



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:07 AM UTC

PDB ID : 7TE6 / pdb_00007te6
Title : Crystal structure of GluN1b-2B ATD complexed to Fab5 anti-GluN2B antibody
Authors : Regan, M.; Tajima, N.; Furukawa, H.
Deposited on : 2022-01-04
Resolution : 4.55 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
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

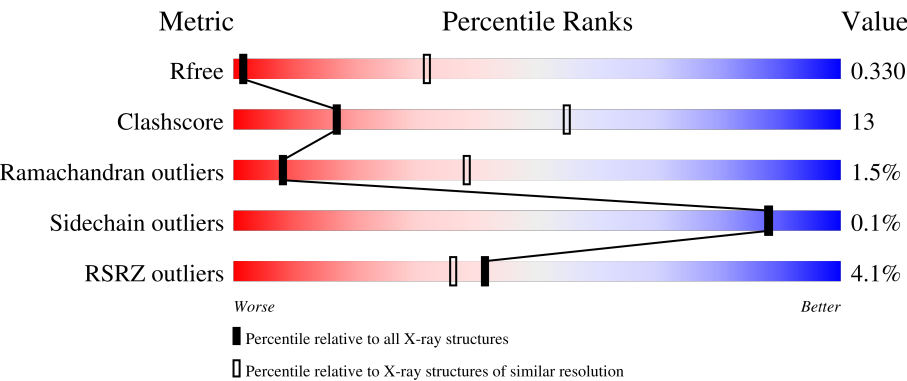
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.55 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	1000 (5.20-3.92)
Clashscore	190562	1009 (5.14-3.94)
Ramachandran outliers	187476	1067 (5.22-3.90)
Sidechain outliers	187428	1049 (5.22-3.90)
RSRZ outliers	180081	1136 (5.22-3.90)

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	383	%69%20%•10%
1	E	383	5%68%21%•10%
2	B	364	2%68%21%•10%
2	F	364	5%64%23%••10%
3	C	221	3%67%27%•••

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Mol	Chain	Length	Quality of chain
3	G	221	10% 61% 32%
4	D	215	3% 76% 23%
4	H	215	4% 73% 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17193 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2714	1729	472	502	11			
1	E	345	Total	C	N	O	S	0	0	0
			2706	1725	470	500	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	conflict	UNP A0A1L8F5J9
A	371	GLN	ASN	conflict	UNP A0A1L8F5J9
E	61	GLN	ASN	conflict	UNP A0A1L8F5J9
E	371	GLN	ASN	conflict	UNP A0A1L8F5J9

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2584	1653	407	510	14			
2	F	327	Total	C	N	O	S	0	0	0
			2571	1645	404	508	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	conflict	UNP Q00960
F	348	ASP	ASN	conflict	UNP Q00960

- Molecule 3 is a protein called Fab5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1633	1030	269	325	9			

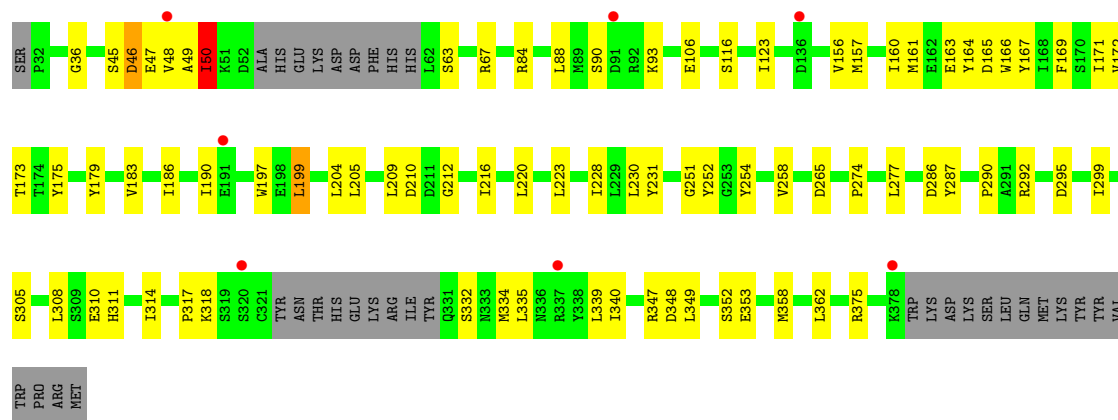
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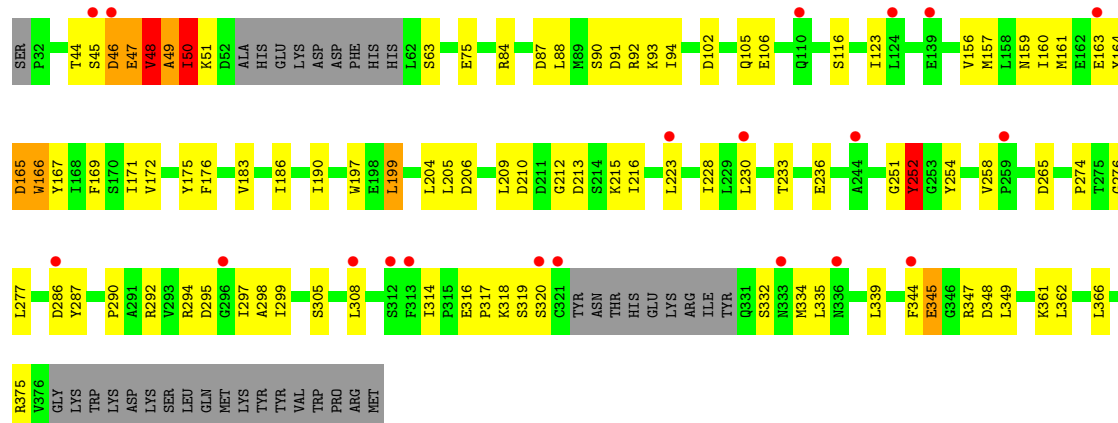
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	214	Total	C	N	O	S	0	0	0
			1629	1028	268	324	9			

- Molecule 4 is a protein called Fab5 light chain.

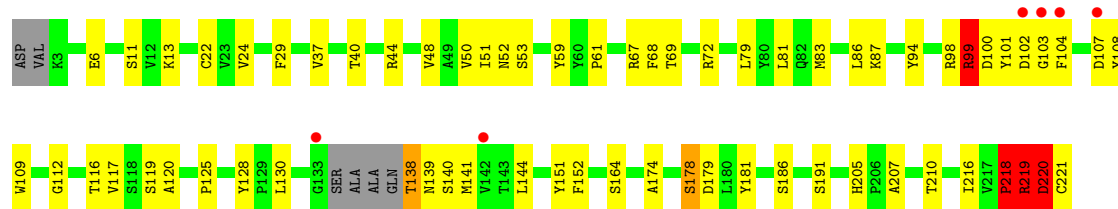
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	215	Total	C	N	O	S	0	0	0
			1678	1046	287	339	6			
4	H	215	Total	C	N	O	S	0	0	0
			1678	1046	287	339	6			



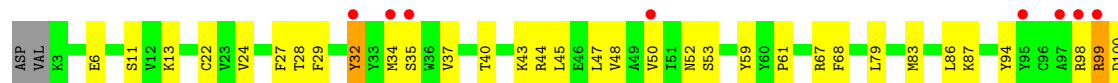
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

