE:CE1	1:B:92:TYR:HB2	2.44	0.53
1:B:63:MET:HE1	1:B:77:ARG:HH11	1.73	0.53
1:B:396:LYS:HG3	1:B:397:PRO:N	2.23	0.53
1:D:263:SER:HB2	1:D:264:PRO:HD2	1.90	0.53
1:B:10:VAL:HG11	1:B:32:THR:HG23	1.89	0.53
1:B:262:PRO:HB3	1:B:301:TYR:CZ	2.43	0.53
1:C:14:THR:CG2	1:C:29:TRP:HA	2.32	0.53
1:D:121:ILE:HG13	1:D:133:GLU:O	2.07	0.53
1:B:10:VAL:CG1	1:B:11:PRO:HD3	2.37	0.53
1:C:202:SER:O	1:C:203:SER:OG	2.19	0.53
1:C:357:TYR:O	1:C:358:LYS:HB2	2.08	0.53
1:D:91:ASP:HB3	1:D:93:TYR:HE1	1.74	0.53
1:C:207:ARG:HD2	1:D:233:PHE:CZ	2.43	0.53
1:C:330:THR:HA	1:C:388:SER:HB2	1.90	0.53
1:D:170:LEU:C	1:D:171:HIS:HD1	2.17	0.53
1:D:151:ILE:HD11	1:D:196:THR:HG23	1.90	0.53
1:A:130:PHE:N	1:A:179:LEU:O	2.33	0.53
1:A:328:GLN:HE21	1:A:328:GLN:N	2.06	0.53
1:C:317:TYR:HA	1:C:319:HIS:HE1	1.73	0.53
1:C:170:LEU:HD12	1:C:170:LEU:N	2.19	0.53
1:B:372:LEU:HD21	1:B:378:MET:HB2	1.91	0.53
1:B:393:VAL:HG12	1:B:394:ARG:H	1.74	0.53
1:B:381:PRO:O	1:B:382:GLN:NE2	2.42	0.53
1:C:261:ARG:HB2	1:C:302:THR:OG1	2.09	0.53
1:A:23:ASN:ND2	1:A:24:ARG:HG2	2.24	0.53
1:B:67:CYS:SG	1:B:68:PRO:HD2	2.48	0.53
1:C:390:CYS:CB	1:C:412:TYR:HB2	2.40	0.52
1:A:43:LEU:HB3	1:A:54:VAL:HB	1.91	0.52
1:B:140:ASP:OD1	1:B:140:ASP:N	2.41	0.52
1:C:383:LEU:O	1:C:385:PRO:HD2	2.09	0.52
1:D:33:GLU:CD	1:D:33:GLU:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:HD13	1:D:146:LEU:HD13	1.91	0.52
1:C:278:PRO:HB2	1:C:279:GLN:HA	1.91	0.52
1:A:36:GLN:N	1:A:36:GLN:OE1	2.41	0.52
1:B:344:LYS:O	1:B:346:PRO:HD3	2.09	0.52
1:D:61:LYS:HG3	1:D:62:LEU:H	1.72	0.52
1:B:21:TYR:HE1	1:B:85:PHE:CG	2.28	0.52
1:C:321:GLN:O	1:C:322:MET:HE3	2.10	0.52
1:C:325:PRO:HA	1:C:339:HIS:O	2.08	0.52
1:A:252:GLY:O	1:B:10:VAL:HG12	2.10	0.52
1:B:54:VAL:HG13	1:B:80:ILE:CG2	2.40	0.52
1:C:43:LEU:HD11	1:C:93:TYR:HB3	1.91	0.52
1:C:46:HIS:C	1:C:50:LYS:HE2	2.35	0.52
1:A:18:TYR:HD1	1:B:318:TYR:HB3	1.74	0.52
1:A:350:ASP:OD2	1:A:398:ILE:HG23	2.10	0.52
1:C:10:VAL:HA	1:C:13:LYS:HE3	1.92	0.52
1:B:323:GLU:OE1	1:B:394:ARG:N	2.43	0.52
1:B:340:TRP:HH2	1:B:372:LEU:HD23	1.75	0.52
1:A:229:ASN:O	1:A:244:TRP:HA	2.10	0.51
1:C:337:SER:HA	1:C:379:ASP:HA	1.93	0.51
1:A:232:CYS:HA	1:A:242:CYS:HA	1.92	0.51
1:A:348:TYR:HB2	1:A:349:ILE:HG23	1.92	0.51
1:A:372:LEU:HD11	1:A:378:MET:HG3	1.90	0.51
1:A:394:ARG:HG3	1:A:405:TRP:CE3	2.44	0.51
1:B:324:PRO:HD2	1:B:342:THR:HG22	1.93	0.51
1:C:12:LEU:HD12	1:D:310:GLN:HB3	1.90	0.51
1:A:101:LEU:HB2	1:B:226:GLN:HG2	1.93	0.51
1:C:8:GLU:O	1:C:13:LYS:HE2	2.11	0.51
1:A:113:VAL:HG13	1:A:198:LEU:HD11	1.92	0.51
1:A:207:ARG:HD3	1:B:233:PHE:CE1	2.46	0.51
1:B:46:HIS:HB2	1:B:92:TYR:HB3	1.92	0.51
1:B:319:HIS:NE2	1:B:397:PRO:HG3	2.26	0.51
1:B:113:VAL:HG12	1:B:205:SER:O	2.11	0.51
1:B:329:GLN:NE2	1:B:333:ALA:H	2.08	0.51
1:B:343:GLN:N	1:B:344:LYS:HB2	2.25	0.51
1:C:188:SER:HB2	1:C:190:TYR:HE1	1.74	0.51
1:C:357:TYR:CE1	1:C:388:SER:O	2.63	0.51
1:B:277:GLU:OE2	1:B:285:ARG:NH1	2.44	0.51
1:A:38:LEU:HD11	1:B:249:GLN:HG3	1.92	0.51
1:C:247:TRP:HD1	1:C:249:GLN:HB2	1.76	0.51
1:C:372:LEU:HD11	1:C:378:MET:HG3	1.92	0.51
1:C:170:LEU:CD1	1:C:170:LEU:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:NH2	1:A:211:TRP:CE2	2.79	0.50
1:C:15:LEU:HD13	1:D:312:LYS:HE2	1.92	0.50
1:A:10:VAL:HG21	1:A:32:THR:HG23	1.94	0.50
1:A:323:GLU:O	1:A:409:SER:HB3	2.11	0.50
1:A:15:LEU:HD23	1:A:29:TRP:HB3	1.93	0.50
