



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2014 – 07:17 PM EDT

PDB ID : 1TYE
Title : Structural basis for allostery in integrins and binding of ligand-mimetic therapeutics to the platelet receptor for fibrinogen
Authors : Xiao, T.; Takagi, J.; Collier, B.S.; Wang, J.-H.; Springer, T.A.
Deposited on : 2004-07-07
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

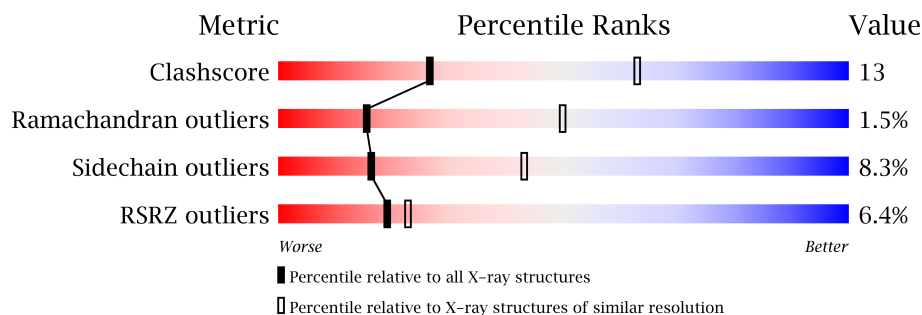
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	452	
1	C	452	
1	E	452	
2	B	440	
2	D	440	
2	F	440	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	B	1006	-	X
3	NAG	D	1007	-	X
3	NAG	F	1015	-	X
6	CAC	B	1301	X	-
6	CAC	D	1302	X	-

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Mol	Type	Chain	Res	Geometry	Electron density
6	CAC	F	1303	X	-
8	CA	B	1403	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21019 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

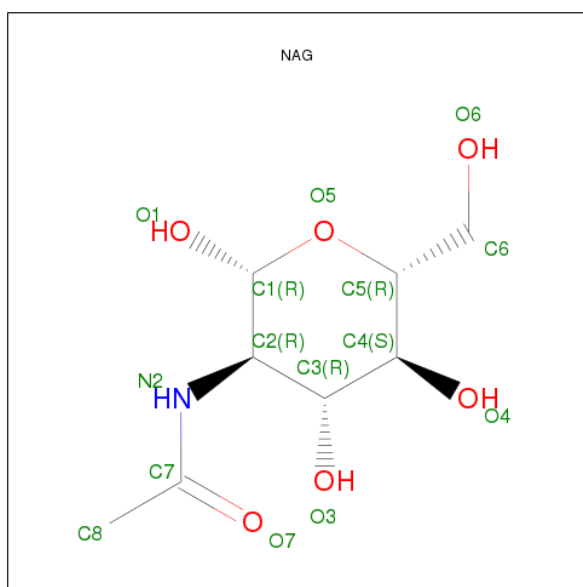
- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			
1	C	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			
1	E	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			
2	D	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			
2	F	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

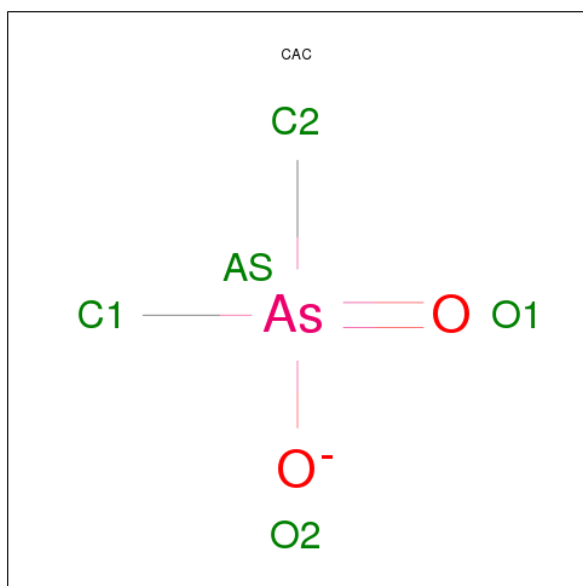
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	4	Total	C	N	O	0	0
			50	28	2	20		
4	F	4	Total	C	N	O	0	0
			50	28	2	20		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	As	C	O	0	0
			5	1	2	2		
6	D	1	Total	As	C	O	0	0
			5	1	2	2		
6	F	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