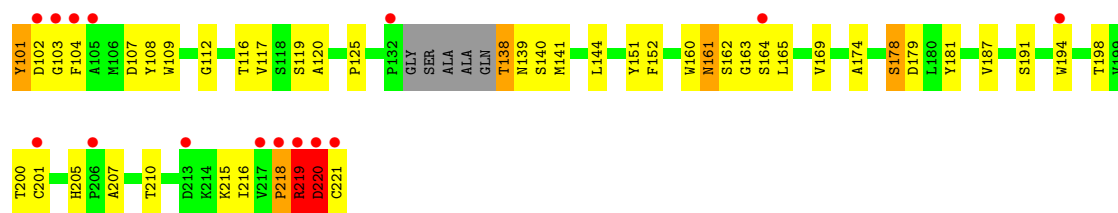


• Molecule 3: Fab5 heavy chain

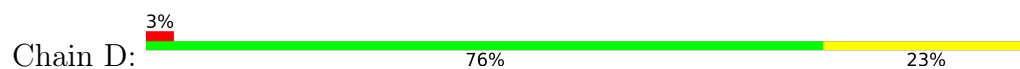


• Molecule 3: Fab5 heavy chain

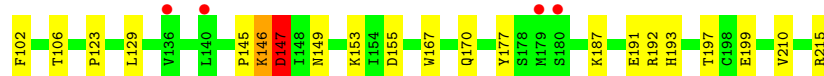
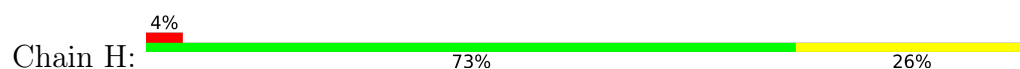




● Molecule 4: Fab5 light chain



● Molecule 4: Fab5 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.92Å 124.92Å 407.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 4.55 24.98 – 4.55	Depositor EDS
% Data completeness (in resolution range)	93.3 (24.98-4.55) 92.6 (24.98-4.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.62Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.282 , 0.324 0.285 , 0.330	Depositor DCC
R_{free} test set	920 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	17193	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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

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	0.29	1/2768 (0.0%)	0.58	4/3751 (0.1%)
1	E	0.34	0/2760	0.72	10/3740 (0.3%)
2	B	0.25	0/2635	0.68	7/3576 (0.2%)
2	F	0.35	0/2622	0.77	12/3560 (0.3%)
3	C	0.36	0/1672	0.76	6/2280 (0.3%)
3	G	0.41	1/1668 (0.1%)	0.81	8/2275 (0.4%)
4	D	0.33	1/1721 (0.1%)	0.65	2/2340 (0.1%)
4	H	0.34	1/1721 (0.1%)	0.70	4/2340 (0.2%)
All	All	0.33	4/17567 (0.0%)	0.70	53/23862 (0.2%)

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	2
1	E	0	4
2	B	0	3
2	F	0	3
3	C	0	5
3	G	0	5
4	H	0	2
All	All	0	24

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	194	TRP	CB-CG	7.73	1.74	1.50
4	H	149	ASN	CA-CB	5.74	1.64	1.53
4	D	149	ASN	CA-CB	5.71	1.64	1.53
1	A	379	ASN	CB-CG	-5.00	1.39	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	LYS	CA-C-N	-9.91	107.77	121.84
1	E	51	LYS	C-N-CA	-9.91	107.77	121.84
2	B	48	VAL	CA-C-N	-9.83	106.81	122.24
2	B	48	VAL	C-N-CA	-9.83	106.81	122.24
2	F	47	GLU	CA-C-N	9.49	139.05	121.97
2	F	47	GLU	C-N-CA	9.49	139.05	121.97
1	E	53	HIS	CA-C-N	-9.37	102.89	121.91
1	E	53	HIS	C-N-CA	-9.37	102.89	121.91
1	E	392	TYR	CA-CB-CG	8.29	128.83	113.90
1	A	379	ASN	CB-CA-C	-7.73	99.29	111.51
3	G	219	ARG	CA-C-N	-7.63	106.97	121.54
3	G	219	ARG	C-N-CA	-7.63	106.97	121.54
1	E	52	ARG	CB-CA-C	-7.44	105.68	116.54
4	H	147	ASP	CA-C-N	-7.39	112.98	123.03
4	H	147	ASP	C-N-CA	-7.39	112.98	123.03
2	F	50	ILE	CA-C-N	6.64	135.49	122.61
2	F	50	ILE	C-N-CA	6.64	135.49	122.61
4	H	146	LYS	CA-C-N	6.54	134.03	121.54
4	H	146	LYS	C-N-CA	6.54	134.03	121.54
2	B	50	ILE	CA-C-N	-6.46	113.66	122.77
2	B	50	ILE	C-N-CA	-6.46	113.66	122.77
2	B	90	SER	CA-C-N	-6.29	109.95	121.52
2	B	90	SER	C-N-CA	-6.29	109.95	121.52
3	G	32	TYR	CA-CB-CG	6.20	125.05	113.90
2	F	90	SER	CA-C-N	6.15	128.80	120.44
2	F	90	SER	C-N-CA	6.15	128.80	120.44
3	G	219	ARG	CB-CA-C	-6.05	98.38	110.42
2	F	47	GLU	CB-CA-C	5.95	122.26	110.42
1	A	55	THR	N-CA-C	-5.68	98.24	108.58
1	E	379	ASN	CB-CA-C	-5.61	99.25	110.42
3	G	138	THR	CA-C-N	5.56	131.72	121.70
3	G	138	THR	C-N-CA	5.56	131.72	121.70
3	C	138	THR	CA-C-N	5.55	131.70	121.70
3	C	138	THR	C-N-CA	5.55	131.70	121.70
2	B	50	ILE	O-C-N	-5.50	115.69	122.57
2	F	159	ASN	CA-C-N	-5.47	110.88	120.29
2	F	159	ASN	C-N-CA	-5.47	110.88	120.29
4	D	147	ASP	CA-C-N	5.44	128.09	122.27
4	D	147	ASP	C-N-CA	5.44	128.09	122.27
2	F	48	VAL	CA-C-N	5.39	131.84	121.54
2	F	48	VAL	C-N-CA	5.39	131.84	121.54
1	E	52	ARG	N-CA-C	5.37	116.23	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	219	ARG	CA-CB-CG	5.29	124.68	114.10
3	C	164	SER	CA-C-N	5.20	130.08	122.85
3	C	164	SER	C-N-CA	5.20	130.08	122.85
1	A	391	SER	CA-C-N	-5.18	113.37	121.87
1	A	391	SER	C-N-CA	-5.18	113.37	121.87
3	G	219	ARG	N-CA-C	5.13	121.72	110.80
2	F	252	TYR	CA-CB-CG	-5.04	104.84	113.90
3	G	220	ASP	CB-CA-C	5.03	120.43	110.42
3	C	220	ASP	CB-CA-C	5.03	120.43	110.42
1	E	54	PHE	CA-C-N	5.00	130.68	123.13
1	E	54	PHE	C-N-CA	5.00	130.68	123.13