1:B:67:CYS:HG	1:B:73:CYS:CB	2.25	0.50
1:B:350:ASP:HB3	1:B:374:ARG:HH21	1.76	0.50
1:D:62:LEU:H	1:D:62:LEU:CD1	2.24	0.50
1:D:126:SER:HB3	1:D:129:HIS:NE2	2.26	0.50
1:C:109:LEU:HD11	1:D:240:LEU:HD13	1.93	0.50
1:C:244:TRP:HE1	1:C:286:TYR:HD2	1.58	0.50
1:A:318:TYR:HB3	1:B:18:TYR:CD1	2.47	0.50
1:B:394:ARG:HE	1:B:405:TRP:HB3	1.77	0.50
1:A:354:GLN:NE2	1:A:371:ASN:OD1	2.44	0.50
1:B:140:ASP:HB2	1:B:141:SER:HA	1.94	0.50
1:A:181:PRO:C	1:A:183:LEU:H	2.20	0.50
1:D:149:LYS:HZ1	1:D:199:SER:HB3	1.75	0.50
1:A:181:PRO:O	1:A:182:LYS:HB2	2.12	0.49
1:B:20:ASP:OD1	1:B:24:ARG:NE	2.44	0.49
1:B:244:TRP:NE1	1:B:286:TYR:HD2	2.09	0.49
1:D:93:TYR:N	1:D:93:TYR:CD1	2.80	0.49
1:D:179:LEU:HB3	1:D:184:PHE:CZ	2.43	0.49
1:C:155:VAL:HG23	1:C:194:VAL:HG22	1.93	0.49
1:D:93:TYR:N	1:D:93:TYR:HD1	2.10	0.49
1:C:9:THR:OG1	1:D:310:GLN:HG3	2.11	0.49
1:C:105:LEU:HD22	1:C:106:MET:N	2.27	0.49
1:B:30:ALA:HB1	1:B:73:CYS:HB2	1.93	0.49
1:B:310:GLN:HA	1:B:310:GLN:HE21	1.77	0.49
1:B:316:SER:HA	1:B:318:TYR:N	2.27	0.49
1:B:357:TYR:CD2	1:B:380:LEU:HD23	2.47	0.49
1:D:92:TYR:C	1:D:93:TYR:HD1	2.20	0.49
1:D:130:PHE:HB2	1:D:179:LEU:O	2.11	0.49
1:A:11:PRO:HA	1:A:30:ALA:O	2.13	0.49
1:B:25:ILE:HB	1:B:80:ILE:HD11	1.94	0.49
1:B:158:LYS:HD3	1:B:159:ARG:O	2.13	0.49
1:C:314:ILE:O	1:C:318:TYR:CE1	2.65	0.49
1:A:381:PRO:C	1:A:382:GLN:HG3	2.37	0.49
1:B:34:ASP:OD1	1:D:224:LYS:NZ	2.39	0.49
1:B:67:CYS:HB2	1:B:73:CYS:SG	2.51	0.49
1:A:276:LYS:HD3	1:A:286:TYR:CE1	2.47	0.49
1:B:321:GLN:O	1:B:406:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HG23	1:A:318:TYR:CD2	2.47	0.49
1:D:160:LEU:HD22	1:D:189:ILE:HB	1.94	0.49
1:A:356:GLN:HG3	1:A:369:THR:HG22	1.95	0.49
1:B:357:TYR:HE2	1:B:380:LEU:HD23	1.68	0.49
1:C:25:ILE:HD12	1:C:80:ILE:HD12	1.95	0.49
1:C:161:GLN:CD	1:C:161:GLN:H	2.19	0.49
1:A:314:ILE:HB	1:B:93:TYR:HE1	1.78	0.49
1:D:127:GLY:H	1:D:129:HIS:CD2	2.30	0.49
1:A:292:VAL:HG21	1:B:109:LEU:HD21	1.94	0.48
1:C:34:ASP:HB3	1:D:249:GLN:HB3	1.95	0.48
1:C:47:GLN:N	1:C:50:LYS:HE2	2.28	0.48
1:C:398:ILE:O	1:C:399:SER:OG	2.23	0.48
1:D:150:ASP:HB2	1:D:202:SER:HB2	1.94	0.48
1:D:160:LEU:HD13	1:D:189:ILE:O	2.13	0.48
1:D:232:CYS:HA	1:D:242:CYS:HA	1.94	0.48
1:A:204:LEU:H	1:A:204:LEU:HD12	1.78	0.48
1:C:322:MET:CE	1:C:344:LYS:HE3	2.43	0.48
1:C:317:TYR:OH	1:D:87:ASN:O	2.31	0.48
1:C:385:PRO:O	1:C:386:ASP:CB	2.61	0.48
1:D:180:GLU:O	1:D:183:LEU:HB2	2.13	0.48
1:A:9:THR:HG23	1:A:11:PRO:HD2	1.96	0.48
1:A:195:ARG:HB3	1:A:211:TRP:CE3	2.48	0.48
1:B:20:ASP:CG	1:B:24:ARG:HE	2.20	0.48
1:A:189:ILE:HD12	1:D:280:ALA:HB2	1.96	0.48
1:B:21:TYR:HE1	1:B:85:PHE:CD2	2.31	0.48
1:C:14:THR:HG22	1:C:29:TRP:CA	2.33	0.48
1:C:62:LEU:HB3	1:C:65:SER:O	2.12	0.48
1:B:330:THR:HG22	1:B:387:THR:HG22	1.95	0.48
1:D:276:LYS:HD2	1:D:286:TYR:HE1	1.77	0.48
1:A:14:THR:HG21	1:A:30:ALA:HB3	1.96	0.48
1:A:39:ILE:HD12	1:A:40:ASN:H	1.79	0.48
1:A:155:VAL:CG1	1:A:170:LEU:HB2	2.42	0.48
1:B:338:LEU:CD2	1:B:357:TYR:OH	2.60	0.48
1:C:314:ILE:HG21	1:D:17:CYS:O	2.14	0.48
1:A:46:HIS:HB2	1:A:92:TYR:HB3	1.95	0.48
1:A:91:ASP:HB3	1:A:93:TYR:HE1	1.78	0.48
1:B:382:GLN:HG2	1:B:383:LEU:N	2.28	0.48
1:C:292:VAL:HG11	1:D:109:LEU:HD21	1.96	0.48
1:D:256:PHE:C	1:D:308:LEU:HD13	2.39	0.48
1:B:45:TYR:O	1:B:51:ILE:O	2.32	0.48
1:B:327:LEU:HD21	1:B:389:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:HIS:HB3	1:B:353:PHE:CE1	2.49	0.48
