



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:39 am GMT

PDB ID : 2IFG  
Title : Structure of the extracellular segment of human TRKA in complex with nerve growth factor  
Authors : He, X.; Garcia, K.C.  
Deposited on : 2006-09-20  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

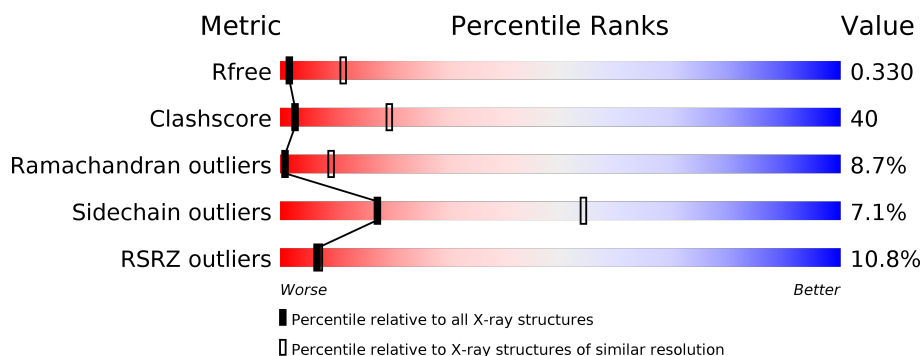
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	347	
1	B	347	
2	E	120	
2	F	120	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NDG	B	395	-	-	-	X
7	NDG	B	392	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7483 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 High affinity nerve growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2659	1662	479	501	17			
1	B	347	Total	C	N	O	S	0	0	0
			2659	1662	479	501	17			

- Molecule 2 is a protein called Beta-nerve growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	108	Total	C	N	O	S	0	0	0
			857	540	152	157	8			
2	F	109	Total	C	N	O	S	0	0	0
			862	543	153	158	8			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	B	3	Total	C	N	O	0	0
			39	22	2	15		
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	B	3	Total	C	N	O	0	0
			39	22	2	15		

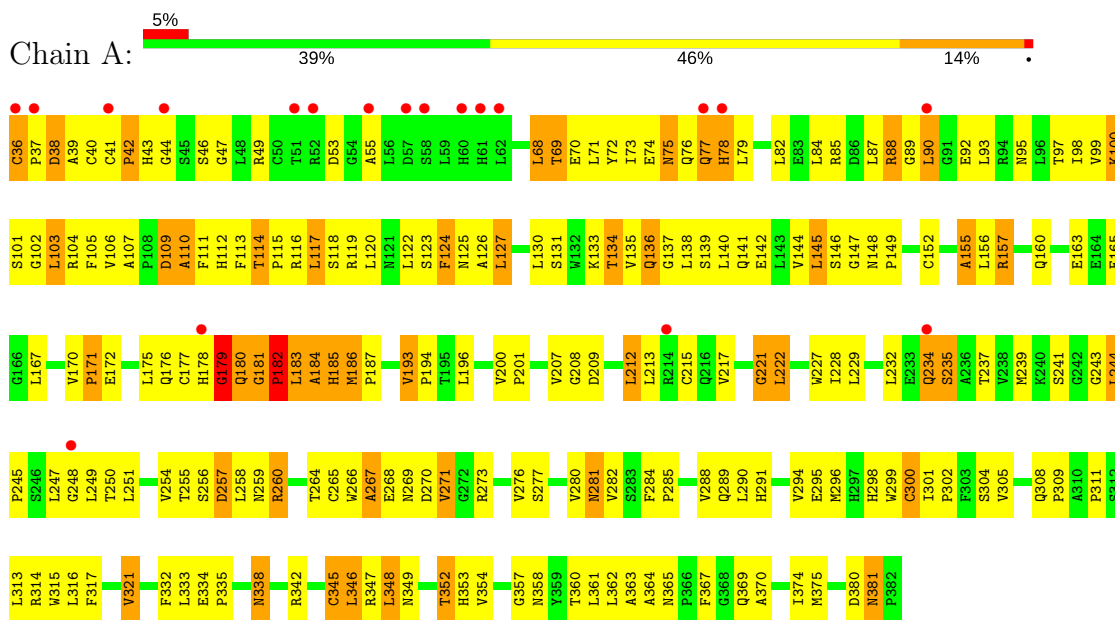
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	B	3	Total	C	N	O	0	0
			39	22	2	15		

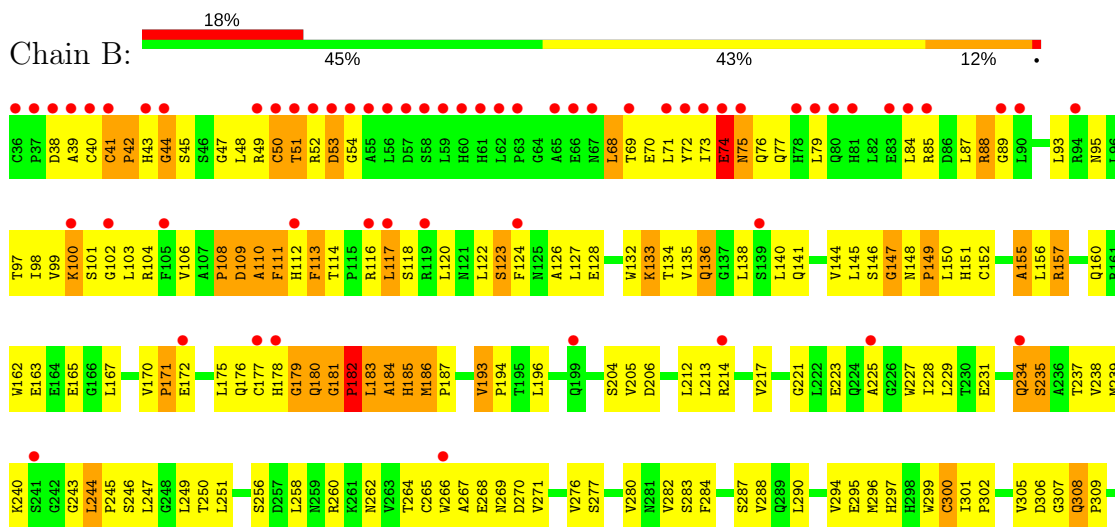
### 3 Residue-property plots

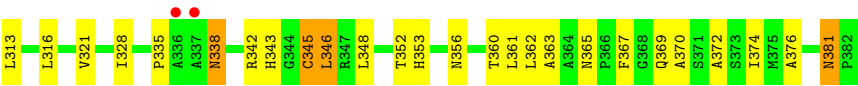
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: High affinity nerve growth factor receptor

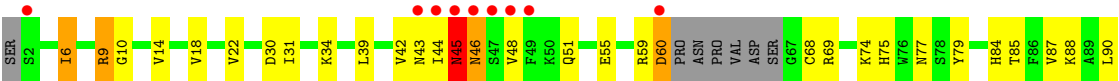


- Molecule 1: High affinity nerve growth factor receptor

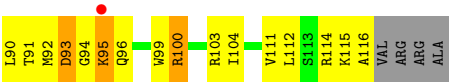
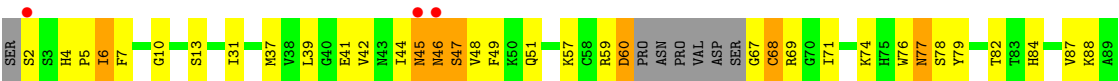




• Molecule 2: Beta-nerve growth factor



• Molecule 2: Beta-nerve growth factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.22Å 81.68Å 115.75Å 90.00° 104.15° 90.00°	Depositor
Resolution (Å)	12.00 – 3.40 11.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.40) 98.7 (11.99-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.43Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.297 , 0.331 0.299 , 0.330	Depositor DCC
$R_{free}$ test set	1289 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 86.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.063 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	7483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.47	1/2720 (0.0%)	0.83	7/3705 (0.2%)
1	B	0.41	0/2720	0.81	9/3705 (0.2%)
2	E	0.42	0/875	0.70	0/1178
2	F	0.41	0/880	0.70	1/1185 (0.1%)
All	All	0.43	1/7195 (0.0%)	0.80	17/9773 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	THR	C-N	5.46	1.44	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	PRO	O-C-N	11.90	141.74	122.70
1	B	181	GLY	N-CA-C	-10.42	87.05	113.10
1	A	181	GLY	N-CA-C	-8.85	90.98	113.10
1	B	185	HIS	N-CA-C	-8.80	87.23	111.00
1	A	185	HIS	N-CA-C	-8.55	87.91	111.00
1	B	346	LEU	N-CA-C	-7.85	89.81	111.00
1	A	181	GLY	C-N-CD	-7.50	104.11	120.60
1	A	346	LEU	N-CA-C	-7.44	90.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	GLY	N-CA-C	-7.41	94.57	113.10
1	B	149	PRO	CA-C-N	-7.36	101.00	117.20
1	A	182	PRO	N-CA-C	7.27	130.99	112.10
1	B	182	PRO	N-CA-C	6.75	129.66	112.10
1	A	345	CYS	CA-CB-SG	5.70	124.26	114.00
1	B	345	CYS	CA-CB-SG	5.69	124.25	114.00
1	A	179	GLY	N-CA-C	-5.68	98.90	113.10
1	B	179	GLY	N-CA-C	-5.28	99.91	113.10
2	F	77	ASN	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	LEU	Mainchain

## 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	2659	0	2573	254	0
1	B	2659	0	2574	227	0
2	E	857	0	832	46	0
2	F	862	0	837	62	0
3	A	28	0	25	5	0
3	B	28	0	25	0	0
4	A	39	0	34	1	0
4	B	39	0	34	2	0
5	A	39	0	34	6	0
5	B	78	0	68	0	0
6	A	78	0	68	2	0
6	B	39	0	34	0	0
7	A	39	0	34	0	0
7	B	39	0	34	0	0
All	All	7483	0	7206	581	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 40.