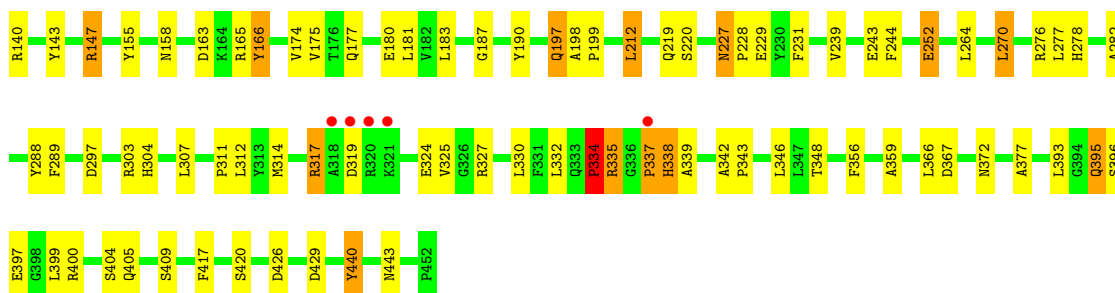
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Ca 2 2	0	0
8	E	4	Total Ca 4 4	0	0
8	B	2	Total Ca 2 2	0	0
8	C	4	Total Ca 4 4	0	0
8	A	4	Total Ca 4 4	0	0
8	F	2	Total Ca 2 2	0	0

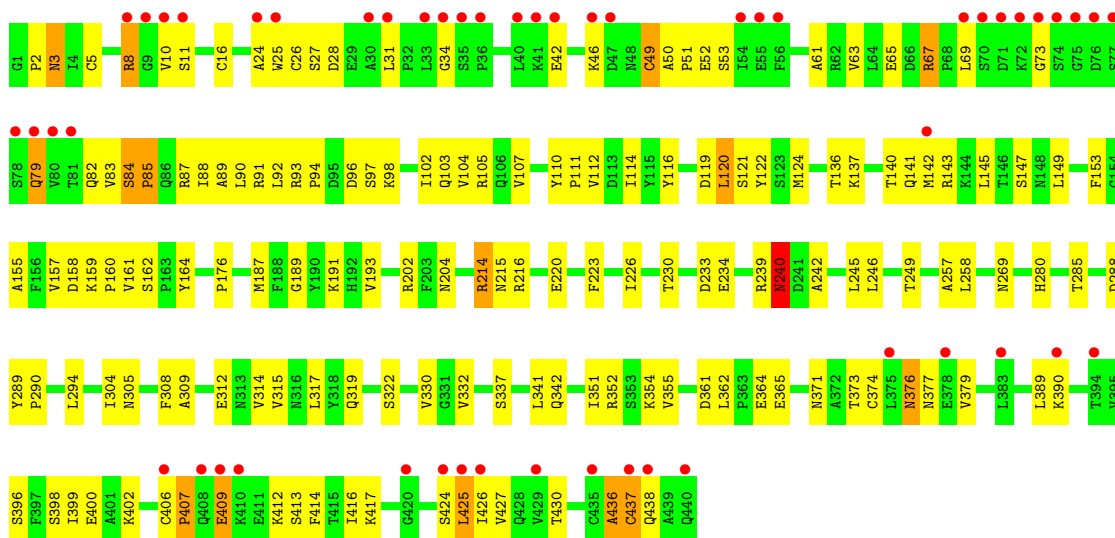
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	22	Total O 22 22	0	0
9	B	16	Total O 16 16	0	0
9	C	20	Total O 20 20	0	0
9	D	19	Total O 19 19	0	0
9	E	28	Total O 28 28	0	0
9	F	15	Total O 15 15	0	0