1:A:47:GLN:H	1:A:50:LYS:CG	2.27	0.47
1:A:332:ASN:ND2	1:A:332:ASN:O	2.46	0.47
1:B:337:SER:HA	1:B:379:ASP:HA	1.95	0.47
1:D:150:ASP:CB	1:D:202:SER:HB2	2.44	0.47
1:B:354:GLN:NE2	1:B:371:ASN:OD1	2.43	0.47
1:C:148:SER:O	1:C:151:ILE:HG22	2.14	0.47
1:D:38:LEU:HD23	1:D:38:LEU:H	1.79	0.47
1:D:119:LYS:O	1:D:135:SER:OG	2.26	0.47
1:A:46:HIS:HA	1:A:50:LYS:CD	2.44	0.47
1:A:258:LEU:HD22	1:A:288:CYS:HB3	1.95	0.47
1:A:411:GLU:H	1:A:411:GLU:HG2	1.44	0.47
1:B:223:ASP:O	1:B:224:LYS:HB3	2.14	0.47
1:C:14:THR:HG21	1:C:62:LEU:HD11	1.85	0.47
1:C:105:LEU:HB3	1:D:230:LEU:HD12	1.96	0.47
1:A:325:PRO:HD2	1:A:410:ASN:CG	2.40	0.47
1:B:107:VAL:HG23	1:B:112:HIS:CD2	2.50	0.47
1:B:193:ARG:NH2	1:B:211:TRP:CE2	2.83	0.47
1:B:349:ILE:HG22	1:B:350:ASP:N	2.29	0.47
1:C:21:TYR:O	1:C:85:PHE:CZ	2.66	0.47
1:C:186:PRO:HA	1:C:220:GLN:NE2	2.30	0.47
1:C:259:PHE:HB2	1:C:304:SER:OG	2.15	0.47
1:B:383:LEU:HB3	1:B:385:PRO:HD2	1.96	0.47
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.77	0.47
1:A:41:MET:HE2	1:B:253:SER:O	2.14	0.47
1:B:54:VAL:HG13	1:B:80:ILE:HG23	1.97	0.47
1:C:356:GLN:OE1	1:C:367:SER:HB3	2.14	0.47
1:A:103:ILE:HG13	1:A:104:GLN:N	2.30	0.47
1:A:325:PRO:O	1:A:410:ASN:ND2	2.47	0.47
1:D:50:LYS:O	1:D:52:GLN:N	2.46	0.47
1:A:9:THR:CG2	1:B:310:GLN:HG2	2.45	0.47
1:A:189:ILE:CD1	1:D:280:ALA:HB2	2.45	0.47
1:C:322:MET:HE1	1:C:344:LYS:CE	2.45	0.47
1:D:144:SER:O	1:D:144:SER:OG	2.13	0.47
1:A:93:TYR:N	1:A:93:TYR:CD1	2.82	0.47
1:B:21:TYR:CE1	1:B:85:PHE:CG	3.02	0.47
1:C:47:GLN:H	1:C:50:LYS:CB	2.27	0.47
1:C:315:MET:HE1	1:D:90:ASN:OD1	2.15	0.47
1:C:329:GLN:HG2	1:C:330:THR:H	1.80	0.47
1:D:157:TYR:HE1	1:D:170:LEU:HD13	1.78	0.47
1:B:25:ILE:HD12	1:B:80:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLU:OE1	1:B:393:VAL:HB	2.15	0.46
1:C:262:PRO:HA	1:C:301:TYR:CE1	2.51	0.46
1:D:231:GLN:O	1:D:242:CYS:HA	2.15	0.46
1:A:357:TYR:HA	1:A:390:CYS:O	2.16	0.46
1:B:396:LYS:HB3	1:B:405:TRP:CZ3	2.50	0.46
1:C:244:TRP:HZ3	1:C:258:LEU:HD22	1.80	0.46
1:B:124:SER:OG	1:B:131:LEU:HB2	2.15	0.46
1:B:340:TRP:CE3	1:B:376:ASN:HA	2.51	0.46
1:C:17:CYS:HB2	1:D:314:ILE:CD1	2.46	0.46
1:C:113:VAL:HG12	1:C:205:SER:O	2.16	0.46
1:A:350:ASP:OD2	1:A:399:SER:HB3	2.16	0.46
1:B:383:LEU:C	1:B:385:PRO:HD2	2.40	0.46
1:C:107:VAL:HG22	1:C:107:VAL:O	2.16	0.46
1:C:350:ASP:OD1	1:C:398:ILE:HG23	2.14	0.46
1:D:149:LYS:CE	1:D:150:ASP:HA	2.46	0.46
1:A:320:ILE:HG23	1:A:321:GLN:N	2.30	0.46
1:A:346:PRO:HG2	1:A:351:HIS:NE2	2.30	0.46
1:C:319:HIS:NE2	1:D:21:TYR:CD1	2.83	0.46
1:A:184:PHE:CE2	1:A:217:TRP:HZ2	2.34	0.46
1:B:181:PRO:C	1:B:183:LEU:H	2.24	0.46
1:B:340:TRP:CZ3	1:B:353:PHE:HB2	2.50	0.46
1:B:394:ARG:HB3	1:B:405:TRP:CZ3	2.51	0.46
1:D:123:ILE:HD12	1:D:131:LEU:O	2.15	0.46
1:C:96:GLN:HB2	1:C:97:PRO:HD2	1.97	0.46
1:C:317:TYR:O	1:C:402:ASP:O	2.33	0.46
1:C:343:GLN:HG2	1:C:345:ILE:HG12	1.98	0.46
1:D:319:HIS:H	1:D:319:HIS:CD2	2.34	0.46
1:A:324:PRO:O	1:A:340:TRP:HA	2.16	0.46
1:D:130:PHE:HB2	1:D:179:LEU:HB2	1.97	0.46
1:A:16:GLU:HB2	1:A:64:TRP:HB2	1.98	0.45
1:A:136:VAL:HG21	1:A:153:PHE:CZ	2.51	0.45
1:A:367:SER:O	1:A:367:SER:OG	2.24	0.45
1:C:25:ILE:HD13	1:C:82:TYR:HB2	1.98	0.45
1:C:18:TYR:CE1	1:D:318:TYR:HB3	2.51	0.45
1:C:138:LEU:HA	1:D:237:ILE:HD11	1.98	0.45
1:C:350:ASP:OD2	1:C:398:ILE:HD13	2.15	0.45