All (581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:O	1:A:178:HIS:HB2	1.31	1.25
1:B:149:PRO:O	1:B:178:HIS:HB2	1.38	1.19
1:B:74:GLU:HB3	1:B:99:VAL:HG13	1.33	1.08
1:A:260:ARG:HH22	5:A:386:NAG:H62	1.20	1.06
1:B:149:PRO:O	1:B:178:HIS:CB	2.04	1.05
1:B:185:HIS:O	1:B:186:MET:HB2	1.56	1.02
1:A:185:HIS:O	1:A:186:MET:HB2	1.57	0.97
1:A:181:GLY:N	1:A:182:PRO:HD3	1.79	0.97
3:A:1:NAG:H3	3:A:2:NDG:H2	1.44	0.95
1:B:104:ARG:HA	1:B:127:LEU:HA	1.44	0.95
1:B:196:LEU:HD21	1:B:217:VAL:HG22	1.49	0.95
2:E:14:VAL:HG22	2:E:68:CYS:HB3	1.49	0.94
1:A:176:GLN:HB3	1:A:182:PRO:O	1.67	0.92
1:B:193:VAL:HG12	1:B:194:PRO:HD2	1.51	0.92
2:F:47:SER:HB3	2:F:49:PHE:HE1	1.33	0.92
2:F:46:ASN:HD22	2:F:46:ASN:C	1.73	0.92
1:A:163:GLU:OE1	1:A:184:ALA:HB1	1.71	0.91
1:B:335:PRO:HB3	1:B:342:ARG:HH11	1.35	0.91
1:A:196:LEU:HD21	1:A:217:VAL:HG22	1.54	0.90
1:A:193:VAL:HG12	1:A:194:PRO:HD2	1.51	0.90
1:A:178:HIS:C	1:A:180:GLN:H	1.76	0.89
1:A:149:PRO:O	1:A:178:HIS:CB	2.21	0.88
1:A:178:HIS:O	1:A:180:GLN:N	2.06	0.88
1:A:42:PRO:HD2	1:A:49:ARG:O	1.75	0.86
1:B:42:PRO:HG2	1:B:49:ARG:HB2	1.58	0.86
1:B:163:GLU:OE1	1:B:184:ALA:HB1	1.76	0.86
1:A:180:GLN:HG2	1:A:182:PRO:HG3	1.56	0.85
1:B:176:GLN:HB3	1:B:182:PRO:O	1.75	0.85
1:A:352:THR:HG21	2:F:31:ILE:HD11	1.59	0.85
1:A:212:LEU:HD23	1:A:212:LEU:H	1.42	0.84
1:B:74:GLU:HA	1:B:99:VAL:O	1.77	0.84
1:B:118:SER:O	1:B:141:GLN:N	2.12	0.83
1:B:149:PRO:C	1:B:178:HIS:HB2	1.99	0.83
1:A:74:GLU:HA	1:A:99:VAL:O	1.79	0.83
1:B:262:ASN:ND2	4:B:383:NAG:H61	1.94	0.82
1:A:260:ARG:HG2	1:A:338:ASN:HA	1.61	0.82
1:B:146:SER:C	1:B:148:ASN:N	2.24	0.82
1:B:157:ARG:HE	1:B:160:GLN:HG2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HD12	1:A:346:LEU:HD23	1.59	0.82
1:A:290:LEU:HD23	1:A:374:ILE:HG22	1.62	0.82
1:A:118:SER:O	1:A:141:GLN:N	2.12	0.82
1:A:181:GLY:N	1:A:182:PRO:CD	2.36	0.81
1:A:130:LEU:HD11	1:A:134:THR:HG21	1.63	0.81
1:A:177:CYS:O	1:A:180:GLN:HA	1.81	0.81
1:A:176:GLN:CB	1:A:182:PRO:O	2.27	0.81
1:B:365:ASN:HD21	1:B:367:PHE:HD2	1.29	0.81
1:A:228:ILE:HD11	1:A:266:TRP:HE1	1.46	0.81
1:B:146:SER:H	1:B:148:ASN:HD22	1.29	0.81
1:B:145:LEU:O	1:B:175:LEU:HD21	1.81	0.80
1:B:99:VAL:HA	1:B:123:SER:O	1.82	0.80
1:B:52:ARG:HG2	1:B:53:ASP:H	1.45	0.79
1:B:186:MET:HG2	1:B:187:PRO:HD2	1.64	0.78
1:A:157:ARG:HE	1:A:160:GLN:HG2	1.47	0.78
1:B:178:HIS:C	1:B:180:GLN:H	1.84	0.78
1:A:260:ARG:HB3	1:A:338:ASN:HA	1.66	0.78
1:B:74:GLU:HB3	1:B:99:VAL:CG1	2.14	0.78
2:E:30:ASP:OD2	2:E:34:LYS:HB3	1.84	0.77
1:A:288:VAL:HG22	1:A:305:VAL:HG23	1.66	0.77
1:B:288:VAL:HG22	1:B:305:VAL:HG23	1.66	0.77
1:A:157:ARG:O	1:A:160:GLN:HB3	1.85	0.77
1:A:145:LEU:O	1:A:175:LEU:HD21	1.85	0.76
1:A:178:HIS:C	1:A:180:GLN:N	2.33	0.76
1:B:335:PRO:HD3	1:B:342:ARG:HH12	1.50	0.76
1:A:75:ASN:H	1:A:100:LYS:HB2	1.48	0.76
1:A:353:HIS:HB2	1:A:381:ASN:HB3	1.69	0.75
2:F:95:LYS:CD	2:F:95:LYS:H	1.99	0.75
1:A:180:GLN:C	1:A:182:PRO:HD3	2.06	0.75
1:B:284:PHE:CE1	1:B:308:GLN:HB2	2.22	0.75
1:A:186:MET:HG2	1:A:187:PRO:HD2	1.69	0.74
2:E:104:ILE:HD13	2:E:104:ILE:H	1.52	0.74
1:A:123:SER:HB3	1:A:144:VAL:HG12	1.69	0.74
1:A:40:CYS:SG	1:A:41:CYS:N	2.57	0.74
2:F:46:ASN:ND2	2:F:46:ASN:C	2.41	0.74
2:E:91:THR:OG1	2:E:100:ARG:HG3	1.88	0.73
1:B:228:ILE:HD11	1:B:266:TRP:HE1	1.53	0.73
1:A:176:GLN:CA	1:A:182:PRO:O	2.36	0.73
5:A:386:NAG:H61	5:A:387:NDG:H8C3	1.70	0.73
1:B:146:SER:C	1:B:148:ASN:H	1.90	0.73
2:E:43:ASN:HB3	2:E:48:VAL:HG12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD11	1:A:87:LEU:HD11	1.72	0.72
1:B:176:GLN:HE21	1:B:183:LEU:HD13	1.53	0.72
1:A:264:THR:OG1	1:A:277:SER:HB3	1.89	0.72
1:B:178:HIS:CG	1:B:179:GLY:N	2.57	0.72
2:F:88:LYS:HE2	2:F:99:TRP:O	1.90	0.72
2:F:77:ASN:OD1	2:F:115:LYS:HB3	1.90	0.71
1:B:178:HIS:C	1:B:180:GLN:N	2.40	0.70
1:A:353:HIS:CB	1:A:381:ASN:HB3	2.20	0.70
2:F:47:SER:HB3	2:F:49:PHE:CE1	2.23	0.70
1:B:212:LEU:H	1:B:212:LEU:HD23	1.55	0.70
1:A:281:ASN:HD22	5:A:386:NAG:C7	2.05	0.70
1:B:135:VAL:O	1:B:138:LEU:HG	1.91	0.70
1:B:157:ARG:O	1:B:160:GLN:HB3	1.92	0.69
1:B:176:GLN:CB	1:B:182:PRO:O	2.39	0.69
1:B:283:SER:HA	1:B:308:GLN:HB3	1.75	0.69
2:E:55:GLU:OE2	2:E:104:ILE:HB	1.92	0.69
2:E:14:VAL:CG2	2:E:68:CYS:HB3	2.21	0.69
1:B:181:GLY:N	1:B:182:PRO:CD	2.53	0.68
1:B:284:PHE:N	1:B:308:GLN:O	2.24	0.68
2:F:42:VAL:HG23	2:F:90:LEU:HD22	1.75	0.68
1:B:335:PRO:HB3	1:B:342:ARG:NH1	2.07	0.68
1:B:145:LEU:O	1:B:146:SER:HB3	1.93	0.68
1:B:97:THR:HG22	1:B:99:VAL:HG12	1.74	0.68
1:A:149:PRO:C	1:A:178:HIS:HB2	2.13	0.68
1:B:52:ARG:HG2	1:B:53:ASP:N	2.09	0.68
1:A:103:LEU:HD11	1:A:106:VAL:HG22	1.76	0.67
1:A:260:ARG:NH2	5:A:386:NAG:H62	2.03	0.67
1:A:75:ASN:H	1:A:100:LYS:CB	2.08	0.67
1:B:175:LEU:O	1:B:183:LEU:HB2	1.96	0.66
1:B:183:LEU:HG	1:B:184:ALA:N	2.10	0.66
1:A:178:HIS:CG	1:A:179:GLY:N	2.62	0.66
1:B:185:HIS:O	1:B:186:MET:CB	2.36	0.66
1:B:196:LEU:HB3	1:B:276:VAL:HG11	1.78	0.66
1:A:260:ARG:CG	1:A:338:ASN:HA	2.25	0.66
1:A:254:VAL:HG11	1:A:282:VAL:HG11	1.77	0.66
2:F:41:GLU:HA	2:F:49:PHE:O	1.96	0.65
1:A:99:VAL:HA	1:A:123:SER:O	1.96	0.65
1:A:180:GLN:CG	1:A:182:PRO:HG3	2.25	0.65
1:A:98:ILE:HB	1:A:122:LEU:HD23	1.78	0.65
1:A:179:GLY:O	1:A:180:GLN:HB2	1.95	0.65
2:E:104:ILE:HD13	2:E:104:ILE:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:CG	1:B:49:ARG:HB2	2.27	0.65
2:E:6:ILE:HD13	2:E:10:GLY:HA3	1.77	0.65
1:A:227:TRP:HZ2	1:A:247:LEU:O	1.80	0.64
1:B:98:ILE:HB	1:B:122:LEU:HD23	1.78	0.64
1:A:155:ALA:HA	1:A:271:VAL:HB	1.78	0.64
1:A:185:HIS:O	1:A:186:MET:CB	2.34	0.64
3:A:1:NAG:H5	3:A:2:NDG:N2	2.13	0.64
1:B:148:ASN:CB	1:B:150:LEU:HG	2.27	0.64
1:B:196:LEU:HD13	1:B:276:VAL:HG12	1.79	0.64
1:A:221:GLY:HA3	1:A:269:ASN:HB2	1.80	0.64
1:A:84:LEU:HD13	1:A:112:HIS:HB3	1.80	0.63
1:A:374:ILE:HD12	1:A:375:MET:H	1.63	0.63
1:A:296:MET:CE	2:E:6:ILE:HD12	2.28	0.63
1:A:288:VAL:HG23	1:A:370:ALA:HB3	1.80	0.63
1:B:104:ARG:CZ	1:B:128:GLU:HB2	2.28	0.63
1:B:43:HIS:ND1	1:B:44:GLY:N	2.46	0.63
2:E:14:VAL:HB	2:F:112:LEU:HD11	1.81	0.63
1:A:109:ASP:O	1:A:110:ALA:C	2.36	0.62
1:A:260:ARG:HG2	1:A:338:ASN:CA	2.28	0.62
1:A:260:ARG:CB	1:A:338:ASN:HA	2.28	0.62
1:B:146:SER:N	1:B:148:ASN:HD22	1.98	0.62
1:B:176:GLN:CA	1:B:182:PRO:O	2.47	0.62
1:A:288:VAL:HG21	1:A:363:ALA:HB3	1.81	0.62
2:F:46:ASN:HD22	2:F:47:SER:N	1.96	0.62
1:B:288:VAL:HG21	1:B:363:ALA:HB3	1.82	0.62