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	LYS	Mainchain
1	A	54	PHE	Mainchain
2	B	252	TYR	Peptide
2	B	46	ASP	Mainchain
2	B	50	ILE	Mainchain
3	C	218	PRO	Mainchain
3	C	219	ARG	Peptide
3	C	220	ASP	Peptide,Mainchain
3	C	99	ARG	Peptide
1	E	379	ASN	Mainchain
1	E	51	LYS	Peptide,Mainchain
1	E	54	PHE	Mainchain
2	F	252	TYR	Peptide
2	F	46	ASP	Mainchain
2	F	50	ILE	Mainchain
3	G	218	PRO	Mainchain
3	G	219	ARG	Peptide
3	G	220	ASP	Peptide,Mainchain
3	G	99	ARG	Peptide
4	H	73	THR	Peptide
4	H	74	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	2714	0	2744	52	1
1	E	2706	0	2738	59	1
2	B	2584	0	2551	55	0
2	F	2571	0	2535	79	2
3	C	1633	0	1595	52	0
3	G	1629	0	1592	91	0
4	D	1678	0	1600	37	0
4	H	1678	0	1600	47	0
All	All	17193	0	16955	435	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (435) 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)
3:G:161:ASN:HD22	3:G:165:LEU:HD12	1.27	0.97
3:G:198:THR:HG21	3:G:215:LYS:HE3	1.46	0.97
1:E:381:LYS:HG2	1:E:382:LEU:H	1.29	0.96
3:G:219:ARG:H	3:G:220:ASP:HA	1.36	0.90
2:F:46:ASP:C	2:F:48:VAL:H	1.81	0.84
2:F:294:ARG:NE	2:F:345:GLU:OE2	2.08	0.84
3:G:32:TYR:CE1	3:G:98:ARG:HB2	2.12	0.84
1:E:341:LEU:HA	2:F:210:ASP:HB2	1.60	0.83
2:F:48:VAL:O	2:F:50:ILE:N	2.12	0.81
3:G:32:TYR:HE1	3:G:98:ARG:CB	1.95	0.79
3:G:32:TYR:HE1	3:G:98:ARG:HB2	1.47	0.78
2:B:287:TYR:O	2:B:292:ARG:NH1	2.17	0.78
2:F:286:ASP:OD2	2:F:375:ARG:NH1	2.16	0.78
3:G:102:ASP:N	3:G:103:GLY:HA3	1.98	0.78
2:F:287:TYR:OH	2:F:347:ARG:NH1	2.17	0.78
2:F:287:TYR:O	2:F:292:ARG:NH1	2.17	0.77
2:F:47:GLU:O	2:F:51:LYS:HE3	1.84	0.77
3:C:102:ASP:N	3:C:103:GLY:HA3	1.98	0.76
2:F:87:ASP:O	2:F:91:ASP:HB2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:SER:H	2:F:47:GLU:HG3	1.51	0.76
1:A:379:ASN:HB2	1:A:381:LYS:HG3	1.68	0.75
2:F:252:TYR:OH	2:F:276:GLY:HA3	1.87	0.74
3:G:99:ARG:NE	3:G:104:PHE:O	2.19	0.74
3:C:219:ARG:H	3:C:220:ASP:HA	1.51	0.74
3:G:160:TRP:O	3:G:163:GLY:N	2.14	0.72
3:C:138:THR:HA	3:C:139:ASN:HB2	1.70	0.72
3:G:138:THR:HA	3:G:139:ASN:HB2	1.70	0.72
1:A:218:PHE:HZ	1:A:248:ASP:HB3	1.55	0.72
1:E:218:PHE:HZ	1:E:248:ASP:HB3	1.55	0.72
1:E:381:LYS:HG2	1:E:382:LEU:N	2.04	0.71
2:F:93:LYS:HB2	2:F:317:PRO:HG2	1.74	0.70
1:E:377:LEU:HD12	1:E:381:LYS:O	1.92	0.70
1:A:55:THR:HB	1:A:58:ILE:O	1.92	0.69
1:E:379:ASN:O	1:E:380:ARG:HB2	1.92	0.69
2:F:344:PHE:CZ	2:F:349:LEU:HD13	2.27	0.69
4:H:71:SER:O	4:H:74:ASP:HB3	1.92	0.68
3:G:219:ARG:HH12	4:H:123:PRO:HG2	1.59	0.68
1:A:218:PHE:CZ	1:A:248:ASP:HB3	2.29	0.67
3:C:141:MET:HE3	3:C:191:SER:H	1.60	0.67
3:G:141:MET:HE3	3:G:191:SER:H	1.60	0.67
1:A:157:LEU:HD21	1:A:392:TYR:OH	1.95	0.67
1:E:218:PHE:CZ	1:E:248:ASP:HB3	2.29	0.67
4:D:84:GLU:N	4:D:84:GLU:OE1	2.27	0.66
2:B:358:MET:O	4:H:192:ARG:NH1	2.29	0.65
2:F:106:GLU:OE1	2:F:106:GLU:N	2.30	0.65
3:G:160:TRP:HB3	3:G:201:CYS:HA	1.77	0.65
3:G:160:TRP:HZ2	3:G:169:VAL:HG22	1.61	0.65
2:B:205:LEU:HD13	2:B:216:ILE:HG23	1.79	0.65
3:C:98:ARG:HH12	3:C:99:ARG:CD	2.09	0.64
3:G:29:PHE:O	3:G:32:TYR:HB3	1.98	0.64
3:G:161:ASN:HD22	3:G:165:LEU:CD1	2.06	0.64
2:B:106:GLU:N	2:B:106:GLU:OE1	2.30	0.64
2:F:344:PHE:CE2	2:F:349:LEU:HD13	2.33	0.63
2:F:205:LEU:HD13	2:F:216:ILE:HG23	1.79	0.63
2:F:48:VAL:HA	2:F:51:LYS:HD2	1.81	0.62
3:C:98:ARG:HH12	3:C:99:ARG:HD2	1.62	0.62
3:G:32:TYR:CZ	3:G:34:MET:HB3	2.35	0.62
3:C:100:ASP:HB3	3:C:103:GLY:C	2.24	0.62
1:E:328:GLY:O	1:E:332:ASN:ND2	2.33	0.62
3:G:104:PHE:HE1	4:H:36:TYR:CZ	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:161:ASN:ND2	3:G:165:LEU:HD12	2.07	0.62
2:B:347:ARG:HB2	2:B:349:LEU:HD11	1.82	0.62
2:F:92:ARG:HD2	2:F:94:ILE:HD11	1.82	0.62
1:A:296:LYS:O	1:A:298:GLU:N	2.33	0.61
3:G:219:ARG:N	3:G:220:ASP:HA	2.04	0.61
1:A:226:THR:O	1:A:230:LEU:HG	2.01	0.61
1:A:328:GLY:O	1:A:332:ASN:ND2	2.33	0.61
2:F:46:ASP:C	2:F:48:VAL:N	2.52	0.61
3:G:220:ASP:OD1	3:G:221:CYS:N	2.32	0.61
2:F:274:PRO:HG2	2:F:277:LEU:HD21	1.82	0.60
1:A:54:PHE:C	1:A:56:ARG:N	2.58	0.60
2:F:63:SER:OG	2:F:305:SER:OG	2.14	0.60
3:G:219:ARG:HB2	3:G:219:ARG:CZ	2.31	0.60