1:B:10:VAL:O	1:B:14:THR:OG1	2.28	0.45
1:B:235:ASP:C	1:B:237:ILE:H	2.24	0.45
1:B:372:LEU:CD2	1:B:378:MET:HB2	2.46	0.45
1:A:158:LYS:HD2	1:A:162:ASP:HB2	1.98	0.45
1:B:244:TRP:CZ3	1:B:258:LEU:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLN:OE1	1:C:394:ARG:NH1	2.49	0.45
1:D:194:VAL:O	1:D:212:SER:OG	2.27	0.45
1:D:224:LYS:HG3	1:D:247:TRP:CD1	2.51	0.45
1:A:349:ILE:HG21	1:A:401:TYR:CE2	2.52	0.45
1:A:19:ASN:OD1	1:B:318:TYR:O	2.34	0.45
1:A:330:THR:HA	1:A:388:SER:HB3	1.98	0.45
1:B:164:TRP:NE1	1:B:214:GLU:OE2	2.48	0.45
1:B:338:LEU:HD12	1:B:378:MET:O	2.17	0.45
1:C:109:LEU:HD12	1:C:109:LEU:HA	1.66	0.45
1:A:107:VAL:O	1:A:107:VAL:HG22	2.17	0.45
1:A:327:LEU:H	1:A:327:LEU:HG	1.36	0.45
1:B:105:LEU:HD22	1:B:106:MET:N	2.32	0.45
1:C:349:ILE:HG21	1:C:401:TYR:CG	2.52	0.45
1:D:74:VAL:HA	1:D:75:PRO:HD3	1.78	0.45
1:D:290:LEU:HA	1:D:291:PRO:HD3	1.83	0.45
1:B:121:ILE:HG13	1:B:133:GLU:O	2.17	0.45
1:B:354:GLN:O	1:B:393:VAL:HA	2.16	0.45
1:B:113:VAL:O	1:B:206:GLY:HA3	2.17	0.45
1:B:152:GLU:HG2	1:B:153:PHE:H	1.81	0.45
1:C:9:THR:O	1:C:13:LYS:HG3	2.16	0.45
1:C:230:LEU:HD12	1:D:105:LEU:HB3	1.99	0.45
1:D:107:VAL:HG23	1:D:112:HIS:CG	2.52	0.45
1:D:119:LYS:HG2	1:D:120:ASP:N	2.32	0.45
1:D:158:LYS:NZ	1:D:162:ASP:O	2.32	0.45
1:A:394:ARG:HD3	1:A:408:TRP:CZ2	2.52	0.45
1:C:383:LEU:O	1:C:385:PRO:CD	2.64	0.45
1:D:234:PHE:HD1	1:D:239:SER:O	1.99	0.45
1:A:358:LYS:O	1:A:390:CYS:N	2.36	0.44
1:B:15:LEU:HD22	1:B:27:CYS:SG	2.57	0.44
1:C:353:PHE:CD1	1:C:395:VAL:HG22	2.51	0.44
1:D:261:ARG:HD3	1:D:266:ALA:O	2.17	0.44
1:D:15:LEU:HG	1:D:95:PHE:CZ	2.53	0.44
1:D:164:TRP:CD2	1:D:193:ARG:NH1	2.86	0.44
1:A:376:ASN:O	1:A:376:ASN:ND2	2.46	0.44
1:B:128:ASP:OD1	1:B:129:HIS:N	2.50	0.44
1:B:185:LEU:HD21	1:B:229:ASN:CG	2.42	0.44
1:A:351:HIS:HB2	1:A:374:ARG:CG	2.47	0.44
1:B:39:ILE:HD12	1:B:40:ASN:H	1.83	0.44
1:C:136:VAL:HG21	1:C:153:PHE:CZ	2.53	0.44
1:C:383:LEU:C	1:C:385:PRO:CD	2.87	0.44
1:D:136:VAL:HG21	1:D:153:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:HB2	1:A:216:HIS:CE1	2.52	0.44
1:C:157:TYR:HE1	1:C:170:LEU:CD1	2.30	0.44
1:C:386:ASP:HB3	1:C:387:THR:H	1.56	0.44
1:C:315:MET:HA	1:D:91:ASP:HB2	2.00	0.44
1:C:322:MET:O	1:C:323:GLU:HB2	2.18	0.44
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.79	0.44
1:A:57:GLU:O	1:A:77:ARG:N	2.45	0.44
1:C:101:LEU:HD13	1:D:256:PHE:CZ	2.52	0.44
1:C:342:THR:OG1	1:C:344:LYS:HG2	2.17	0.44
1:C:351:HIS:HB3	1:C:353:PHE:CE1	2.53	0.44
1:D:154:GLU:HB3	1:D:197:ARG:HD3	2.00	0.44
1:D:306:LYS:HA	1:D:306:LYS:HD3	1.61	0.44
1:A:140:ASP:N	1:A:140:ASP:OD1	2.51	0.43
1:B:9:THR:HB	1:B:11:PRO:HD2	2.00	0.43
1:B:278:PRO:HG2	1:B:279:GLN:HA	2.00	0.43
1:B:337:SER:HA	1:B:378:MET:O	2.18	0.43
1:C:323:GLU:OE1	1:C:395:VAL:HG21	2.18	0.43
1:D:231:GLN:N	1:D:243:SER:O	2.47	0.43
1:C:35:ALA:HB1	1:C:39:ILE:HG22	2.00	0.43
1:C:183:LEU:HB3	1:C:184:PHE:CE1	2.53	0.43
1:D:256:PHE:HD2	1:D:305:VAL:HG12	1.82	0.43
1:A:157:TYR:CZ	1:A:168:SER:HB2	2.53	0.43
1:B:29:TRP:CH2	1:B:76:ARG:HG3	2.53	0.43
1:B:340:TRP:CH2	1:B:372:LEU:HD23	2.54	0.43
1:D:123:ILE:HD12	1:D:131:LEU:C	2.44	0.43
1:A:386:ASP:OD1	1:A:387:THR:OG1	2.35	0.43
1:C:164:TRP:CH2	1:C:193:ARG:HG3	2.54	0.43
1:B:149:LYS:HE3	1:B:149:LYS:HB2	1.92	0.43
1:B:234:PHE:HD1	1:B:239:SER:O	2.01	0.43
1:B:383:LEU:CB	1:B:385:PRO:HD2	2.49	0.43
1:D:144:SER:O	1:D:145:TRP:HB2	2.18	0.43