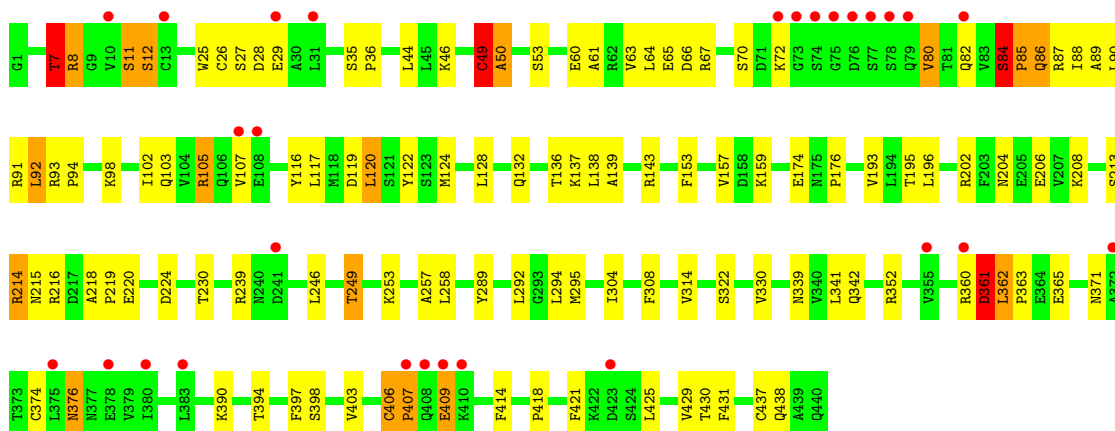
• Molecule 2: Integrin beta-3

Chain B:



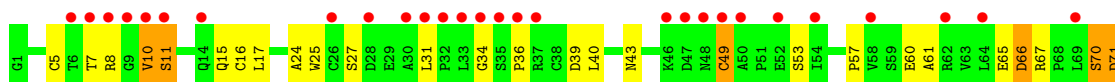
• Molecule 2: Integrin beta-3

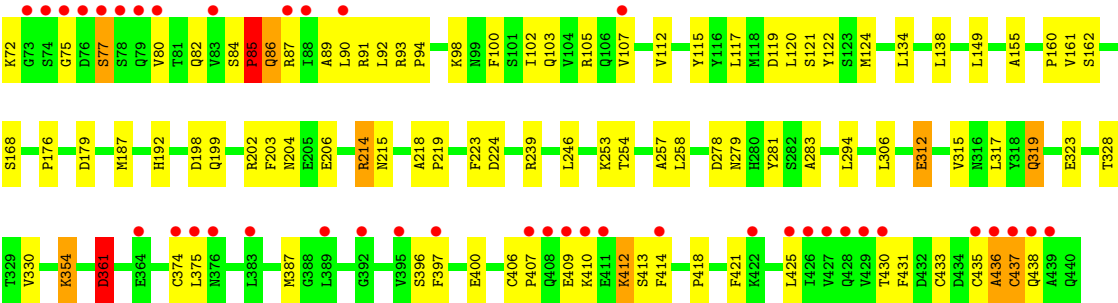
Chain D:



• Molecule 2: Integrin beta-3

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	332.09Å 332.09Å 88.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 47.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.90) 98.3 (47.28-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.254 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.8	EDS
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 121498 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21019	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, CA, CAC, 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	0.75	9/3564 (0.3%)	0.86	11/4857 (0.2%)
1	C	0.60	7/3564 (0.2%)	0.95	17/4857 (0.4%)
1	E	0.61	4/3564 (0.1%)	0.88	12/4857 (0.2%)
2	B	0.40	0/3461	0.80	6/4693 (0.1%)
2	D	0.68	5/3461 (0.1%)	0.78	9/4693 (0.2%)
2	F	0.39	0/3461	0.73	9/4693 (0.2%)
All	All	0.59	25/21075 (0.1%)	0.84	64/28650 (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	4
1	C	0	5
1	E	0	3
2	D	0	3
2	F	0	1
All	All	0	16