2:F:332:SER:N	3:G:102:ASP:O	2.33	0.60
4:H:193:HIS:O	4:H:215:ARG:NH2	2.25	0.60
2:F:318:LYS:HE3	2:F:320:SER:HB2	1.84	0.60
2:F:223:LEU:HD13	2:F:228:ILE:HD13	1.84	0.60
4:H:44:PRO:O	4:H:46:GLN:NE2	2.28	0.60
2:B:274:PRO:HG2	2:B:277:LEU:HD21	1.82	0.60
3:G:22:CYS:SG	3:G:79:LEU:HB3	2.41	0.60
3:G:107:ASP:HB3	3:G:108:TYR:CD1	2.37	0.60
3:C:219:ARG:H	3:C:220:ASP:CA	2.14	0.60
3:G:160:TRP:HB2	3:G:200:THR:O	2.02	0.60
3:C:107:ASP:HB3	3:C:108:TYR:CD1	2.37	0.60
3:C:22:CYS:SG	3:C:79:LEU:HB3	2.41	0.60
4:D:53:LYS:HB3	4:D:57:ASN:HB2	1.84	0.59
4:H:53:LYS:HB3	4:H:57:ASN:HB2	1.84	0.59
2:B:63:SER:OG	2:B:305:SER:OG	2.14	0.59
2:F:230:LEU:HB3	2:F:258:VAL:HG22	1.84	0.59
3:G:37:VAL:HG21	3:G:109:TRP:CZ3	2.38	0.59
4:H:42:HIS:CE1	4:H:48:PRO:HG3	2.37	0.59
2:B:223:LEU:HD13	2:B:228:ILE:HD13	1.84	0.59
3:C:37:VAL:HG21	3:C:109:TRP:CZ3	2.38	0.59
1:E:226:THR:O	1:E:230:LEU:HG	2.01	0.59
4:D:42:HIS:CE1	4:D:48:PRO:HG3	2.37	0.59
3:C:24:VAL:HG11	3:C:29:PHE:HD1	1.68	0.58
3:C:98:ARG:NH1	3:C:99:ARG:HB3	2.18	0.58
2:F:46:ASP:OD1	2:F:49:ALA:HB3	2.04	0.58
2:F:44:THR:HA	2:F:47:GLU:OE2	2.02	0.58
2:F:156:VAL:HG21	2:F:362:LEU:HD22	1.86	0.58
3:G:13:LYS:HG2	3:G:119:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:LYS:HG2	3:C:119:SER:HA	1.85	0.58
1:E:53:HIS:O	1:E:54:PHE:HD1	1.87	0.58
3:G:24:VAL:HG11	3:G:29:PHE:HD1	1.68	0.58
3:G:160:TRP:C	3:G:162:SER:N	2.62	0.58
2:B:156:VAL:HG21	2:B:362:LEU:HD22	1.86	0.57
2:B:45:SER:OG	2:B:46:ASP:N	2.37	0.57
4:D:193:HIS:O	4:D:215:ARG:NH2	2.25	0.57
2:F:84:ARG:O	2:F:88:LEU:HG	2.05	0.57
3:G:160:TRP:CZ2	3:G:169:VAL:HG22	2.40	0.57
2:B:230:LEU:HB3	2:B:258:VAL:HG22	1.85	0.57
2:B:46:ASP:OD1	2:B:49:ALA:HB3	2.04	0.56
1:A:54:PHE:O	1:A:56:ARG:N	2.38	0.56
3:C:100:ASP:HB3	3:C:104:PHE:N	2.21	0.56
3:G:34:MET:HG3	3:G:79:LEU:HD13	1.87	0.56
4:H:38:HIS:CE1	4:H:93:GLN:HB3	2.41	0.56
3:G:160:TRP:C	3:G:160:TRP:CD1	2.84	0.56
4:D:38:HIS:CE1	4:D:93:GLN:HB3	2.41	0.56
2:F:45:SER:OG	2:F:46:ASP:N	2.37	0.55
2:B:84:ARG:O	2:B:88:LEU:HG	2.05	0.55
2:B:165:ASP:HA	2:B:167:TYR:CZ	2.42	0.55
2:F:298:ALA:HB3	2:F:344:PHE:CZ	2.41	0.55
1:A:143:PRO:HG2	1:A:146:HIS:HB2	1.89	0.55
1:E:25:LYS:N	1:E:57:LYS:O	2.40	0.55
1:A:36:LYS:O	1:A:39:GLU:HB2	2.06	0.55
2:F:48:VAL:C	2:F:51:LYS:HB2	2.31	0.55
2:F:334:MET:HB2	3:G:104:PHE:HZ	1.72	0.55
1:E:143:PRO:HG2	1:E:146:HIS:HB2	1.88	0.54
4:D:24:ARG:HD3	4:H:167:TRP:CE2	2.42	0.54
4:H:43:LYS:HB2	4:H:46:GLN:HG3	1.88	0.54
4:H:146:LYS:HG2	4:H:177:TYR:CZ	2.43	0.54
2:B:93:LYS:HB3	2:B:317:PRO:HG2	1.88	0.54
1:A:344:ARG:HD2	2:B:210:ASP:HB3	1.90	0.54
3:C:130:LEU:HB3	4:D:122:PHE:CD2	2.43	0.54
3:G:219:ARG:HH22	4:H:123:PRO:HG3	1.73	0.54
1:E:270:VAL:CG2	1:E:274:GLU:HB2	2.38	0.53
1:E:148:ALA:HA	1:E:151:TRP:CE3	2.44	0.53
1:A:270:VAL:CG2	1:A:274:GLU:HB2	2.38	0.53
4:D:146:LYS:HG2	4:D:177:TYR:CZ	2.43	0.53
3:G:35:SER:OG	3:G:99:ARG:HD2	2.09	0.53
1:A:148:ALA:HA	1:A:151:TRP:CE3	2.44	0.53
3:C:219:ARG:N	3:C:220:ASP:HA	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:SER:HB2	4:D:139:PHE:CD2	2.44	0.53
2:B:348:ASP:C	2:B:349:LEU:HG	2.31	0.52
1:A:294:ASN:O	1:A:301:HIS:NE2	2.42	0.52
4:D:149:ASN:ND2	4:H:74:ASP:OD2	2.42	0.52
3:G:6:GLU:CD	3:G:112:GLY:H	2.18	0.52
4:H:42:HIS:NE2	4:H:48:PRO:HG3	2.25	0.52
4:D:42:HIS:NE2	4:D:48:PRO:HG3	2.25	0.52
3:G:100:ASP:OD2	4:H:53:LYS:NZ	2.43	0.52
1:A:124:ARG:NH1	1:A:272:GLU:OE1	2.40	0.52
3:C:219:ARG:N	3:C:220:ASP:O	2.43	0.51
3:G:205:HIS:HB3	3:G:210:THR:HG22	1.93	0.51
1:E:55:THR:HG23	1:E:58:ILE:O	2.10	0.51
4:H:43:LYS:HB2	4:H:46:GLN:CG	2.40	0.51
2:F:348:ASP:C	2:F:349:LEU:HG	2.31	0.51
4:D:39:TRP:CZ3	4:D:92:CYS:HB2	2.46	0.51
1:E:294:ASN:O	1:E:301:HIS:NE2	2.42	0.51
1:E:316:LEU:O	1:E:319:MET:HB2	2.11	0.51
1:E:341:LEU:CA	2:F:210:ASP:HB2	2.37	0.51
3:C:205:HIS:HB3	3:C:210:THR:HG22	1.93	0.51
3:G:125:PRO:HB3	3:G:151:TYR:HB3	1.93	0.51
3:G:32:TYR:CD1	3:G:98:ARG:HB2	2.44	0.51
3:G:160:TRP:CH2	3:G:187:VAL:HG22	2.46	0.51
3:G:32:TYR:HE1	3:G:98:ARG:HB3	1.74	0.51
2:F:175:TYR:CZ	2:F:204:LEU:HD21	2.46	0.51
2:F:252:TYR:HH	2:F:276:GLY:HA3	1.75	0.51
4:H:187:LYS:O	4:H:191:GLU:HB2	2.11	0.51