1:A:176:GLN:HE21	1:A:183:LEU:HD13	1.64	0.62
1:B:244:LEU:H	1:B:245:PRO:HD2	1.64	0.62
1:A:99:VAL:HG23	1:A:123:SER:C	2.20	0.62
1:B:213:LEU:HD23	1:B:249:LEU:O	2.00	0.62
1:B:288:VAL:HG21	1:B:363:ALA:CB	2.28	0.62
1:A:97:THR:HG22	1:A:99:VAL:HG12	1.79	0.62
1:A:365:ASN:HD21	1:A:367:PHE:HD1	1.48	0.62
1:B:290:LEU:HD23	1:B:374:ILE:HG22	1.82	0.62
1:B:70:GLU:HG2	1:B:95:ASN:HD22	1.66	0.61
1:A:296:MET:HE3	2:E:6:ILE:HD12	1.81	0.61
1:B:146:SER:HB3	1:B:175:LEU:HD21	1.81	0.61
1:B:50:CYS:O	1:B:52:ARG:N	2.35	0.60
1:A:362:LEU:HB3	1:A:369:GLN:HE21	1.65	0.60
2:F:6:ILE:HD13	2:F:10:GLY:HA3	1.82	0.60
1:A:119:ARG:HD3	1:A:142:GLU:OE1	2.00	0.60
2:E:6:ILE:CD1	2:E:10:GLY:HA3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD21	1:A:249:LEU:HD12	1.83	0.60
1:B:99:VAL:HG22	1:B:100:LYS:N	2.17	0.60
2:F:67:GLY:HA2	2:F:78:SER:O	2.01	0.60
1:B:180:GLN:C	1:B:182:PRO:HD3	2.22	0.60
2:E:44:ILE:O	2:E:46:ASN:N	2.35	0.60
1:A:249:LEU:HD13	1:A:250:THR:N	2.16	0.59
1:B:177:CYS:O	1:B:180:GLN:HG3	2.03	0.59
1:B:163:GLU:CD	1:B:184:ALA:HB1	2.22	0.59
1:A:244:LEU:H	1:A:245:PRO:HD2	1.66	0.59
1:A:316:LEU:HD23	1:A:321:VAL:HA	1.85	0.59
1:B:97:THR:CG2	1:B:99:VAL:HG12	2.32	0.59
1:A:348:LEU:HD22	1:A:348:LEU:N	2.18	0.59
1:B:149:PRO:O	1:B:178:HIS:CA	2.51	0.59
2:F:47:SER:O	2:F:49:PHE:HD1	1.86	0.59
1:A:43:HIS:ND1	1:A:44:GLY:N	2.51	0.59
1:A:249:LEU:C	1:A:249:LEU:HD13	2.23	0.58
1:B:227:TRP:HZ2	1:B:247:LEU:O	1.86	0.58
1:B:352:THR:HG21	2:E:31:ILE:HD11	1.85	0.58
1:B:353:HIS:HA	1:B:356:ASN:OD1	2.02	0.58
2:F:45:ASN:O	2:F:46:ASN:ND2	2.35	0.58
1:A:316:LEU:HG	1:A:362:LEU:HD21	1.83	0.58
1:A:42:PRO:HG2	1:A:49:ARG:HB2	1.84	0.58
1:B:103:LEU:HD21	1:B:106:VAL:HG22	1.85	0.58
1:B:118:SER:C	1:B:140:LEU:HD12	2.24	0.58
1:B:177:CYS:N	1:B:182:PRO:O	2.36	0.58
2:F:91:THR:OG1	2:F:100:ARG:HG3	2.04	0.58
1:A:99:VAL:HG23	1:A:123:SER:O	2.04	0.58
1:B:269:ASN:HD21	1:B:271:VAL:HG13	1.68	0.58
1:B:123:SER:HB3	1:B:144:VAL:HG12	1.85	0.58
1:B:99:VAL:HG23	1:B:124:PHE:HB2	1.86	0.58
1:B:365:ASN:ND2	1:B:367:PHE:HD2	2.00	0.58
1:B:43:HIS:CD2	1:B:47:GLY:HA3	2.39	0.58
1:B:110:ALA:O	1:B:112:HIS:N	2.37	0.57
1:B:72:TYR:HB3	1:B:74:GLU:OE2	2.03	0.57
1:B:297:HIS:HA	2:F:13:SER:OG	2.03	0.57
1:A:358:ASN:CG	6:A:389:NDG:HA	2.08	0.57
1:A:193:VAL:HG12	1:A:194:PRO:CD	2.31	0.57
1:A:98:ILE:HB	1:A:122:LEU:CD2	2.33	0.57
1:B:290:LEU:HD13	1:B:372:ALA:HB3	1.87	0.57
1:B:316:LEU:HB2	1:B:360:THR:HB	1.86	0.57
2:E:87:VAL:HG23	2:E:104:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:HA	1:A:182:PRO:O	2.03	0.57
1:A:237:THR:HG22	1:A:251:LEU:CD2	2.35	0.57
1:B:345:CYS:SG	2:F:6:ILE:HG13	2.45	0.57
1:A:215:CYS:HB2	1:A:227:TRP:CH2	2.39	0.57
1:A:98:ILE:O	1:A:98:ILE:HG22	2.05	0.57
1:A:73:ILE:HG22	1:A:73:ILE:O	2.05	0.57
1:B:99:VAL:HG23	1:B:123:SER:C	2.25	0.57
1:B:145:LEU:O	1:B:175:LEU:CD2	2.52	0.57
1:B:237:THR:HG22	1:B:251:LEU:CD2	2.34	0.56
1:B:296:MET:CE	2:F:6:ILE:HD12	2.35	0.56
1:B:99:VAL:CG2	1:B:124:PHE:HB2	2.35	0.56
2:F:95:LYS:HD2	2:F:96:GLN:HE21	1.70	0.56
2:E:9:ARG:HG2	2:E:9:ARG:HH11	1.71	0.56
1:B:186:MET:HG2	1:B:187:PRO:CD	2.33	0.56
1:B:306:ASP:OD1	1:B:307:GLY:N	2.39	0.56
1:B:181:GLY:N	1:B:182:PRO:HD3	2.20	0.56
1:A:234:GLN:HG2	1:A:257:ASP:HB2	1.88	0.56
1:B:170:VAL:N	1:B:171:PRO:CD	2.69	0.56
1:A:88:ARG:HH11	1:A:113:PHE:HZ	1.54	0.56
1:B:229:LEU:N	1:B:229:LEU:HD12	2.21	0.56
1:A:243:GLY:C	1:A:244:LEU:HD22	2.26	0.55
1:A:97:THR:CG2	1:A:99:VAL:HG12	2.36	0.55
1:A:229:LEU:HD12	1:A:229:LEU:N	2.21	0.55
2:E:6:ILE:O	2:E:6:ILE:HD13	2.06	0.55
1:B:296:MET:HE3	2:F:6:ILE:HD12	1.87	0.55
1:A:296:MET:HE1	2:E:6:ILE:HG23	1.89	0.55
1:A:177:CYS:H	1:A:182:PRO:C	2.09	0.55
1:B:183:LEU:C	1:B:185:HIS:H	2.10	0.55
1:A:352:THR:OG1	1:A:354:VAL:HG22	2.07	0.55
1:A:288:VAL:CG2	1:A:363:ALA:HB3	2.36	0.55
1:B:98:ILE:O	1:B:98:ILE:HG22	2.07	0.55
2:E:85:THR:HG23	2:E:104:ILE:HD11	1.87	0.55
1:A:268:GLU:HG2	1:A:273:ARG:HB2	1.89	0.55
1:A:70:GLU:HG2	1:A:95:ASN:HB2	1.88	0.55
1:B:148:ASN:HB3	1:B:150:LEU:HG	1.89	0.55
2:E:85:THR:HG22	2:E:106:THR:HB	1.88	0.55
1:A:75:ASN:N	1:A:100:LYS:HB2	2.21	0.54
1:B:179:GLY:O	1:B:180:GLN:HB2	2.05	0.54
1:B:264:THR:OG1	1:B:277:SER:HB3	2.07	0.54
1:A:75:ASN:N	1:A:100:LYS:O	2.41	0.54
1:B:362:LEU:HB3	1:B:369:GLN:HE21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:HD2	1:B:49:ARG:O	2.08	0.54
1:A:146:SER:O	1:A:147:GLY:C	2.46	0.54
2:F:68:CYS:HB2	2:F:71:ILE:HD13	1.89	0.54
1:A:69:THR:HA	1:A:93:LEU:HA	1.88	0.53
1:B:183:LEU:O	1:B:185:HIS:O	2.26	0.53
1:B:225:ALA:HB1	1:B:247:LEU:HD21	1.89	0.53
2:F:115:LYS:O	2:F:116:ALA:HB3	2.07	0.53
1:A:196:LEU:HD13	1:A:276:VAL:HG12	1.90	0.53
1:B:178:HIS:CG	1:B:179:GLY:H	2.25	0.53
2:F:74:LYS:O	2:F:115:LYS:HD2	2.09	0.53
1:A:165:GLU:HB3	1:A:167:LEU:HG	1.90	0.53
1:A:200:VAL:HB	1:A:201:PRO:HD2	1.89	0.53
1:A:267:ALA:O	1:A:273:ARG:HG3	2.08	0.53
1:A:266:TRP:O	1:A:267:ALA:HB2	2.08	0.53
1:A:333:LEU:HB3	2:E:9:ARG:NH2	2.24	0.53
1:B:290:LEU:HD11	1:B:361:LEU:HB3	1.91	0.53
1:A:186:MET:HG2	1:A:187:PRO:CD	2.37	0.53
1:A:288:VAL:HG21	1:A:363:ALA:CB	2.39	0.53
1:A:43:HIS:CD2	1:A:47:GLY:HA3	2.43	0.53
2:F:42:VAL:HG13	2:F:44:ILE:HD11	1.89	0.53
1:B:155:ALA:HA	1:B:271:VAL:HB	1.89	0.53
1:B:196:LEU:CD2	1:B:217:VAL:HG22	2.32	0.53
1:A:104:ARG:HG2	1:A:104:ARG:HH11	1.73	0.53
1:B:103:LEU:HD21	1:B:106:VAL:CG2	2.38	0.53
2:F:42:VAL:HG13	2:F:44:ILE:CD1	2.38	0.53
1:B:104:ARG:O	1:B:127:LEU:HD12	2.09	0.53
1:B:84:LEU:HD13	1:B:112:HIS:HB3	1.91	0.53
1:B:85:ARG:O	1:B:85:ARG:HD2	2.08	0.53
1:A:123:SER:O	1:A:124:PHE:C	2.47	0.53
1:A:157:ARG:HE	1:A:160:GLN:CG	2.17	0.53
1:A:163:GLU:CD	1:A:184:ALA:HB1	2.28	0.53
1:A:209:ASP:O	1:A:254:VAL:HG23	2.08	0.53
1:A:85:ARG:HD2	1:A:85:ARG:O	2.07	0.53
1:A:165:GLU:CB	1:A:167:LEU:HG	2.40	0.52
1:A:256:SER:C	1:A:258:LEU:H	2.12	0.52
1:A:317:PHE:HE1	1:A:357:GLY:HA3	1.74	0.52
4:A:383:NAG:H83	4:A:383:NAG:O3	2.09	0.52
1:B:128:GLU:OE1	1:B:151:HIS:HB2	2.10	0.52
1:B:149:PRO:CA	1:B:178:HIS:HB2	2.39	0.52
1:B:73:ILE:HG22	1:B:73:ILE:O	2.09	0.52
1:A:123:SER:HB3	1:A:144:VAL:CG1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TRP:O	1:B:134:THR:N	2.43	0.52
1:B:348:LEU:HD22	1:B:348:LEU:N	2.24	0.52
1:A:186:MET:O	1:A:187:PRO:C	2.47	0.52
2:E:85:THR:O	2:E:104:ILE:HD13	2.09	0.52
1:B:301:ILE:HD12	1:B:346:LEU:HD23	1.91	0.52