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	85	PRO	N-CD	28.23	1.87	1.47
1	A	101	SER	CB-OG	22.05	1.71	1.42
1	A	123	GLU	CB-CG	17.06	1.84	1.52
1	E	123	GLU	C-N	-16.41	0.96	1.34
1	E	122	ALA	C-N	13.02	1.64	1.34
1	A	122	ALA	C-N	-12.71	1.04	1.34
1	C	117	GLU	CA-C	12.18	1.84	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	100	TRP	C-N	-11.80	1.06	1.34
1	C	101	SER	C-N	-11.77	1.06	1.34
1	C	100	TRP	C-N	-10.62	1.09	1.34
2	D	84	SER	C-N	-9.09	1.17	1.34
1	C	118	LYS	N-CA	-8.10	1.30	1.46
1	A	123	GLU	C-N	6.81	1.49	1.34
2	D	8	ARG	CB-CG	-6.72	1.34	1.52
1	C	123	GLU	N-CA	6.46	1.59	1.46
1	C	122	ALA	C-O	-6.27	1.11	1.23
1	A	28	ASP	CB-CG	-6.20	1.38	1.51
2	D	7	THR	C-N	-6.17	1.19	1.34
1	A	124	LYS	N-CA	-5.88	1.34	1.46
1	A	451	GLN	CB-CG	-5.83	1.36	1.52
1	A	334	PRO	N-CD	5.47	1.55	1.47
1	A	123	GLU	C-O	5.38	1.33	1.23
1	C	122	ALA	C-N	-5.38	1.21	1.34
2	D	85	PRO	CB-CG	5.34	1.76	1.50
1	E	123	GLU	CB-CG	-5.16	1.42	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	SER	C-N-CD	-26.08	63.23	120.60
1	C	101	SER	O-C-N	-24.91	82.84	122.70
1	E	123	GLU	O-C-N	-18.48	93.12	122.70
1	C	334	PRO	CA-N-CD	-16.12	88.93	111.50
1	A	122	ALA	O-C-N	-15.63	97.70	122.70
1	A	122	ALA	CA-C-N	15.40	151.09	117.20
1	C	101	SER	CA-C-N	14.37	148.82	117.20
2	D	85	PRO	CA-N-CD	-14.20	91.61	111.50
1	E	100	TRP	O-C-N	-12.67	102.43	122.70
1	E	100	TRP	C-N-CA	12.19	152.18	121.70
1	C	100	TRP	O-C-N	-11.90	103.66	122.70
1	E	123	GLU	CA-C-N	11.29	142.03	117.20
1	A	337	PRO	CA-N-CD	-11.03	96.06	111.50
2	D	84	SER	O-C-N	-10.66	100.84	121.10
1	A	122	ALA	C-N-CA	10.15	147.07	121.70
1	C	100	TRP	C-N-CA	10.02	146.76	121.70
1	C	117	GLU	O-C-N	10.02	138.73	122.70
1	C	122	ALA	CB-CA-C	9.85	124.88	110.10
1	C	101	SER	C-N-CA	9.79	146.18	121.70
1	E	334	PRO	CA-N-CD	-9.48	98.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	PRO	CA-N-CD	-9.07	98.80	111.50
1	E	101	SER	N-CA-CB	-8.74	97.39	110.50
2	B	8	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	E	100	TRP	CA-C-N	8.20	135.23	117.20
1	C	336	GLY	C-N-CD	-8.01	102.98	120.60
2	D	85	PRO	N-CD-CG	-7.79	91.52	103.20
2	F	361	ASP	CB-CG-OD2	-7.70	111.37	118.30
2	D	85	PRO	N-CA-CB	7.55	112.36	103.30
1	A	102	ASP	N-CA-C	7.47	131.16	111.00
2	F	85	PRO	N-CA-CB	-7.46	94.35	103.30
2	F	436	ALA	N-CA-C	-7.28	91.35	111.00
1	C	102	ASP	N-CA-C	7.25	130.57	111.00
2	D	84	SER	CA-C-N	7.23	137.33	117.10
1	A	102	ASP	N-CA-CB	-7.16	97.72	110.60
1	C	123	GLU	O-C-N	-7.15	111.27	122.70
1	C	100	TRP	CA-C-N	6.98	132.56	117.20
1	C	122	ALA	C-N-CA	6.97	139.12	121.70
2	F	85	PRO	CB-CA-C	6.91	129.27	112.00
2	F	11	SER	N-CA-C	6.83	129.43	111.00
1	E	337	PRO	CA-N-CD	-6.79	102.00	111.50
1	A	122	ALA	N-CA-C	-6.75	92.78	111.00