2:B:50:ILE:HG22	2:B:50:ILE:O	2.11	0.50
3:C:6:GLU:CD	3:C:112:GLY:H	2.18	0.50
2:B:164:TYR:O	2:B:165:ASP:C	2.50	0.50
2:B:175:TYR:CZ	2:B:204:LEU:HD21	2.46	0.50
2:B:295:ASP:O	2:B:299:ILE:HG13	2.12	0.50
3:C:51:ILE:HD13	3:C:72:ARG:HG3	1.94	0.50
3:G:100:ASP:O	3:G:101:TYR:HB3	2.09	0.50
3:G:29:PHE:CE1	3:G:32:TYR:HE2	2.29	0.50
4:H:39:TRP:CH2	4:H:75:PHE:HB3	2.46	0.50
3:C:125:PRO:HB3	3:C:151:TYR:HB3	1.93	0.50
3:G:178:SER:OG	3:G:179:ASP:N	2.45	0.50
1:A:316:LEU:O	1:A:319:MET:HB2	2.11	0.49
1:E:296:LYS:O	1:E:298:GLU:N	2.45	0.49
2:B:172:VAL:HG21	2:B:223:LEU:HD11	1.94	0.49
1:E:281:ARG:HD2	1:E:282:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:ILE:HG12	2:F:290:PRO:HG3	1.94	0.49
2:F:172:VAL:HG21	2:F:223:LEU:HD11	1.94	0.49
2:F:295:ASP:O	2:F:299:ILE:HG13	2.12	0.49
1:A:160:TRP:CG	1:A:239:VAL:HG21	2.48	0.49
2:B:358:MET:O	4:H:192:ARG:NH2	2.45	0.49
2:B:50:ILE:HG12	2:B:290:PRO:HG3	1.94	0.49
3:C:178:SER:OG	3:C:179:ASP:N	2.45	0.49
2:F:50:ILE:HG22	2:F:50:ILE:O	2.11	0.49
2:B:36:GLY:HA2	2:B:67:ARG:HB3	1.95	0.48
2:B:165:ASP:HA	2:B:167:TYR:CE1	2.48	0.48
1:E:124:ARG:NH1	1:E:272:GLU:OE1	2.40	0.48
3:G:218:PRO:HB2	3:G:220:ASP:O	2.14	0.48
1:E:131:LYS:HE3	2:F:175:TYR:CE1	2.47	0.48
2:B:47:GLU:C	2:B:49:ALA:N	2.69	0.48
4:D:16:GLY:HA2	4:D:81:PRO:HB2	1.96	0.48
1:A:71:ALA:HB1	1:A:106:PRO:HB3	1.95	0.48
3:C:218:PRO:HB2	3:C:220:ASP:O	2.14	0.48
4:D:84:GLU:HG2	4:D:172:SER:O	2.14	0.48
1:E:36:LYS:O	1:E:39:GLU:HB2	2.14	0.48
1:E:71:ALA:HB1	1:E:106:PRO:HB3	1.95	0.48
1:E:150:VAL:HG12	1:E:154:MET:HE2	1.96	0.48
1:E:160:TRP:CG	1:E:239:VAL:HG21	2.48	0.48
2:F:46:ASP:CG	2:F:49:ALA:HB3	2.39	0.48
3:G:160:TRP:CB	3:G:201:CYS:HA	2.42	0.48
2:B:46:ASP:CG	2:B:49:ALA:HB3	2.39	0.48
2:B:173:THR:HG1	2:B:179:TYR:HD1	1.59	0.48
2:F:160:ILE:O	2:F:163:GLU:N	2.48	0.47
2:B:286:ASP:OD2	2:B:375:ARG:NH2	2.47	0.47
4:H:16:GLY:HA2	4:H:81:PRO:HB2	1.95	0.47
3:G:219:ARG:HH22	4:H:123:PRO:CG	2.27	0.47
2:B:340:ILE:HD12	2:B:353:GLU:HA	1.96	0.47
4:D:153:LYS:HB2	4:D:197:THR:OG1	2.15	0.47
1:E:79:CYS:HA	1:E:83:ILE:HB	1.95	0.47
3:C:11:SER:HA	3:C:116:THR:O	2.14	0.47
4:D:39:TRP:O	4:D:50:LEU:HD12	2.15	0.47
3:G:32:TYR:CD1	3:G:98:ARG:HD2	2.50	0.47
4:H:153:LYS:HB2	4:H:197:THR:OG1	2.15	0.47
2:F:175:TYR:C	2:F:176:PHE:HD1	2.22	0.47
3:G:43:LYS:O	4:H:91:TYR:OH	2.33	0.47
1:A:79:CYS:HA	1:A:83:ILE:HB	1.95	0.47
3:C:220:ASP:OD1	3:C:221:CYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:HG21	1:E:107:ILE:HG12	1.97	0.47
3:G:11:SER:HA	3:G:116:THR:O	2.14	0.47
3:C:98:ARG:NH1	3:C:99:ARG:CB	2.77	0.46
1:E:331:GLY:HA2	2:F:75:GLU:CD	2.40	0.46
1:A:82:LEU:HB3	1:A:87:VAL:HG11	1.96	0.46
1:E:129:SER:OG	1:E:139:ARG:NH2	2.49	0.46
2:F:165:ASP:O	2:F:167:TYR:N	2.49	0.46
4:H:54:TYR:HB2	4:H:57:ASN:OD1	2.16	0.46
1:A:129:SER:OG	1:A:139:ARG:NH2	2.49	0.46
1:E:290:LEU:HA	1:E:373:SER:O	2.16	0.46
2:F:210:ASP:CG	2:F:212:GLY:H	2.24	0.46
1:A:150:VAL:HG12	1:A:154:MET:HE2	1.96	0.46
1:A:392:TYR:CG	1:A:393:ILE:N	2.84	0.46
3:C:67:ARG:C	3:C:68:PHE:HD1	2.24	0.46
1:E:318:GLU:HG3	1:E:318:GLU:O	2.15	0.46
3:G:67:ARG:C	3:G:68:PHE:HD1	2.24	0.46
3:G:101:TYR:C	3:G:103:GLY:HA3	2.41	0.46
4:H:21:ILE:HG21	4:H:106:THR:HG21	1.97	0.46
1:A:78:VAL:HG21	1:A:107:ILE:HG12	1.97	0.46
1:A:379:ASN:O	1:A:380:ARG:CB	2.64	0.46
1:E:344:ARG:HA	2:F:209:LEU:HD22	1.97	0.46
1:A:379:ASN:HB2	1:A:381:LYS:CG	2.43	0.46
3:C:40:THR:HG22	3:C:44:ARG:O	2.16	0.46
3:C:101:TYR:C	3:C:103:GLY:HA3	2.41	0.46
1:E:285:ASP:HA	1:E:377:LEU:HD23	1.97	0.46
3:G:52:ASN:OD1	3:G:53:SER:N	2.49	0.46
4:H:145:PRO:HB2	4:H:147:ASP:HB3	1.98	0.46
1:A:285:ASP:HA	1:A:377:LEU:HD23	1.97	0.46
4:D:54:TYR:HB2	4:D:57:ASN:OD1	2.16	0.46
2:B:160:ILE:O	2:B:163:GLU:HB3	2.16	0.45
2:B:251:GLY:O	2:B:254:TYR:HB2	2.16	0.45
4:D:199:GLU:HG2	4:D:210:VAL:HG22	1.98	0.45
1:E:82:LEU:HB3	1:E:87:VAL:HG11	1.96	0.45
2:F:251:GLY:O	2:F:254:TYR:HB2	2.16	0.45
1:E:238:ARG:HD3	1:E:238:ARG:HA	1.80	0.45
3:G:104:PHE:CE1	4:H:36:TYR:CZ	3.02	0.45
1:A:94:HIS:N	1:A:122:THR:OG1	2.50	0.45
1:A:290:LEU:HA	1:A:373:SER:O	2.16	0.45
2:B:210:ASP:CG	2:B:212:GLY:H	2.24	0.45