1:A:313:LEU:HD22	1:A:361:LEU:HD11	1.91	0.52
2:F:39:LEU:HD23	2:F:90:LEU:O	2.10	0.52
1:A:170:VAL:N	1:A:171:PRO:CD	2.73	0.51
3:A:1:NAG:H5	3:A:2:NDG:C7	2.39	0.51
1:B:178:HIS:O	1:B:180:GLN:N	2.19	0.51
1:A:103:LEU:O	1:A:127:LEU:HD13	2.11	0.51
1:B:110:ALA:C	1:B:112:HIS:H	2.14	0.51
1:A:334:GLU:OE2	1:A:335:PRO:HD2	2.10	0.51
1:A:89:GLY:O	1:A:90:LEU:C	2.48	0.51
1:B:244:LEU:N	1:B:245:PRO:HD2	2.25	0.51
2:F:95:LYS:HE2	2:F:95:LYS:H	1.76	0.51
1:A:295:GLU:HB2	1:A:299:TRP:CE2	2.45	0.51
2:F:95:LYS:CE	2:F:95:LYS:H	2.22	0.51
1:A:177:CYS:N	1:A:182:PRO:O	2.44	0.51
1:A:332:PHE:HB3	1:A:342:ARG:NH2	2.24	0.51
2:E:14:VAL:HG23	2:E:69:ARG:O	2.11	0.51
1:B:186:MET:O	1:B:187:PRO:C	2.46	0.51
1:B:256:SER:HA	1:B:282:VAL:HG21	1.93	0.51
1:B:308:GLN:HA	1:B:309:PRO:C	2.31	0.51
1:B:40:CYS:SG	1:B:49:ARG:C	2.89	0.51
2:F:48:VAL:HG23	2:F:48:VAL:O	2.10	0.51
1:A:146:SER:C	1:A:148:ASN:N	2.58	0.51
1:A:170:VAL:O	1:A:171:PRO:C	2.49	0.51
1:A:183:LEU:C	1:A:185:HIS:H	2.12	0.51
1:B:48:LEU:HB2	1:B:71:LEU:HD23	1.91	0.51
1:B:75:ASN:O	1:B:76:GLN:HG3	2.11	0.51
1:A:110:ALA:O	1:A:112:HIS:N	2.41	0.50
1:B:40:CYS:O	1:B:41:CYS:SG	2.70	0.50
1:B:271:VAL:HG13	1:B:271:VAL:O	2.11	0.50
2:E:79:TYR:CE1	2:E:111:VAL:HB	2.47	0.50
1:A:317:PHE:CE1	1:A:357:GLY:HA3	2.46	0.50
1:A:308:GLN:HA	1:A:309:PRO:C	2.32	0.50
2:F:2:SER:HA	2:F:7:PHE:CE2	2.46	0.50
1:A:176:GLN:NE2	1:A:183:LEU:HD13	2.25	0.50
1:A:176:GLN:HA	1:A:183:LEU:HA	1.92	0.50
1:B:135:VAL:O	1:B:136:GLN:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:HB2	1:B:299:TRP:CE2	2.46	0.50
1:A:178:HIS:CG	1:A:179:GLY:H	2.27	0.50
1:B:69:THR:HA	1:B:93:LEU:HA	1.94	0.50
2:F:68:CYS:HB2	2:F:71:ILE:CD1	2.42	0.50
1:A:43:HIS:HB2	1:A:49:ARG:HG3	1.94	0.49
1:B:300:CYS:SG	1:B:302:PRO:HG3	2.52	0.49
2:E:59:ARG:O	2:E:60:ASP:C	2.50	0.49
2:F:13:SER:O	2:F:69:ARG:NH1	2.45	0.49
1:B:152:CYS:HA	1:B:156:LEU:HD12	1.93	0.49
2:E:112:LEU:N	2:E:112:LEU:HD12	2.27	0.49
1:A:133:LYS:O	1:A:134:THR:C	2.51	0.49
1:B:93:LEU:HD23	1:B:93:LEU:C	2.33	0.49
1:A:237:THR:HG22	1:A:251:LEU:HD23	1.94	0.49
1:A:353:HIS:CG	1:A:381:ASN:HB3	2.47	0.49
1:A:93:LEU:HD23	1:A:93:LEU:C	2.31	0.49
1:B:223:GLU:HB2	1:B:268:GLU:O	2.11	0.49
2:F:93:ASP:O	2:F:96:GLN:HB2	2.11	0.49
1:B:213:LEU:HD21	1:B:249:LEU:HD12	1.95	0.49
1:B:88:ARG:HA	1:B:113:PHE:CE2	2.47	0.49
2:E:88:LYS:HE3	2:E:99:TRP:C	2.32	0.49
1:A:104:ARG:HG3	1:A:126:ALA:O	2.13	0.49
1:B:353:HIS:CD2	1:B:381:ASN:HB3	2.47	0.49
3:A:2:NDG:H6C2	3:A:2:NDG:O3	2.13	0.48
1:A:284:PHE:CE1	1:A:308:GLN:HB3	2.47	0.48
1:A:43:HIS:CD2	1:A:49:ARG:HE	2.30	0.48
1:B:283:SER:CA	1:B:308:GLN:O	2.61	0.48
1:B:40:CYS:SG	1:B:49:ARG:O	2.71	0.48
1:A:254:VAL:CG1	1:A:282:VAL:HG11	2.43	0.48
1:A:284:PHE:HB2	1:A:285:PRO:HD2	1.95	0.48
1:B:108:PRO:CB	1:B:133:LYS:HB3	2.43	0.48
1:A:109:ASP:O	1:A:112:HIS:N	2.47	0.48
1:A:40:CYS:SG	1:A:49:ARG:O	2.72	0.48
1:B:238:VAL:N	1:B:250:THR:O	2.47	0.48
1:A:74:GLU:HG2	1:A:99:VAL:CG1	2.44	0.48
1:B:264:THR:HG22	1:B:265:CYS:N	2.29	0.48
2:F:6:ILE:HD13	2:F:10:GLY:CA	2.44	0.48
1:A:104:ARG:HD3	1:A:105:PHE:HE1	1.79	0.48
1:B:182:PRO:O	1:B:183:LEU:HB3	2.14	0.47
1:B:288:VAL:CG2	1:B:363:ALA:HB3	2.43	0.47
1:B:43:HIS:CD2	1:B:49:ARG:HE	2.32	0.47
1:B:93:LEU:HD21	1:B:95:ASN:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:CZ2	1:A:346:LEU:HB2	2.47	0.47
1:B:246:SER:C	1:B:247:LEU:HD12	2.34	0.47
1:A:135:VAL:O	1:A:138:LEU:HG	2.15	0.47
1:A:259:ASN:ND2	1:A:282:VAL:HG23	2.30	0.47
2:F:47:SER:O	2:F:49:PHE:CD1	2.67	0.47
1:B:99:VAL:CG2	1:B:100:LYS:N	2.77	0.47
1:B:149:PRO:O	1:B:178:HIS:N	2.47	0.47
1:B:183:LEU:O	1:B:185:HIS:N	2.33	0.47
2:E:42:VAL:HG22	2:E:43:ASN:N	2.30	0.47
1:B:176:GLN:HA	1:B:182:PRO:O	2.13	0.47
1:B:356:ASN:HA	1:B:376:ALA:O	2.14	0.47
1:B:74:GLU:O	1:B:75:ASN:HB2	2.14	0.47
1:A:107:ALA:O	1:A:109:ASP:N	2.47	0.47
1:A:106:VAL:HG23	1:A:127:LEU:HD11	1.97	0.47
1:A:113:PHE:O	1:A:115:PRO:HD3	2.15	0.47
1:A:70:GLU:HB3	1:A:72:TYR:HE1	1.80	0.47
1:A:93:LEU:HD21	1:A:95:ASN:C	2.35	0.47
1:B:98:ILE:HB	1:B:122:LEU:CD2	2.42	0.47
1:A:182:PRO:O	1:A:183:LEU:HB3	2.14	0.47
1:A:316:LEU:HB2	1:A:360:THR:HB	1.96	0.47
1:B:165:GLU:HB2	1:B:167:LEU:HG	1.97	0.47
1:B:328:ILE:HG12	1:B:348:LEU:HD12	1.97	0.47
1:B:313:LEU:HG	1:B:361:LEU:HD11	1.96	0.47
1:A:212:LEU:HD23	1:A:212:LEU:N	2.19	0.46
1:A:290:LEU:HD23	1:A:374:ILE:CG2	2.40	0.46
2:E:44:ILE:O	2:E:45:ASN:C	2.53	0.46
2:E:95:LYS:HG3	2:E:96:GLN:HG2	1.97	0.46
1:A:152:CYS:HA	1:A:156:LEU:HD12	1.97	0.46
2:F:39:LEU:HD23	2:F:90:LEU:C	2.36	0.46
1:A:99:VAL:CG2	1:A:124:PHE:HB2	2.45	0.46
1:B:270:ASP:OD2	1:B:271:VAL:HG12	2.15	0.46
1:B:68:LEU:HD23	1:B:68:LEU:N	2.31	0.46
1:A:75:ASN:O	1:A:76:GLN:HG3	2.16	0.46
1:A:84:LEU:CD1	1:A:112:HIS:HB3	2.44	0.46
1:A:281:ASN:ND2	5:A:386:NAG:C7	2.73	0.46
1:A:365:ASN:ND2	1:A:367:PHE:HD1	2.11	0.46
1:A:53:ASP:HA	1:A:76:GLN:HG2	1.97	0.46
1:A:183:LEU:HD21	1:A:185:HIS:ND1	2.30	0.46
1:A:349:ASN:O	2:F:103:ARG:NH2	2.49	0.46
1:A:37:PRO:O	1:A:38:ASP:HB2	2.16	0.46
1:A:281:ASN:HD22	5:A:386:NAG:C8	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:C	1:A:136:GLN:HE21	2.18	0.46
1:A:193:VAL:CG1	1:A:194:PRO:HD2	2.34	0.46
1:B:104:ARG:HG3	1:B:126:ALA:O	2.16	0.46
1:B:87:LEU:N	1:B:87:LEU:HD12	2.30	0.46
1:A:256:SER:O	1:A:258:LEU:N	2.47	0.46
1:A:68:LEU:HD23	1:A:68:LEU:N	2.30	0.46
1:B:85:ARG:C	1:B:85:ARG:HD2	2.37	0.46
2:F:37:MET:HB2	2:F:92:MET:HB2	1.98	0.46
1:A:244:LEU:N	1:A:245:PRO:HD2	2.30	0.46
1:A:260:ARG:HG2	1:A:338:ASN:N	2.31	0.46
1:B:247:LEU:HD12	1:B:247:LEU:N	2.31	0.46
2:E:39:LEU:HD22	2:E:39:LEU:N	2.31	0.46
2:F:57:LYS:HA	2:F:82:THR:HG23	1.97	0.46
1:A:103:LEU:HB3	1:A:125:ASN:HD21	1.81	0.45
1:A:213:LEU:N	1:A:213:LEU:HD23	2.31	0.45
1:A:241:SER:HB3	1:A:248:GLY:HA3	1.98	0.45
1:A:239:MET:HB3	1:A:249:LEU:HD23	1.98	0.45
1:A:271:VAL:O	1:A:271:VAL:HG22	2.15	0.45
1:B:183:LEU:CG	1:B:184:ALA:N	2.69	0.45
1:B:234:GLN:O	1:B:235:SER:HB2	2.16	0.45
1:A:183:LEU:O	1:A:185:HIS:N	2.37	0.45
1:B:316:LEU:HD23	1:B:321:VAL:HA	1.98	0.45
1:A:102:GLY:O	1:A:103:LEU:C	2.54	0.45
1:A:110:ALA:C	1:A:112:HIS:H	2.20	0.45
1:B:249:LEU:C	1:B:249:LEU:HD13	2.37	0.45
2:F:59:ARG:O	2:F:60:ASP:C	2.54	0.45
1:A:353:HIS:CD2	1:A:381:ASN:HB2	2.52	0.45
1:B:148:ASN:HB2	1:B:150:LEU:HG	1.98	0.45
1:B:283:SER:HA	1:B:308:GLN:O	2.17	0.45
2:F:95:LYS:HD2	2:F:95:LYS:H	1.77	0.45