1:D:14:THR:HG21	1:D:30:ALA:HB3	2.01	0.43
1:D:38:LEU:HD23	1:D:38:LEU:N	2.33	0.43
1:B:400:ASP:HB3	1:B:401:TYR:HD1	1.83	0.43
1:C:17:CYS:HB2	1:D:314:ILE:HD13	2.01	0.43
1:C:28:SER:HB2	1:C:63:MET:HE3	2.00	0.43
1:D:72:ARG:HG3	1:D:73:CYS:N	2.33	0.43
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.78	0.43
1:B:277:GLU:OE2	1:B:287:ARG:HD3	2.19	0.43
1:C:184:PHE:CD1	1:C:184:PHE:N	2.86	0.43
1:D:154:GLU:OE1	1:D:195:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:HIS:HB2	1:C:374:ARG:HA	1.99	0.43
1:A:23:ASN:O	1:A:82:TYR:HB3	2.18	0.43
1:A:136:VAL:HG21	1:A:153:PHE:HZ	1.84	0.43
1:B:347:LYS:HE2	1:B:347:LYS:HB3	1.92	0.43
1:C:109:LEU:HG	1:D:234:PHE:CD2	2.54	0.43
1:C:353:PHE:CD1	1:C:353:PHE:N	2.86	0.43
1:A:91:ASP:HB2	1:B:315:MET:H	1.84	0.42
1:A:340:TRP:CZ3	1:A:375:VAL:O	2.72	0.42
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.76	0.42
1:B:20:ASP:OD2	1:B:24:ARG:NH2	2.52	0.42
1:C:185:LEU:HD21	1:C:229:ASN:CB	2.47	0.42
1:C:396:LYS:HB2	1:C:405:TRP:CE3	2.54	0.42
1:A:50:LYS:HD2	1:A:51:ILE:N	2.33	0.42
1:B:400:ASP:HB3	1:B:401:TYR:CD1	2.54	0.42
1:B:7:GLU:N	1:B:7:GLU:OE2	2.51	0.42
1:B:261:ARG:HG2	1:B:266:ALA:O	2.19	0.42
1:B:382:GLN:HG2	1:B:383:LEU:H	1.84	0.42
1:C:22:THR:OG1	1:C:23:ASN:N	2.52	0.42
1:C:278:PRO:CB	1:C:279:GLN:HA	2.49	0.42
1:C:369:THR:OG1	1:C:370:GLU:N	2.51	0.42
1:A:240:LEU:HD22	1:A:290:LEU:HD11	2.00	0.42
1:A:320:ILE:HG23	1:A:321:GLN:H	1.83	0.42
1:A:394:ARG:NH2	1:A:405:TRP:CD1	2.87	0.42
1:B:339:HIS:O	1:B:340:TRP:HD1	2.03	0.42
1:C:12:LEU:CD1	1:D:310:GLN:HB3	2.48	0.42
1:D:258:LEU:HD11	1:D:303:VAL:HG12	2.02	0.42
1:A:105:LEU:HD22	1:A:106:MET:H	1.82	0.42
1:A:159:ARG:HG3	1:A:162:ASP:OD2	2.18	0.42
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.84	0.42
1:C:260:TYR:CD2	1:C:290:LEU:HD13	2.54	0.42
1:C:100:ASP:OD1	1:C:100:ASP:N	2.49	0.42
1:C:391:ALA:O	1:C:411:GLU:HB2	2.19	0.42
1:C:197:ARG:HG2	1:C:208:PRO:HB3	2.00	0.42
1:A:59:SER:OG	1:A:60:GLU:N	2.53	0.42
1:C:29:TRP:CH2	1:C:76:ARG:HG3	2.54	0.42
1:C:63:MET:HB2	1:C:64:TRP:CE3	2.54	0.42
1:C:99:ARG:NE	1:D:223:ASP:OD2	2.53	0.42
1:C:202:SER:C	1:C:204:LEU:H	2.27	0.42
1:C:247:TRP:HE1	1:C:249:GLN:NE2	2.18	0.42
1:C:353:PHE:N	1:C:353:PHE:HD1	2.17	0.42
1:D:293:PRO:HG2	1:D:294:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.72	0.42
1:A:396:LYS:HB2	1:A:405:TRP:CD2	2.55	0.42
1:B:22:THR:OG1	1:B:23:ASN:N	2.52	0.42
1:B:70:SER:OG	1:B:71:HIS:ND1	2.52	0.42
1:C:140:ASP:HA	1:C:141:SER:HA	1.54	0.42
1:A:33:GLU:OE2	1:A:72:ARG:HG2	2.20	0.42
1:A:236:GLY:C	1:A:237:ILE:HG13	2.44	0.42
1:A:244:TRP:CZ3	1:A:258:LEU:HD13	2.55	0.42
1:A:317:TYR:O	1:A:318:TYR:CD1	2.72	0.42
1:B:86:SER:OG	1:B:89:ASP:N	2.53	0.42
1:B:353:PHE:CD1	1:B:353:PHE:N	2.88	0.42
1:C:21:TYR:O	1:C:85:PHE:CE1	2.73	0.42
1:A:180:GLU:H	1:A:180:GLU:CD	2.28	0.41
1:D:273:PRO:O	1:D:288:CYS:HB2	2.20	0.41
1:B:356:GLN:O	1:B:356:GLN:HG2	2.21	0.41
1:C:239:SER:HB2	1:C:241:HIS:HE1	1.85	0.41
1:D:116:PRO:HA	1:D:117:PRO:HD2	1.94	0.41
1:B:342:THR:CG2	1:B:344:LYS:HD3	2.46	0.41
1:C:63:MET:HE1	1:C:77:ARG:HE	1.85	0.41
1:A:136:VAL:H	1:A:175:PHE:HE2	1.68	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.79	0.41
1:A:247:TRP:CE3	1:A:283:TYR:CE1	3.07	0.41
1:A:318:TYR:HB3	1:B:18:TYR:HD1	1.85	0.41
1:B:62:LEU:HD12	1:B:65:SER:H	1.86	0.41
1:B:319:HIS:CD2	1:B:397:PRO:CG	3.02	0.41