2:F:344:PHE:CE1	2:F:349:LEU:HD13	2.50	0.45
3:C:50:VAL:HG22	3:C:59:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HB3	1:A:228:LEU:HD22	1.99	0.45
3:C:138:THR:HA	3:C:139:ASN:CB	2.45	0.45
1:E:94:HIS:N	1:E:122:THR:OG1	2.50	0.45
1:E:333:THR:O	2:F:105:GLN:NE2	2.50	0.45
3:G:40:THR:HG22	3:G:44:ARG:O	2.16	0.45
3:C:48:VAL:O	3:C:61:PRO:HD2	2.17	0.45
3:C:52:ASN:OD1	3:C:53:SER:N	2.49	0.45
3:G:29:PHE:CE1	3:G:32:TYR:CE2	3.05	0.45
3:G:34:MET:SD	3:G:34:MET:N	2.90	0.45
3:G:219:ARG:N	3:G:220:ASP:CA	2.77	0.45
3:G:219:ARG:NH1	4:H:123:PRO:HG2	2.31	0.45
4:H:41:GLN:HB3	4:H:51:LEU:HD22	1.99	0.45
4:H:155:ASP:OD2	4:H:193:HIS:ND1	2.33	0.45
1:A:379:ASN:O	1:A:380:ARG:HB2	2.17	0.45
4:D:21:ILE:HG21	4:D:106:THR:HG21	1.98	0.45
4:D:41:GLN:HB3	4:D:51:LEU:HD22	1.99	0.45
4:D:4:LEU:HD22	4:D:23:CYS:SG	2.57	0.44
3:G:50:VAL:HG22	3:G:59:TYR:HB3	1.98	0.44
2:B:308:LEU:HB2	2:B:314:ILE:HG12	1.99	0.44
2:F:308:LEU:HB2	2:F:314:ILE:HG12	1.99	0.44
3:G:47:LEU:HD22	4:H:100:TYR:HB2	1.99	0.44
2:F:252:TYR:HA	2:F:254:TYR:H	1.83	0.44
4:H:4:LEU:HD22	4:H:23:CYS:SG	2.57	0.44
1:A:270:VAL:HG12	1:A:288:ILE:O	2.17	0.44
2:F:318:LYS:C	2:F:320:SER:H	2.25	0.44
3:G:100:ASP:O	3:G:100:ASP:CG	2.59	0.44
3:G:160:TRP:HB2	3:G:161:ASN:H	1.49	0.44
1:A:67:HIS:CG	1:A:95:PRO:HB3	2.52	0.44
2:F:176:PHE:HD1	2:F:176:PHE:N	2.16	0.44
1:A:113:PHE:O	1:A:115:ARG:NH1	2.42	0.44
3:C:144:LEU:HB3	3:C:216:ILE:HD13	2.00	0.44
1:E:216:LEU:HB3	1:E:228:LEU:HD22	1.99	0.44
4:D:50:LEU:HD23	4:D:59:GLU:OE2	2.17	0.44
2:F:171:ILE:HG21	2:F:183:VAL:HG12	1.99	0.44
4:H:50:LEU:HD23	4:H:59:GLU:OE2	2.17	0.44
2:B:47:GLU:C	2:B:49:ALA:H	2.26	0.44
2:B:169:PHE:CE1	2:B:199:LEU:HD13	2.53	0.44
1:E:270:VAL:HG12	1:E:288:ILE:O	2.17	0.44
2:F:48:VAL:HA	2:F:51:LYS:CD	2.47	0.44
3:G:94:TYR:O	3:G:112:GLY:HA2	2.18	0.44
2:B:171:ILE:HG21	2:B:183:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:HIS:CG	1:E:95:PRO:HB3	2.53	0.44
1:E:296:LYS:O	1:E:296:LYS:HG2	2.17	0.44
3:G:48:VAL:O	3:G:61:PRO:HD2	2.17	0.44
3:G:144:LEU:HB3	3:G:216:ILE:HD13	2.00	0.43
4:D:39:TRP:CE2	4:D:77:LEU:HB2	2.53	0.43
4:H:74:ASP:CG	4:H:74:ASP:O	2.61	0.43
3:C:94:TYR:O	3:C:112:GLY:HA2	2.18	0.43
4:H:199:GLU:HG2	4:H:210:VAL:HG22	1.98	0.43
2:B:157:MET:O	2:B:161:MET:HG3	2.19	0.43
2:B:352:SER:HA	2:B:358:MET:HE3	2.00	0.43
3:C:104:PHE:HE1	4:D:36:TYR:CZ	2.36	0.43
1:E:59:GLN:HG2	1:E:60:LEU:N	2.34	0.43
2:F:298:ALA:HB3	2:F:344:PHE:CE1	2.54	0.43
2:F:169:PHE:CE1	2:F:199:LEU:HD13	2.53	0.43
3:G:27:PHE:CE2	3:G:98:ARG:NH2	2.87	0.43
1:A:59:GLN:HG2	1:A:60:LEU:N	2.34	0.43
2:B:335:LEU:O	2:B:339:LEU:N	2.51	0.43
2:F:157:MET:O	2:F:161:MET:HG3	2.19	0.43
2:F:176:PHE:N	2:F:176:PHE:CD1	2.84	0.43
1:A:220:PRO:HB3	1:A:248:ASP:OD2	2.19	0.43
3:C:83:MET:HB3	3:C:86:LEU:HD21	2.00	0.43
1:E:220:PRO:HB3	1:E:248:ASP:OD2	2.19	0.43
2:F:335:LEU:O	2:F:339:LEU:N	2.51	0.43
2:B:63:SER:HG	2:B:305:SER:HG	1.58	0.43
2:F:186:ILE:O	2:F:190:ILE:HG12	2.19	0.43
3:C:99:ARG:HG2	3:C:100:ASP:N	2.34	0.42
3:G:160:TRP:O	3:G:162:SER:N	2.52	0.42
4:H:51:LEU:HD21	4:H:66:PHE:CE2	2.54	0.42
2:B:186:ILE:O	2:B:190:ILE:HG12	2.19	0.42
1:A:288:ILE:HA	1:A:375:MET:O	2.18	0.42
4:D:43:LYS:O	4:D:46:GLN:HB3	2.19	0.42
4:D:87:THR:HG21	4:D:170:GLN:HB3	2.01	0.42
3:G:99:ARG:NH2	4:H:100:TYR:CE2	2.87	0.42
4:H:87:THR:HG21	4:H:170:GLN:HB3	2.01	0.42
2:B:116:SER:HB2	2:B:123:ILE:HD12	2.02	0.42
4:D:51:LEU:HD21	4:D:66:PHE:CE2	2.54	0.42
2:F:206:ASP:HB3	2:F:215:LYS:HE2	2.01	0.42
3:G:45:LEU:HB2	4:H:102:PHE:CG	2.55	0.42
3:G:164:SER:O	3:G:165:LEU:HD23	2.20	0.42
3:C:120:ALA:HB3	3:C:152:PHE:CE2	2.55	0.42
3:C:128:TYR:HB3	4:D:125:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:PRO:O	4:D:101:THR:HG23	2.20	0.42
2:F:344:PHE:HD1	2:F:345:GLU:HG3	1.84	0.42
2:B:310:GLU:HA	4:D:98:ASN:HB3	2.02	0.42
2:B:334:MET:SD	4:D:36:TYR:HE2	2.43	0.42
3:C:98:ARG:HH11	3:C:99:ARG:HB3	1.84	0.42
2:F:361:LYS:HD3	2:F:361:LYS:HA	1.83	0.42
3:G:83:MET:HB3	3:G:86:LEU:HD21	2.00	0.42
4:D:98:ASN:CG	4:D:99:PRO:HD3	2.45	0.42
1:A:139:ARG:NH2	1:A:143:PRO:HB3	2.35	0.42