1:A:98:ILE:HG21	1:A:103:LEU:HD22	1.99	0.45
1:A:120:LEU:HD11	1:A:122:LEU:HG	1.99	0.45
3:A:1:NAG:H5	3:A:2:NDG:O7	2.16	0.45
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.82	0.45
2:E:90:LEU:HB2	2:E:99:TRP:HZ3	1.81	0.45
1:A:227:TRP:CE3	1:A:265:CYS:HB3	2.51	0.45
1:A:345:CYS:SG	2:E:6:ILE:HG13	2.56	0.45
1:A:127:LEU:HB2	1:A:148:ASN:OD1	2.17	0.45
1:B:73:ILE:O	1:B:75:ASN:N	2.43	0.45
1:B:51:THR:HG23	1:B:74:GLU:OE1	2.16	0.45
1:B:68:LEU:HD12	1:B:71:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:LEU:HD22	2:F:39:LEU:N	2.32	0.45
1:B:108:PRO:HB3	1:B:133:LYS:HB3	1.98	0.44
1:B:100:LYS:N	1:B:124:PHE:O	2.50	0.44
1:A:207:VAL:HG22	1:A:208:GLY:N	2.32	0.44
1:A:87:LEU:N	1:A:87:LEU:HD12	2.32	0.44
1:B:136:GLN:HE21	1:B:136:GLN:C	2.19	0.44
1:A:125:ASN:OD1	1:A:126:ALA:N	2.45	0.44
1:A:353:HIS:HB3	1:A:380:ASP:O	2.16	0.44
1:B:163:GLU:OE2	1:B:184:ALA:CB	2.66	0.44
1:B:51:THR:O	1:B:52:ARG:HB2	2.17	0.44
2:F:87:VAL:CG2	2:F:104:ILE:HD11	2.47	0.44
1:A:100:LYS:N	1:A:124:PHE:O	2.48	0.44
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.76	0.44
4:B:383:NAG:O3	4:B:384:NDG:H2	2.18	0.44
2:E:9:ARG:HG2	2:E:9:ARG:NH1	2.32	0.44
1:A:145:LEU:O	1:A:175:LEU:CD2	2.62	0.44
1:A:314:ARG:HH21	1:A:362:LEU:HG	1.83	0.44
1:A:68:LEU:HD12	1:A:71:LEU:HG	1.99	0.44
1:A:78:HIS:O	1:A:79:LEU:HB3	2.17	0.44
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.73	0.44
1:B:52:ARG:CG	1:B:53:ASP:H	2.23	0.44
1:B:177:CYS:H	1:B:182:PRO:C	2.21	0.44
1:A:212:LEU:CD2	1:A:212:LEU:H	2.23	0.44
1:A:271:VAL:O	1:A:271:VAL:HG13	2.18	0.44
1:A:229:LEU:HD23	1:A:232:LEU:HD12	1.99	0.44
1:B:288:VAL:HG21	1:B:363:ALA:HB2	1.98	0.44
1:A:99:VAL:HG22	1:A:100:LYS:N	2.33	0.43
1:B:183:LEU:C	1:B:185:HIS:N	2.72	0.43
2:E:99:TRP:C	2:E:100:ARG:HG2	2.37	0.43
2:F:59:ARG:O	2:F:59:ARG:CG	2.66	0.43
1:A:183:LEU:C	1:A:185:HIS:N	2.72	0.43
1:A:100:LYS:O	1:A:101:SER:OG	2.33	0.43
1:A:288:VAL:HG23	1:A:370:ALA:CB	2.45	0.43
1:A:36:CYS:HA	1:A:37:PRO:HA	1.83	0.43
1:B:163:GLU:OE2	1:B:184:ALA:HB1	2.17	0.43
1:B:53:ASP:HA	1:B:76:GLN:HA	2.00	0.43
1:A:114:THR:O	1:A:114:THR:HG23	2.18	0.43
1:B:343:HIS:CD2	2:F:5:PRO:HG2	2.53	0.43
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.84	0.43
1:A:221:GLY:O	1:A:222:LEU:HB2	2.19	0.43
1:A:288:VAL:CG2	1:A:363:ALA:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:O	1:A:126:ALA:HB3	2.18	0.43
1:A:118:SER:C	1:A:140:LEU:HD12	2.39	0.43
1:A:254:VAL:HG12	1:A:255:THR:O	2.19	0.43
1:A:258:LEU:HD21	1:A:280:VAL:HG21	2.01	0.43
1:B:104:ARG:HA	1:B:127:LEU:CA	2.32	0.43
1:B:120:LEU:N	1:B:140:LEU:HD11	2.33	0.43
1:B:146:SER:O	1:B:148:ASN:N	2.49	0.43
1:B:221:GLY:HA3	1:B:269:ASN:HB2	2.01	0.43
2:F:94:GLY:C	2:F:96:GLN:H	2.22	0.43
1:B:243:GLY:C	1:B:244:LEU:HD22	2.38	0.43
2:F:42:VAL:CG1	2:F:44:ILE:HD11	2.48	0.43
1:A:298:HIS:ND1	1:A:347:ARG:NH2	2.66	0.43
2:E:14:VAL:HB	2:F:112:LEU:CD1	2.48	0.43
1:A:75:ASN:O	1:A:76:GLN:CG	2.67	0.42
1:B:114:THR:HG21	1:B:117:LEU:HD12	2.01	0.42
2:F:87:VAL:HG21	2:F:104:ILE:HD11	2.00	0.42
1:A:138:LEU:O	1:A:139:SER:HB2	2.19	0.42
1:A:316:LEU:HG	1:A:362:LEU:CD2	2.47	0.42
1:B:99:VAL:HB	1:B:123:SER:OG	2.19	0.42
1:A:301:ILE:HB	1:A:346:LEU:HB3	2.00	0.42
1:A:84:LEU:HB2	1:A:109:ASP:CG	2.39	0.42
1:A:291:HIS:HB2	1:A:302:PRO:HB2	2.01	0.42
1:B:172:GLU:CD	1:B:172:GLU:H	2.23	0.42
1:B:205:VAL:HG12	1:B:206:ASP:N	2.34	0.42
1:A:374:ILE:HD12	1:A:375:MET:N	2.34	0.42
1:A:308:GLN:HA	1:A:308:GLN:HE21	1.85	0.42
1:B:109:ASP:OD2	1:B:112:HIS:HB2	2.19	0.42
1:B:146:SER:O	1:B:147:GLY:C	2.55	0.42
1:B:176:GLN:HA	1:B:183:LEU:CB	2.50	0.42
1:B:41:CYS:N	1:B:42:PRO:CD	2.83	0.42
2:F:79:TYR:CE1	2:F:111:VAL:HB	2.55	0.42
1:B:74:GLU:O	1:B:100:LYS:HB2	2.20	0.42
1:B:123:SER:O	1:B:124:PHE:C	2.58	0.42
1:B:288:VAL:CG2	1:B:363:ALA:CB	2.95	0.42
1:A:234:GLN:O	1:A:235:SER:HB2	2.20	0.42
1:B:114:THR:HG23	1:B:114:THR:O	2.20	0.42
2:E:22:VAL:CG2	2:E:55:GLU:HG3	2.49	0.42
2:E:74:LYS:C	2:E:75:HIS:HD2	2.23	0.42
2:E:84:HIS:ND1	2:E:103:ARG:NH1	2.67	0.42
2:F:99:TRP:HA	2:F:99:TRP:CE3	2.54	0.42
1:A:295:GLU:HB2	1:A:299:TRP:CZ2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:O	1:A:40:CYS:HB2	2.17	0.41
1:A:82:LEU:HD11	1:A:87:LEU:CD1	2.47	0.41
1:B:162:TRP:HB3	1:B:170:VAL:HG21	2.02	0.41
1:B:54:GLY:N	1:B:76:GLN:HG2	2.34	0.41
1:B:99:VAL:HG23	1:B:123:SER:O	2.19	0.41
2:F:88:LYS:HD2	2:F:88:LYS:HA	1.88	0.41
1:B:111:PHE:O	1:B:112:HIS:C	2.58	0.41
1:B:43:HIS:CD2	1:B:49:ARG:NE	2.88	0.41
2:F:76:TRP:CZ3	2:F:114:ARG:HG3	2.55	0.41
2:F:90:LEU:HB2	2:F:99:TRP:HZ3	1.84	0.41
1:A:288:VAL:HG12	1:A:289:GLN:N	2.35	0.41
1:A:300:CYS:O	1:A:302:PRO:HD3	2.21	0.41
1:B:183:LEU:HD21	1:B:185:HIS:ND1	2.35	0.41
1:B:269:ASN:ND2	1:B:271:VAL:CG1	2.84	0.41
1:B:288:VAL:HG23	1:B:370:ALA:HB3	2.01	0.41
1:A:311:PRO:HA	1:A:364:ALA:O	2.21	0.41
1:A:335:PRO:HB3	1:A:342:ARG:NH1	2.36	0.41
1:A:87:LEU:O	1:A:89:GLY:N	2.54	0.41
1:A:247:LEU:HD12	1:A:247:LEU:N	2.35	0.41
1:A:92:GLU:HG3	1:A:92:GLU:O	2.21	0.41
1:B:335:PRO:HD3	1:B:342:ARG:NH1	2.26	0.41
1:A:104:ARG:HA	1:A:126:ALA:O	2.21	0.41
1:A:244:LEU:N	1:A:244:LEU:HD22	2.35	0.41
1:A:74:GLU:H	1:A:74:GLU:HG3	1.65	0.41
1:B:258:LEU:HD23	1:B:280:VAL:HG11	2.02	0.41
2:E:18:VAL:HG13	2:E:18:VAL:O	2.20	0.41
2:E:99:TRP:CE3	2:E:99:TRP:HA	2.55	0.41
2:F:95:LYS:CD	2:F:96:GLN:HE21	2.33	0.41
1:A:289:GLN:HG2	1:A:304:SER:HB2	2.03	0.41
2:E:45:ASN:O	2:E:46:ASN:CG	2.59	0.41
1:A:172:GLU:H	1:A:172:GLU:CD	2.25	0.41
1:B:109:ASP:O	1:B:110:ALA:C	2.59	0.41
1:B:110:ALA:C	1:B:112:HIS:N	2.75	0.41
1:B:287:SER:C	1:B:288:VAL:HG23	2.42	0.41
1:B:87:LEU:O	1:B:89:GLY:N	2.54	0.41
1:A:333:LEU:HB3	2:E:9:ARG:HH21	1.85	0.41
2:F:115:LYS:O	2:F:116:ALA:CB	2.69	0.41
2:F:45:ASN:HD22	2:F:45:ASN:HA	1.62	0.41
1:A:196:LEU:HB3	1:A:276:VAL:HG11	2.03	0.40
1:A:308:GLN:NE2	1:A:309:PRO:HA	2.36	0.40
1:B:214:ARG:NH1	1:B:214:ARG:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:390:NDG:C1	6:A:390:NDG:O6	2.69	0.40
1:B:124:PHE:N	1:B:124:PHE:CD1	2.90	0.40
2:F:4:HIS:HA	2:F:5:PRO:HD3	1.97	0.40
1:B:296:MET:HE1	2:F:6:ILE:HG23	2.02	0.40
2:F:84:HIS:ND1	2:F:103:ARG:NH1	2.69	0.40
1:B:239:MET:O	1:B:240:LYS:HB2	2.22	0.40
2:E:93:ASP:O	2:E:93:ASP:OD1	2.39	0.40
1:B:213:LEU:N	1:B:213:LEU:HD23	2.37	0.40
1:A:196:LEU:HA	1:A:196:LEU:HD23	1.92	0.40
2:E:88:LYS:HE2	2:E:99:TRP:CD1	2.57	0.40