1:C:244:TRP:CE2	1:C:286:TYR:HB2	2.55	0.41
1:A:320:ILE:C	1:A:321:GLN:HG2	2.46	0.41
1:C:136:VAL:HG21	1:C:153:PHE:HZ	1.85	0.41
1:A:50:LYS:HG3	1:A:50:LYS:HZ3	1.68	0.41
1:A:140:ASP:HB2	1:A:141:SER:HA	2.01	0.41
1:B:379:ASP:OD1	1:B:379:ASP:N	2.54	0.41
1:C:184:PHE:HD2	1:C:190:TYR:CE2	2.39	0.41
1:C:262:PRO:O	1:C:263:SER:HB3	2.20	0.41
1:D:8:GLU:O	1:D:13:LYS:HE2	2.20	0.41
1:D:180:GLU:H	1:D:183:LEU:HD23	1.85	0.41
1:A:356:GLN:HB3	1:A:392:ARG:HG3	2.01	0.41
1:B:18:TYR:HD1	1:B:18:TYR:HA	1.66	0.41
1:C:188:SER:HB2	1:C:190:TYR:CE1	2.55	0.41
1:C:281:SER:OG	1:C:282:VAL:N	2.54	0.41
1:D:149:LYS:NZ	1:D:199:SER:HB3	2.35	0.41
1:A:181:PRO:HG3	1:A:220:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HB3	1:B:184:PHE:CE1	2.56	0.41
1:B:382:GLN:O	1:B:383:LEU:HD13	2.21	0.41
1:C:47:GLN:N	1:C:50:LYS:HB2	2.36	0.41
1:C:123:ILE:HG22	1:C:215:VAL:HG22	2.03	0.41
1:C:184:PHE:HD2	1:C:190:TYR:CD2	2.38	0.41
1:D:193:ARG:HD3	1:D:211:TRP:CD1	2.56	0.41
1:D:232:CYS:HA	1:D:241:HIS:O	2.21	0.41
1:D:274:VAL:HA	1:D:288:CYS:HB2	2.03	0.41
1:A:8:GLU:HB3	1:A:12:LEU:CD2	2.51	0.41
1:A:98:ASP:OD1	1:A:98:ASP:N	2.42	0.41
1:A:389:TYR:HA	1:A:390:CYS:HA	1.71	0.41
1:B:150:ASP:HB3	1:B:202:SER:CB	2.46	0.41
1:B:244:TRP:NE1	1:B:286:TYR:CD2	2.88	0.41
1:B:350:ASP:HA	1:B:374:ARG:HE	1.86	0.41
1:C:47:GLN:HB2	1:C:50:LYS:HD3	2.03	0.41
1:C:104:GLN:HG3	1:D:304:SER:HB3	2.02	0.41
1:C:123:ILE:HD12	1:C:131:LEU:O	2.21	0.41
1:D:74:VAL:HG12	1:D:76:ARG:NH1	2.36	0.41
1:D:140:ASP:HA	1:D:141:SER:C	2.46	0.41
1:D:154:GLU:OE1	1:D:195:ARG:NE	2.46	0.41
1:D:258:LEU:HD11	1:D:303:VAL:CG1	2.51	0.41
1:A:260:TYR:CD1	1:A:290:LEU:HD22	2.56	0.41
1:A:343:GLN:N	1:A:344:LYS:HB2	2.35	0.41
1:B:247:TRP:O	1:B:250:THR:HB	2.20	0.41
1:C:39:ILE:HD12	1:C:39:ILE:HA	1.89	0.41
1:C:45:TYR:CG	1:C:50:LYS:HE3	2.56	0.41
1:C:158:LYS:HB3	1:C:167:ALA:HB2	2.02	0.41
1:C:181:PRO:O	1:C:182:LYS:HB2	2.21	0.41
1:A:115:PRO:HG3	1:A:198:LEU:HD21	2.03	0.40
1:A:161:GLN:OE1	1:A:161:GLN:N	2.48	0.40
1:A:394:ARG:HH21	1:A:405:TRP:CG	2.39	0.40
1:B:39:ILE:HD13	1:B:99:ARG:NH2	2.36	0.40
1:C:47:GLN:H	1:C:50:LYS:HB3	1.86	0.40
1:C:142:GLN:HG3	1:C:143:VAL:HG23	2.03	0.40
1:A:17:CYS:SG	1:A:25:ILE:HG22	2.61	0.40
1:A:150:ASP:O	1:A:199:SER:HB2	2.21	0.40
1:B:48:LEU:HB3	1:B:49:ASP:H	1.53	0.40
1:B:144:SER:O	1:B:146:LEU:N	2.40	0.40
1:B:318:TYR:C	1:B:319:HIS:CG	2.99	0.40
1:C:93:TYR:HE1	1:D:314:ILE:HB	1.86	0.40
1:A:157:TYR:HA	1:A:191:ALA:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:HB2	1:A:358:LYS:H	1.64	0.40
1:B:391:ALA:C	1:B:411:GLU:HG2	2.46	0.40
1:C:253:SER:OG	1:D:31:ASP:OD1	2.35	0.40
1:C:389:TYR:N	1:C:389:TYR:CD1	2.90	0.40
1:D:49:ASP:O	1:D:51:ILE:HG12	2.22	0.40
1:D:278:PRO:O	1:D:279:GLN:C	2.63	0.40
1:A:193:ARG:HH22	1:A:211:TRP:NE1	2.18	0.40
1:A:394:ARG:NH2	1:A:405:TRP:CG	2.89	0.40
1:B:278:PRO:CB	1:B:279:GLN:HA	2.52	0.40
1:C:149:LYS:HA	1:C:150:ASP:HA	1.83	0.40
1:B:70:SER:OG	1:B:71:HIS:N	2.54	0.40
1:B:298:HIS:O	1:B:300:GLN:HG2	2.21	0.40
1:C:130:PHE:O	1:C:178:ASN:HA	2.22	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	395/416 (95%)	354 (90%)	36 (9%)	5 (1%)	9	39
1	B	391/416 (94%)	353 (90%)	33 (8%)	5 (1%)	9	39
1	C	398/416 (96%)	355 (89%)	35 (9%)	8 (2%)	6	32
1	D	314/416 (76%)	291 (93%)	20 (6%)	3 (1%)	12	44
All	All	1498/1664 (90%)	1353 (90%)	124 (8%)	21 (1%)	9	38