1:A:165:LEU:HB3	1:A:215:VAL:HG22	2.02	0.42
1:E:165:LEU:HB3	1:E:215:VAL:HG22	2.02	0.42
3:G:32:TYR:CE1	3:G:98:ARG:HD3	2.54	0.42
4:D:155:ASP:OD2	4:D:193:HIS:ND1	2.33	0.42
1:E:288:ILE:HA	1:E:375:MET:O	2.18	0.42
1:E:344:ARG:NE	2:F:213:ASP:OD2	2.50	0.42
2:F:164:TYR:O	2:F:166:TRP:N	2.53	0.42
4:H:99:PRO:O	4:H:101:THR:HG23	2.20	0.42
2:B:164:TYR:O	2:B:166:TRP:N	2.53	0.42
2:B:311:HIS:CE1	4:D:96:TRP:O	2.73	0.42
1:E:124:ARG:O	1:E:143:PRO:HA	2.20	0.42
3:G:218:PRO:O	3:G:219:ARG:HB2	2.19	0.42
3:C:205:HIS:CE1	3:C:207:ALA:HB3	2.55	0.41
3:C:219:ARG:N	3:C:220:ASP:CA	2.78	0.41
2:F:116:SER:HB2	2:F:123:ILE:HD12	2.02	0.41
3:G:34:MET:CG	3:G:79:LEU:HD13	2.49	0.41
3:G:87:LYS:O	3:G:117:VAL:HG11	2.20	0.41
1:A:124:ARG:O	1:A:143:PRO:HA	2.20	0.41
1:E:148:ALA:O	1:E:151:TRP:HB2	2.20	0.41
1:E:139:ARG:NH2	1:E:143:PRO:HB3	2.35	0.41
1:E:214:LYS:HG3	1:E:235:LEU:HD13	2.01	0.41
2:F:297:ILE:HD13	2:F:297:ILE:HA	1.93	0.41
3:G:32:TYR:CE1	3:G:34:MET:HB3	2.55	0.41
3:G:100:ASP:OD2	4:H:53:LYS:HE3	2.20	0.41
3:G:120:ALA:HB3	3:G:152:PHE:CE2	2.55	0.41
4:H:98:ASN:CG	4:H:99:PRO:HD3	2.45	0.41
1:A:74:MET:HE3	1:A:74:MET:HA	2.03	0.41
1:E:53:HIS:O	1:E:54:PHE:CD1	2.70	0.41
2:F:176:PHE:HD2	2:F:233:THR:HG23	1.85	0.41
3:G:138:THR:HA	3:G:139:ASN:CB	2.45	0.41
1:E:319:MET:HB3	1:E:319:MET:HE3	1.77	0.41
3:G:104:PHE:HB3	4:H:100:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:88:ALA:HB3	4:H:90:TYR:CE1	2.56	0.41
1:E:74:MET:HE3	1:E:74:MET:HA	2.03	0.41
2:F:169:PHE:HE2	2:F:197:TRP:HB3	1.86	0.41
2:B:173:THR:HG22	2:B:231:TYR:HB3	2.03	0.41
4:D:88:ALA:HB3	4:D:90:TYR:CE1	2.56	0.41
2:F:45:SER:C	2:F:47:GLU:N	2.79	0.41
3:G:215:LYS:HG2	3:G:216:ILE:N	2.35	0.41
1:A:148:ALA:O	1:A:151:TRP:HB2	2.20	0.41
1:A:214:LYS:HG3	1:A:235:LEU:HD13	2.01	0.41
1:A:238:ARG:HA	1:A:238:ARG:HD3	1.80	0.41
1:A:347:MET:HE3	2:B:209:LEU:HD11	2.02	0.41
2:B:220:LEU:HD23	2:B:220:LEU:HA	1.95	0.41
3:C:140:SER:HA	3:C:141:MET:SD	2.61	0.41
3:C:219:ARG:H	3:C:220:ASP:C	2.28	0.41
3:G:140:SER:HA	3:G:141:MET:SD	2.61	0.41
3:G:160:TRP:O	3:G:161:ASN:C	2.63	0.41
3:G:205:HIS:CE1	3:G:207:ALA:HB3	2.55	0.41
1:A:103:THR:O	1:A:105:THR:N	2.54	0.41
3:C:87:LYS:O	3:C:117:VAL:HG11	2.20	0.41
1:E:32:VAL:HG11	1:E:107:ILE:HD11	2.03	0.41
3:G:174:ALA:HB1	3:G:181:TYR:HB3	2.03	0.41
3:C:174:ALA:HB1	3:C:181:TYR:HB3	2.03	0.40
2:F:318:LYS:HG3	2:F:320:SER:H	1.87	0.40
4:H:129:LEU:HD23	4:H:129:LEU:HA	1.92	0.40
1:A:168:SER:HA	1:A:218:PHE:O	2.21	0.40
2:B:169:PHE:HE2	2:B:197:TRP:HB3	1.86	0.40
2:B:332:SER:HB2	4:D:36:TYR:OH	2.21	0.40
3:C:220:ASP:O	3:C:221:CYS:C	2.63	0.40
1:E:103:THR:O	1:E:105:THR:N	2.54	0.40
2:F:167:TYR:HA	2:F:197:TRP:CE3	2.56	0.40
1:A:30:GLY:HA2	1:A:63:THR:O	2.22	0.40
1:A:74:MET:HG2	1:A:106:PRO:HG2	2.03	0.40
2:B:46:ASP:HB3	2:B:50:ILE:CD1	2.52	0.40
2:B:352:SER:HA	2:B:358:MET:CE	2.51	0.40
2:F:46:ASP:HB3	2:F:50:ILE:CD1	2.52	0.40
3:G:138:THR:CA	3:G:139:ASN:HB2	2.47	0.40
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.85	0.40
3:C:109:TRP:CZ3	4:D:48:PRO:HG2	2.57	0.40
1:E:168:SER:HA	1:E:218:PHE:O	2.21	0.40
1:E:381:LYS:CG	1:E:382:LEU:N	2.80	0.40
2:F:176:PHE:CZ	2:F:236:GLU:OE2	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:316:GLU:HA	2:F:317:PRO:HD3	1.89	0.40
3:G:68:PHE:CE1	3:G:83:MET:HB3	2.56	0.40
4:H:15:LEU:HA	4:H:15:LEU:HD23	1.87	0.40
3:C:69:THR:O	3:C:81:LEU:HD12	2.21	0.40
1:E:30:GLY:HA2	1:E:63:THR:O	2.22	0.40
3:G:32:TYR:HD1	3:G:98:ARG:HD2	1.85	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:NZ	2:F:102:ASP:O[7_455]	2.19	0.01
1:E:51:LYS:NZ	2:F:276:GLY:O[6_564]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	340/383 (89%)	324 (95%)	14 (4%)	2 (1%)	21	58
1	E	339/383 (88%)	314 (93%)	21 (6%)	4 (1%)	10	43
2	B	323/364 (89%)	297 (92%)	22 (7%)	4 (1%)	10	43
2	F	321/364 (88%)	292 (91%)	21 (6%)	8 (2%)	4	26
3	C	211/221 (96%)	193 (92%)	14 (7%)	4 (2%)	6	32
3	G	210/221 (95%)	191 (91%)	14 (7%)	5 (2%)	4	27
4	D	213/215 (99%)	201 (94%)	10 (5%)	2 (1%)	14	49
4	H	213/215 (99%)	200 (94%)	10 (5%)	3 (1%)	9	39
All	All	2170/2366 (92%)	2012 (93%)	126 (6%)	32 (2%)	8	38