There are no symmetry-related clashes.

## 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	345/347 (99%)	250 (72%)	57 (16%)	38 (11%)	0	5
1	B	345/347 (99%)	262 (76%)	47 (14%)	36 (10%)	0	6
2	E	104/120 (87%)	96 (92%)	4 (4%)	4 (4%)	4	29
2	F	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
All	All	899/934 (96%)	710 (79%)	111 (12%)	78 (9%)	1	9

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	78	HIS
1	A	90	LEU
1	A	103	LEU
1	A	110	ALA

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Mol	Chain	Res	Type
1	A	111	PHE
1	A	182	PRO
1	A	186	MET
1	A	271	VAL
1	B	111	PHE
1	B	133	LYS
1	B	182	PRO
1	B	186	MET
2	E	45	ASN
1	A	42	PRO
1	A	88	ARG
1	A	100	LYS
1	A	109	ASP
1	A	116	ARG
1	A	134	THR
1	A	137	GLY
1	A	235	SER
1	A	267	ALA
1	B	42	PRO
1	B	44	GLY
1	B	51	THR
1	B	53	ASP
1	B	75	ASN
1	B	79	LEU
1	B	88	ARG
1	B	100	LYS
1	B	101	SER
1	B	109	ASP
1	B	110	ALA
1	B	116	ARG
1	B	123	SER
1	B	184	ALA
1	B	204	SER
1	B	235	SER
2	E	46	ASN
2	E	93	ASP
1	A	69	THR
1	A	124	PHE
1	A	155	ALA
1	A	180	GLN
1	A	184	ALA
1	A	257	ASP