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	PRO
1	C	323	GLU

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Mol	Chain	Res	Type
1	C	385	PRO
1	A	384	GLU
1	B	51	ILE
1	C	386	ASP
1	D	51	ILE
1	D	143	VAL
1	D	144	SER
1	A	51	ILE
1	C	51	ILE
1	A	331	ALA
1	B	145	TRP
1	A	316	SER
1	A	321	GLN
1	C	281	SER
1	C	337	SER
1	C	325	PRO
1	B	263	SER
1	B	397	PRO
1	C	381	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	368/385 (96%)	271 (74%)	97 (26%)	0	3
1	B	364/385 (94%)	270 (74%)	94 (26%)	0	3
1	C	371/385 (96%)	260 (70%)	111 (30%)	0	2
1	D	291/385 (76%)	212 (73%)	79 (27%)	0	3
All	All	1394/1540 (90%)	1013 (73%)	381 (27%)	0	3

All (381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	15	LEU

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Mol	Chain	Res	Type
1	A	20	ASP
1	A	21	TYR
1	A	23	ASN
1	A	24	ARG
1	A	26	ILE
1	A	27	CYS
1	A	32	THR
1	A	33	GLU
1	A	34	ASP
1	A	38	LEU
1	A	39	ILE
1	A	43	LEU
1	A	50	LYS
1	A	60	GLU
1	A	70	SER
1	A	71	HIS
1	A	72	ARG
1	A	73	CYS
1	A	80	ILE
1	A	85	PHE
1	A	87	ASN
1	A	93	TYR
1	A	99	ARG
1	A	100	ASP
1	A	101	LEU
1	A	103	ILE
1	A	105	LEU
1	A	107	VAL
1	A	109	LEU
1	A	124	SER
1	A	126	SER
1	A	135	SER
1	A	145	TRP
1	A	148	SER
1	A	149	LYS
1	A	150	ASP
1	A	151	ILE
1	A	155	VAL
1	A	158	LYS
1	A	159	ARG
1	A	169	SER
1	A	178	ASN

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Mol	Chain	Res	Type
1	A	180	GLU
1	A	183	LEU
1	A	193	ARG
1	A	194	VAL
1	A	197	ARG
1	A	207	ARG
1	A	210	ARG
1	A	211	TRP
1	A	212	SER
1	A	220	GLN
1	A	224	LYS
1	A	230	LEU
1	A	232	CYS
1	A	237	ILE
1	A	239	SER
1	A	240	LEU
1	A	246	VAL
1	A	250	THR
1	A	258	LEU
1	A	261	ARG
1	A	276	LYS
1	A	292	VAL
1	A	296	SER
1	A	299	SER
1	A	302	THR
1	A	309	GLU
1	A	314	ILE
1	A	316	SER
1	A	322	MET
1	A	327	LEU
1	A	328	GLN
1	A	338	LEU
1	A	339	HIS
1	A	347	LYS
1	A	349	ILE
1	A	354	GLN
1	A	355	VAL
1	A	357	TYR
1	A	359	LYS
1	A	369	THR
1	A	372	LEU
1	A	374	ARG

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	377	SER
1	A	378	MET
1	A	382	GLN
1	A	383	LEU
1	A	384	GLU
1	A	393	VAL
1	A	394	ARG
1	A	395	VAL
1	A	404	ILE
1	A	411	GLU
1	B	15	LEU
1	B	17	CYS
1	B	18	TYR
1	B	20	ASP
1	B	21	TYR
1	B	24	ARG
1	B	26	ILE
1	B	28	SER
1	B	33	GLU
1	B	39	ILE
1	B	42	THR
1	B	47	GLN
1	B	48	LEU
1	B	56	CYS
1	B	58	LEU
1	B	62	LEU
1	B	65	SER
1	B	69	SER
1	B	77	ARG
1	B	78	CYS
1	B	79	VAL
1	B	80	ILE
1	B	84	ARG
1	B	89	ASP
1	B	100	ASP
1	B	105	LEU
1	B	109	LEU
1	B	112	HIS
1	B	113	VAL
1	B	119	LYS
1	B	124	SER

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Mol	Chain	Res	Type
1	B	126	SER
1	B	131	LEU
1	B	135	SER
1	B	137	SER
1	B	144	SER
1	B	145	TRP
1	B	146	LEU
1	B	148	SER
1	B	149	LYS
1	B	151	ILE
1	B	158	LYS
1	B	159	ARG
1	B	161	GLN
1	B	165	GLU
1	B	183	LEU
1	B	187	ASN
1	B	203	SER
1	B	205	SER
1	B	210	ARG
1	B	218	ASP
1	B	220	GLN
1	B	228	GLN
1	B	240	LEU
1	B	250	THR
1	B	271	CYS
1	B	275	VAL
1	B	282	VAL
1	B	294	GLU
1	B	298	HIS
1	B	304	SER
1	B	306	LYS
1	B	310	GLN
1	B	315	MET
1	B	316	SER
1	B	319	HIS
1	B	321	GLN
1	B	323	GLU
1	B	326	ILE
1	B	330	THR
1	B	336	TYR
1	B	338	LEU
1	B	342	THR

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Mol	Chain	Res	Type
1	B	344	LYS
1	B	347	LYS
1	B	353	PHE
1	B	355	VAL
1	B	356	GLN
1	B	359	LYS
1	B	370	GLU
1	B	379	ASP
1	B	380	LEU
1	B	382	GLN
1	B	383	LEU
1	B	384	GLU
1	B	387	THR
1	B	389	TYR
1	B	393	VAL
1	B	394	ARG
1	B	398	ILE
1	B	401	TYR
1	B	404	ILE
1	B	407	GLU
1	B	409	SER
1	C	9	THR
1	C	15	LEU
1	C	18	TYR
1	C	19	ASN
1	C	21	TYR
1	C	23	ASN
1	C	25	ILE
1	C	34	ASP
1	C	41	MET
1	C	47	GLN
1	C	52	GLN
1	C	56	CYS
1	C	58	LEU
1	C	62	LEU
1	C	65	SER
1	C	66	GLU
1	C	69	SER
1	C	70	SER
1	C	72	ARG
1	C	76	ARG
1	C	78	CYS

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Mol	Chain	Res	Type
1	C	79	VAL
1	C	80	ILE
1	C	82	TYR
1	C	83	THR
1	C	84	ARG
1	C	85	PHE
1	C	86	SER
1	C	89	ASP
1	C	100	ASP
1	C	101	LEU
1	C	103	ILE
1	C	104	GLN
1	C	105	LEU
1	C	107	VAL
1	C	113	VAL
1	C	121	ILE
1	C	122	HIS
1	C	126	SER
1	C	133	GLU
1	C	135	SER
1	C	137	SER
1	C	140	ASP
1	C	141	SER
1	C	142	GLN
1	C	146	LEU
1	C	150	ASP
1	C	151	ILE
1	C	161	GLN
1	C	162	ASP
1	C	163	SER
1	C	168	SER
1	C	182	LYS
1	C	183	LEU
1	C	193	ARG
1	C	194	VAL
1	C	196	THR
1	C	205	SER
1	C	214	GLU
1	C	219	SER
1	C	220	GLN
1	C	230	LEU
1	C	232	CYS