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	99	ARG
3	C	218	PRO
3	C	220	ASP
2	F	49	ALA
2	F	165	ASP
2	F	166	TRP
2	F	345	GLU
3	G	161	ASN
4	H	147	ASP
1	A	297	ASN
2	B	318	LYS
4	D	72	GLY
1	E	53	HIS
3	G	219	ARG
4	H	72	GLY
1	A	69	PRO
4	D	55	ALA
1	E	69	PRO
4	H	55	ALA
3	C	178	SER
1	E	380	ARG
3	G	101	TYR
3	G	178	SER
2	B	199	LEU
1	E	297	ASN
2	F	48	VAL
2	F	199	LEU
2	F	319	SER
3	G	28	THR
2	B	265	ASP
2	F	265	ASP
2	B	50	ILE

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	296/329 (90%)	296 (100%)	0	100	100
1	E	295/329 (90%)	295 (100%)	0	100	100
2	B	293/327 (90%)	293 (100%)	0	100	100
2	F	292/327 (89%)	291 (100%)	1 (0%)	86	84
3	C	188/192 (98%)	188 (100%)	0	100	100
3	G	188/192 (98%)	188 (100%)	0	100	100
4	D	190/190 (100%)	190 (100%)	0	100	100
4	H	190/190 (100%)	190 (100%)	0	100	100
All	All	1932/2076 (93%)	1931 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	314	HIS
2	B	110	GLN
3	C	139	ASN
4	D	3	GLN
4	D	41	GLN
4	D	128	GLN
4	D	194	ASN
1	E	94	HIS
3	G	74	ASN
3	G	139	ASN
3	G	170	HIS
4	H	3	GLN
4	H	41	GLN
4	H	128	GLN
4	H	194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	346/383 (90%)	0.27	2 (0%) 85 73	45, 78, 108, 142	0
1	E	345/383 (90%)	0.72	18 (5%) 33 31	57, 91, 123, 158	0
2	B	329/364 (90%)	0.42	7 (2%) 63 50	39, 61, 97, 128	0
2	F	327/364 (89%)	0.72	20 (6%) 27 28	58, 90, 123, 167	0
3	C	215/221 (97%)	0.40	6 (2%) 55 43	54, 85, 141, 179	0
3	G	214/221 (96%)	0.92	23 (10%) 11 15	54, 83, 150, 202	0
4	D	215/215 (100%)	0.39	6 (2%) 55 43	39, 77, 114, 129	0
4	H	215/215 (100%)	0.58	9 (4%) 40 35	50, 78, 103, 123	0
All	All	2206/2366 (93%)	0.55	91 (4%) 41 36	39, 82, 121, 202	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	102	ASP	5.2
1	E	356	THR	4.8
3	G	104	PHE	4.5
3	G	103	GLY	4.3
1	E	135	LEU	4.0
3	C	102	ASP	3.9
4	D	98	ASN	3.7
3	G	97	ALA	3.7
3	G	99	ARG	3.6
3	C	107	ASP	3.6
3	G	213	ASP	3.6
1	E	211	LYS	3.6
2	B	337	ARG	3.5
1	E	210	PRO	3.3
3	G	105	ALA	3.3
1	E	213	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	191	GLU	3.1
3	G	34	MET	3.1
2	F	321	CYS	3.1
3	G	35	SER	3.1
2	B	136	ASP	3.1
3	G	132	PRO	3.0
4	H	97	GLU	3.0
2	F	344	PHE	2.9
3	G	164	SER	2.9
3	G	220	ASP	2.9
3	G	32	TYR	2.8
3	C	104	PHE	2.8
2	F	286	ASP	2.7
3	G	218	PRO	2.7
2	F	336	ASN	2.7
4	H	38	HIS	2.7
2	F	313	PHE	2.7
3	G	221	CYS	2.6
4	H	21	ILE	2.6
2	F	312	SER	2.5
3	C	103	GLY	2.5
1	E	260	ASP	2.5
1	A	56	ARG	2.5
1	E	286	GLY	2.5
2	F	223	LEU	2.4
2	F	110	GLN	2.4
2	B	48	VAL	2.4
4	H	140	LEU	2.4
3	G	95	TYR	2.4
1	E	23	ASP	2.4
1	E	383	VAL	2.4
2	F	124	LEU	2.4
1	E	218	PHE	2.4
3	C	133	GLY	2.4
4	D	136	VAL	2.4
2	F	333	ASN	2.4
4	H	136	VAL	2.3
2	F	45	SER	2.3
4	D	53	LYS	2.3
3	G	194	TRP	2.3
2	B	320	SER	2.3
1	E	379	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	201	CYS	2.3
3	G	217	VAL	2.2
4	H	180	SER	2.2
4	H	179	MET	2.2
4	H	74	ASP	2.2
1	E	94	HIS	2.2
4	D	32	SER	2.2
1	E	133	ILE	2.2
2	F	259	PRO	2.2
1	E	123	THR	2.2
2	F	320	SER	2.2
4	D	42	HIS	2.2
2	F	139	GLU	2.2
1	E	304	ASP	2.1
3	G	98	ARG	2.1
3	G	219	ARG	2.1
2	F	163	GLU	2.1
2	B	91	ASP	2.1
3	G	50	VAL	2.1
4	H	94	HIS	2.1
2	F	244	ALA	2.1
2	B	378	LYS	2.1
2	F	230	LEU	2.1
2	F	46	ASP	2.1
4	D	34	TYR	2.1
1	E	237	ALA	2.1
1	E	288	ILE	2.1
1	A	307	ALA	2.1
3	G	206	PRO	2.1
3	C	142	VAL	2.1
2	F	296	GLY	2.0
1	E	59	GLN	2.0
2	F	308	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.