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Mol	Chain	Res	Type
1	A	270	ASP
1	A	281	ASN
1	B	38	ASP
1	B	41	CYS
1	B	74	GLU
1	B	180	GLN
1	B	267	ALA
1	A	55	ALA
1	A	68	LEU
1	A	75	ASN
1	A	117	LEU
1	A	222	LEU
1	B	39	ALA
1	B	117	LEU
1	B	231	GLU
1	A	46	SER
1	A	77	GLN
1	A	131	SER
1	B	45	SER
1	B	113	PHE
1	B	171	PRO
1	B	338	ASN
1	A	171	PRO
1	B	102	GLY
1	B	108	PRO
1	B	155	ALA
2	E	95	LYS
1	A	221	GLY
1	A	244	LEU
1	A	179	GLY
1	B	244	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/293 (100%)	274 (94%)	19 (6%)	20	58
1	B	293/293 (100%)	277 (94%)	16 (6%)	25	63
2	E	96/106 (91%)	86 (90%)	10 (10%)	8	34
2	F	96/106 (91%)	86 (90%)	10 (10%)	8	34
All	All	778/798 (98%)	723 (93%)	55 (7%)	17	54

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	CYS
1	A	77	GLN
1	A	117	LEU
1	A	127	LEU
1	A	136	GLN
1	A	157	ARG
1	A	182	PRO
1	A	183	LEU
1	A	193	VAL
1	A	212	LEU
1	A	234	GLN
1	A	260	ARG
1	A	294	VAL
1	A	300	CYS
1	A	321	VAL
1	A	338	ASN
1	A	348	LEU
1	A	352	THR
1	A	381	ASN
1	B	50	CYS
1	B	68	LEU
1	B	74	GLU
1	B	77	GLN
1	B	136	GLN
1	B	157	ARG
1	B	182	PRO
1	B	183	LEU
1	B	193	VAL
1	B	234	GLN
1	B	260	ARG

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Mol	Chain	Res	Type
1	B	294	VAL
1	B	300	CYS
1	B	308	GLN
1	B	338	ASN
1	B	381	ASN
2	E	6	ILE
2	E	9	ARG
2	E	45	ASN
2	E	51	GLN
2	E	60	ASP
2	E	77	ASN
2	E	93	ASP
2	E	99	TRP
2	E	100	ARG
2	E	104	ILE
2	F	6	ILE
2	F	45	ASN
2	F	46	ASN
2	F	47	SER
2	F	51	GLN
2	F	60	ASP
2	F	68	CYS
2	F	93	ASP
2	F	95	LYS
2	F	100	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	136	GLN
1	A	176	GLN
1	A	180	GLN
1	A	234	GLN
1	A	253	ASN
1	A	308	GLN
1	A	369	GLN
1	A	381	ASN
1	B	136	GLN
1	B	148	ASN
1	B	176	GLN
1	B	180	GLN

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Mol	Chain	Res	Type
1	B	234	GLN
1	B	253	ASN
1	B	297	HIS
1	B	308	GLN
1	B	369	GLN
2	E	75	HIS
2	F	45	ASN
2	F	46	ASN
2	F	75	HIS
2	F	96	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 ⓘ