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Mol	Chain	Res	Type
1	C	237	ILE
1	C	239	SER
1	C	240	LEU
1	C	242	CYS
1	C	250	THR
1	C	253	SER
1	C	274	VAL
1	C	277	GLU
1	C	279	GLN
1	C	282	VAL
1	C	284	THR
1	C	288	CYS
1	C	292	VAL
1	C	298	HIS
1	C	306	LYS
1	C	308	LEU
1	C	310	GLN
1	C	315	MET
1	C	320	ILE
1	C	322	MET
1	C	326	ILE
1	C	327	LEU
1	C	336	TYR
1	C	338	LEU
1	C	339	HIS
1	C	341	GLU
1	C	342	THR
1	C	347	LYS
1	C	348	TYR
1	C	349	ILE
1	C	356	GLN
1	C	357	TYR
1	C	358	LYS
1	C	359	LYS
1	C	367	SER
1	C	372	LEU
1	C	378	MET
1	C	382	GLN
1	C	383	LEU
1	C	384	GLU
1	C	398	ILE
1	C	400	ASP

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Mol	Chain	Res	Type
1	C	401	TYR
1	C	404	ILE
1	C	406	SER
1	C	407	GLU
1	C	408	TRP
1	C	410	ASN
1	D	7	GLU
1	D	14	THR
1	D	15	LEU
1	D	17	CYS
1	D	20	ASP
1	D	24	ARG
1	D	26	ILE
1	D	27	CYS
1	D	32	THR
1	D	38	LEU
1	D	39	ILE
1	D	48	LEU
1	D	55	SER
1	D	57	GLU
1	D	58	LEU
1	D	62	LEU
1	D	63	MET
1	D	65	SER
1	D	66	GLU
1	D	70	SER
1	D	72	ARG
1	D	82	TYR
1	D	84	ARG
1	D	86	SER
1	D	93	TYR
1	D	98	ASP
1	D	101	LEU
1	D	103	ILE
1	D	105	LEU
1	D	107	VAL
1	D	111	GLN
1	D	113	VAL
1	D	120	ASP
1	D	122	HIS
1	D	133	GLU
1	D	135	SER

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Mol	Chain	Res	Type
1	D	138	LEU
1	D	144	SER
1	D	146	LEU
1	D	147	SER
1	D	148	SER
1	D	149	LYS
1	D	150	ASP
1	D	151	ILE
1	D	154	GLU
1	D	155	VAL
1	D	162	ASP
1	D	168	SER
1	D	177	VAL
1	D	178	ASN
1	D	182	LYS
1	D	183	LEU
1	D	188	SER
1	D	193	ARG
1	D	203	SER
1	D	205	SER
1	D	207	ARG
1	D	211	TRP
1	D	219	SER
1	D	220	GLN
1	D	224	LYS
1	D	226	GLN
1	D	230	LEU
1	D	232	CYS
1	D	239	SER
1	D	242	CYS
1	D	269	GLU
1	D	274	VAL
1	D	277	GLU
1	D	288	CYS
1	D	296	SER
1	D	298	HIS
1	D	299	SER
1	D	307	HIS
1	D	317	TYR
1	D	318	TYR
1	D	319	HIS
1	D	321	GLN

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Mol	Chain	Res	Type
1	D	322	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	228	GLN
1	A	241	HIS
1	A	354	GLN
1	B	171	HIS
1	B	178	ASN
1	B	220	GLN
1	B	228	GLN
1	B	328	GLN
1	B	329	GLN
1	B	382	GLN
1	C	241	HIS
1	C	249	GLN
1	C	310	GLN
1	C	321	GLN
1	C	328	GLN
1	C	356	GLN
1	C	410	ASN
1	D	112	HIS
1	D	178	ASN
1	D	220	GLN
1	D	310	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

4 ligands are 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	NAG	B	501	1	14,14,15	1.21	1 (7%)	17,19,21	0.67	0
2	NAG	D	501	1	14,14,15	0.53	0	17,19,21	0.39	0
2	NAG	A	501	1	14,14,15	0.65	0	17,19,21	0.60	1 (5%)
2	NAG	C	501	1	14,14,15	0.67	0	17,19,21	0.59	0

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	NAG	B	501	1	-	3/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	C	501	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	C1-C2	4.08	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	NAG	C4-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	C	501	NAG	O5-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
2	B	501	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	399/416 (95%)	-0.08	14 (3%) 47 28	59, 121, 191, 245	0
1	B	395/416 (94%)	-0.22	7 (1%) 67 43	54, 100, 229, 299	0
1	C	402/416 (96%)	-0.14	11 (2%) 56 33	58, 113, 195, 262	0
1	D	316/416 (75%)	-0.42	3 (0%) 81 58	62, 99, 153, 240	0
All	All	1512/1664 (90%)	-0.20	35 (2%) 61 38	54, 107, 200, 299	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	TYR	7.7
1	A	334	ALA	6.1
1	C	323	GLU	5.9
1	B	325	PRO	4.3
1	A	329	GLN	4.2
1	C	357	TYR	4.0
1	C	320	ILE	3.3
1	C	391	ALA	3.0
1	B	357	TYR	2.8
1	B	327	LEU	2.7
1	C	344	LYS	2.6
1	A	383	LEU	2.6
1	A	326	ILE	2.5
1	D	322	MET	2.5
1	B	395	VAL	2.5
1	B	334	ALA	2.5
1	A	330	THR	2.5
1	A	17	CYS	2.5
1	A	388	SER	2.5
1	C	334	ALA	2.4
1	B	330	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	320	ILE	2.4
1	A	335	SER	2.3
1	C	316	SER	2.3
1	A	143	VAL	2.3
1	B	320	ILE	2.3
1	C	85	PHE	2.2
1	D	143	VAL	2.2
1	C	325	PRO	2.2
1	A	73	CYS	2.2
1	C	383	LEU	2.1
1	A	26	ILE	2.1
1	C	342	THR	2.1
1	A	359	LYS	2.0
1	A	320	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	NAG	B	501	14/15	0.50	0.12	125,145,155,157	0
2	NAG	D	501	14/15	0.60	0.10	141,157,168,168	0
2	NAG	A	501	14/15	0.62	0.09	136,149,152,153	0
2	NAG	C	501	14/15	0.63	0.10	134,148,158,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.