34 carbohydrates 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	$\# Z  > 2$
3	NAG	A	1	1,3	14,14,15	0.70	0	15,19,21	0.80	0
3	NDG	A	2	3	14,14,15	0.63	0	15,19,21	0.82	1 (6%)
4	NAG	A	383	1,4	14,14,15	0.65	0	15,19,21	0.81	0
4	NDG	A	384	4	14,14,15	0.65	0	15,19,21	0.78	0
4	MAN	A	385	4	11,11,12	0.56	0	13,15,17	0.45	0
5	NAG	A	386	1,5	14,14,15	0.58	0	15,19,21	0.77	0
5	NDG	A	387	5	14,14,15	0.53	0	15,19,21	0.81	0
5	BMA	A	388	5	11,11,12	0.43	0	13,15,17	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NDG	A	389	1,6	14,14,15	0.68	0	15,19,21	0.79	0
6	NDG	A	390	6	14,14,15	0.61	0	15,19,21	0.85	0
6	BMA	A	391	6	11,11,12	0.50	0	13,15,17	0.28	0
7	NDG	A	392	1,7	14,14,15	0.59	0	15,19,21	0.84	0
7	NDG	A	393	7	14,14,15	0.55	0	15,19,21	0.77	0
7	MAN	A	394	7	11,11,12	0.53	0	13,15,17	0.46	0
6	NDG	A	395	1,6	14,14,15	0.61	0	15,19,21	0.91	1 (6%)
6	NDG	A	396	6	14,14,15	0.59	0	15,19,21	0.82	1 (6%)
6	BMA	A	397	6	11,11,12	0.49	0	13,15,17	0.25	0
3	NAG	B	1	1,3	14,14,15	0.46	0	15,19,21	0.73	0
3	NDG	B	2	3	14,14,15	0.52	0	15,19,21	0.77	0
4	NAG	B	383	1,4	14,14,15	0.60	0	15,19,21	0.76	0
4	NDG	B	384	4	14,14,15	0.60	0	15,19,21	0.76	1 (6%)
4	MAN	B	385	4	11,11,12	0.54	0	13,15,17	0.47	0
5	NAG	B	386	1,5	14,14,15	0.60	0	15,19,21	0.70	0
5	NDG	B	387	5	14,14,15	0.57	0	15,19,21	0.84	0
5	BMA	B	388	5	11,11,12	0.47	0	13,15,17	0.29	0
5	NAG	B	389	1,5	14,14,15	0.52	0	15,19,21	0.76	0
5	NDG	B	390	5	14,14,15	0.59	0	15,19,21	0.93	0
5	BMA	B	391	5	11,11,12	0.49	0	13,15,17	0.26	0
7	NDG	B	392	1,7	14,14,15	0.63	0	15,19,21	0.71	0
7	NDG	B	393	7	14,14,15	0.68	0	15,19,21	0.75	0
7	MAN	B	394	7	11,11,12	0.55	0	13,15,17	0.43	0
6	NDG	B	395	1,6	14,14,15	0.61	0	15,19,21	0.75	1 (6%)
6	NDG	B	396	6	14,14,15	0.59	0	15,19,21	0.80	0
6	BMA	B	397	6	11,11,12	0.47	0	13,15,17	0.23	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
3	NAG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	2	3	-	0/6/23/26	0/1/1/1
4	NAG	A	383	1,4	-	0/6/23/26	0/1/1/1
4	NDG	A	384	4	-	0/6/23/26	0/1/1/1
4	MAN	A	385	4	-	0/2/19/22	0/1/1/1
5	NAG	A	386	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	387	5	-	0/6/23/26	0/1/1/1
5	BMA	A	388	5	-	0/2/19/22	0/1/1/1
6	NDG	A	389	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	A	390	6	-	0/6/23/26	0/1/1/1
6	BMA	A	391	6	-	0/2/19/22	0/1/1/1
7	NDG	A	392	1,7	-	0/6/23/26	0/1/1/1
7	NDG	A	393	7	-	0/6/23/26	0/1/1/1
7	MAN	A	394	7	-	0/2/19/22	0/1/1/1
6	NDG	A	395	1,6	-	0/6/23/26	0/1/1/1
6	NDG	A	396	6	-	0/6/23/26	0/1/1/1
6	BMA	A	397	6	-	0/2/19/22	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NDG	B	2	3	-	0/6/23/26	0/1/1/1
4	NAG	B	383	1,4	-	0/6/23/26	0/1/1/1
4	NDG	B	384	4	-	0/6/23/26	0/1/1/1
4	MAN	B	385	4	-	0/2/19/22	0/1/1/1
5	NAG	B	386	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	387	5	-	0/6/23/26	0/1/1/1
5	BMA	B	388	5	-	0/2/19/22	0/1/1/1
5	NAG	B	389	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	390	5	-	0/6/23/26	0/1/1/1
5	BMA	B	391	5	-	0/2/19/22	0/1/1/1
7	NDG	B	392	1,7	-	0/6/23/26	0/1/1/1
7	NDG	B	393	7	-	0/6/23/26	0/1/1/1
7	MAN	B	394	7	-	0/2/19/22	0/1/1/1
6	NDG	B	395	1,6	-	0/6/23/26	0/1/1/1
6	NDG	B	396	6	-	0/6/23/26	0/1/1/1
6	BMA	B	397	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	395	NDG	C2-N2-C7	-2.16	119.78	122.94
3	A	2	NDG	C2-N2-C7	-2.13	119.83	122.94
6	A	396	NDG	C2-N2-C7	-2.07	119.92	122.94
4	B	384	NDG	C2-N2-C7	-2.03	119.98	122.94
6	B	395	NDG	C2-N2-C7	-2.02	120.00	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	4	0
3	A	2	NDG	5	0
4	A	383	NAG	1	0
5	A	386	NAG	6	0
5	A	387	NDG	1	0
6	A	389	NDG	1	0
6	A	390	NDG	1	0
4	B	383	NAG	2	0
4	B	384	NDG	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	347/347 (100%)	-0.12	19 (5%) 26 24	4, 70, 182, 200	0
1	B	347/347 (100%)	0.61	62 (17%) 2 2	15, 122, 195, 200	0
2	E	108/120 (90%)	0.22	13 (12%) 5 5	15, 69, 184, 200	0
2	F	109/120 (90%)	-0.06	4 (3%) 42 38	8, 65, 153, 200	0
All	All	911/934 (97%)	0.21	98 (10%) 6 7	4, 81, 191, 200	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	46	ASN	8.1
1	B	53	ASP	7.4
1	A	58	SER	7.4
1	B	50	CYS	7.3
1	B	60	HIS	7.1
2	E	2	SER	6.7
1	B	61	HIS	6.7
1	B	90	LEU	6.1
1	B	51	THR	6.0
2	E	49	PHE	6.0
1	A	78	HIS	5.5
1	B	41	CYS	5.4
1	B	54	GLY	5.3
1	B	57	ASP	5.3
1	A	62	LEU	4.9
1	B	234	GLN	4.7
1	B	63	PRO	4.7
2	E	45	ASN	4.6
1	A	61	HIS	4.5
1	B	39	ALA	4.4
1	B	52	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	336	ALA	4.3
1	B	178	HIS	4.2
1	B	36	CYS	4.2
1	B	139	SER	4.2
1	A	44	GLY	4.1
1	B	94	ARG	3.9
1	B	89	GLY	3.9
1	B	40	CYS	3.9
1	A	37	PRO	3.8
1	B	55	ALA	3.8
2	E	47	SER	3.7
1	B	102	GLY	3.6
1	B	117	LEU	3.6
1	B	56	LEU	3.6
1	A	36	CYS	3.5
1	B	78	HIS	3.4
1	B	37	PRO	3.4
1	B	199	GLN	3.3
1	A	60	HIS	3.3
1	B	241	SER	3.2
2	E	43	ASN	3.2
2	F	46	ASN	3.1
2	F	45	ASN	3.1
1	B	80	GLN	3.1
1	A	234	GLN	3.1
1	A	51	THR	3.0
1	B	112	HIS	3.0
1	B	65	ALA	3.0
2	F	95	LYS	3.0
1	B	38	ASP	2.9
1	B	73	ILE	2.9
2	E	44	ILE	2.9
1	B	124	PHE	2.9
1	B	75	ASN	2.9
2	E	94	GLY	2.9
1	A	52	ARG	2.8
1	B	85	ARG	2.8
1	B	71	LEU	2.8
1	A	41	CYS	2.8
2	E	95	LYS	2.8
1	A	90	LEU	2.8
2	E	60	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	49	ARG	2.7
1	B	177	CYS	2.6
1	A	178	HIS	2.6
2	E	96	GLN	2.6
2	F	2	SER	2.6
1	A	214	ARG	2.6
1	B	67	ASN	2.5
1	B	266	TRP	2.5
1	B	43	HIS	2.5
1	B	58	SER	2.5
1	B	105	PHE	2.4
1	B	83	GLU	2.4
1	B	81	HIS	2.4
1	A	55	ALA	2.4
1	B	59	LEU	2.4
1	B	84	LEU	2.4
1	B	62	LEU	2.3
1	B	214	ARG	2.3
1	A	57	ASP	2.3
1	B	74	GLU	2.3
1	B	79	LEU	2.3
2	E	48	VAL	2.3
1	A	248	GLY	2.2
1	B	337	ALA	2.2
1	B	225	ALA	2.2
1	B	44	GLY	2.2
1	B	172	GLU	2.2
1	B	66	GLU	2.1
1	B	69	THR	2.1
1	B	119	ARG	2.1
1	B	100	LYS	2.0
1	A	77	GLN	2.0
2	E	93	ASP	2.0
1	B	72	TYR	2.0
1	B	116	ARG	2.0

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

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

### 6.3 Carbohydrates

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NDG	B	395	14/15	0.71	0.42	0.44	200,200,200,200	0
6	NDG	A	395	14/15	0.86	0.26	0.43	107,111,115,122	0
6	NDG	A	389	14/15	0.85	0.23	0.28	89,93,98,105	0
3	NAG	B	1	14/15	0.67	0.27	0.07	170,170,170,170	0
7	NDG	A	392	14/15	0.83	0.26	0.03	177,177,177,177	0
7	NDG	B	392	14/15	0.68	0.42	-0.34	200,200,200,200	0
3	NAG	A	1	14/15	0.87	0.17	-1.56	81,85,90,97	0
6	NDG	A	390	14/15	0.78	0.26	-	184,185,185,185	0
4	NDG	B	384	14/15	0.71	0.36	-	166,166,166,166	0
4	NAG	B	383	14/15	0.87	0.26	-	116,116,116,116	0
5	NDG	B	390	14/15	0.85	0.24	-	131,132,132,132	0
5	BMA	A	388	11/12	0.54	0.65	-	197,197,197,197	0
3	NDG	B	2	14/15	0.62	0.44	-	191,191,191,191	0
5	NAG	B	389	14/15	0.90	0.19	-	75,79,83,85	0
5	NDG	A	387	14/15	0.82	0.33	-	116,121,126,137	0
6	NDG	B	396	14/15	0.78	0.62	-	200,200,200,200	0
7	MAN	A	394	11/12	0.28	0.86	-	200,200,200,200	0
6	BMA	B	397	11/12	0.34	0.62	-	200,200,200,200	0
6	BMA	A	397	11/12	0.26	0.87	-	200,200,200,200	0
5	BMA	B	388	11/12	0.72	0.56	-	180,180,180,180	0
4	MAN	B	385	11/12	0.58	0.53	-	193,193,193,193	0
7	MAN	B	394	11/12	0.70	0.41	-	166,166,166,166	0
5	NAG	B	386	14/15	0.87	0.24	-	116,120,123,123	0
5	NAG	A	386	14/15	0.93	0.22	-	65,69,74,81	0
7	NDG	B	393	14/15	0.45	0.58	-	197,197,197,197	0
5	BMA	B	391	11/12	0.34	0.54	-	200,200,200,200	0
4	MAN	A	385	11/12	-0.04	0.66	-	200,200,200,200	0
6	BMA	A	391	11/12	0.39	0.42	-	194,194,194,194	0
7	NDG	A	393	14/15	0.54	0.56	-	188,188,188,188	0
4	NDG	A	384	14/15	0.46	0.57	-	198,198,198,198	0
3	NDG	A	2	14/15	0.83	0.38	-	165,170,175,186	0
4	NAG	A	383	14/15	0.84	0.33	-	116,116,116,116	0
5	NDG	B	387	14/15	0.88	0.25	-	146,146,146,146	0
6	NDG	A	396	14/15	0.65	0.44	-	191,191,191,191	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.