1	A	334	PRO	N-CA-CB	6.69	111.33	103.30
2	B	409	GLU	N-CA-C	-6.63	93.10	111.00
2	D	84	SER	C-N-CA	6.61	149.76	122.00
1	E	122	ALA	CA-C-N	-6.61	102.66	117.20
2	F	77	SER	N-CA-C	-6.51	93.43	111.00
1	E	123	GLU	CA-CB-CG	6.27	127.19	113.40
2	B	79	GLN	N-CA-C	-6.25	94.13	111.00
1	C	122	ALA	O-C-N	6.12	132.50	122.70
1	A	122	ALA	CA-C-O	-6.10	107.29	120.10
1	C	122	ALA	CA-C-N	-6.09	103.81	117.20
1	E	122	ALA	O-C-N	6.05	132.37	122.70
2	D	409	GLU	N-CA-C	-5.89	95.09	111.00
2	B	2	PRO	N-CA-C	-5.75	97.14	112.10
2	F	72	LYS	N-CA-C	5.75	126.52	111.00
2	B	84	SER	CB-CA-C	5.69	120.90	110.10
1	C	334	PRO	N-CD-CG	5.43	111.34	103.20
2	F	361	ASP	CB-CG-OD1	5.34	123.10	118.30
2	F	409	GLU	N-CA-C	-5.28	96.74	111.00
1	A	270	LEU	CA-CB-CG	5.25	127.38	115.30
2	D	85	PRO	N-CA-C	-5.15	98.71	112.10
1	A	123	GLU	C-N-CA	-5.15	108.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	85	PRO	CA-CB-CG	-5.08	94.34	104.00
1	E	270	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TRP	Mainchain
1	A	122	ALA	Mainchain,Peptide
1	A	28	ASP	Mainchain
1	C	100	TRP	Mainchain,Peptide
1	C	101	SER	Mainchain,Peptide
1	C	123	GLU	Mainchain
2	D	11	SER	Mainchain
2	D	84	SER	Mainchain,Peptide
1	E	100	TRP	Mainchain,Peptide
1	E	123	GLU	Mainchain
2	F	361	ASP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3468	0	3300	85	0
1	C	3468	0	3299	75	0
1	E	3468	0	3297	84	0
2	B	3400	0	3350	110	0
2	D	3400	0	3349	91	0
2	F	3400	0	3350	85	0
3	B	28	0	26	2	0
3	D	28	0	26	0	0
3	E	14	0	13	0	0
3	F	28	0	26	3	0
4	B	50	0	43	6	0
4	F	50	0	43	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	61	0	52	5	0
6	B	5	0	0	1	0
6	D	5	0	0	1	0
6	F	5	0	0	1	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
8	E	4	0	0	0	0
8	F	2	0	0	0	0
9	A	22	0	0	1	0
9	B	16	0	0	0	0
9	C	20	0	0	1	0
9	D	19	0	0	0	0
9	E	28	0	0	1	0
9	F	15	0	0	0	0
All	All	21019	0	20174	541	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (541) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:85:PRO:CB	2:D:85:PRO:CG	1.76	1.59
1:A:123:GLU:CG	1:A:123:GLU:CB	1.84	1.52
1:C:117:GLU:C	1:C:117:GLU:CA	1.84	1.45
1:A:101:SER:CB	1:A:101:SER:OG	1.70	1.38
2:D:85:PRO:CD	2:D:85:PRO:N	1.87	1.37
1:E:91:GLN:HG2	1:E:108:ALA:HB1	1.32	1.11
2:F:66:ASP:HA	2:F:86:GLN:HE22	1.16	1.07
2:F:84:SER:HB2	2:F:103:GLN:H	1.19	1.05
1:A:303:ARG:HD2	1:A:335:ARG:HE	1.21	1.02
2:D:85:PRO:CD	2:D:85:PRO:CA	2.37	1.02
2:F:84:SER:HB3	2:F:85:PRO:HD2	1.41	0.99
2:D:25:TRP:HE1	2:D:27:SER:HB2	1.30	0.96
2:D:85:PRO:CG	2:D:85:PRO:CA	2.44	0.95
2:F:84:SER:HB3	2:F:85:PRO:CD	2.00	0.91
2:B:61:ALA:HB2	2:B:90:LEU:HD12	1.52	0.89
1:E:395:GLN:HG2	1:E:397:GLU:H	1.41	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:61:ALA:HB2	2:D:90:LEU:HD12	1.59	0.85
2:B:67:ARG:H	2:B:67:ARG:HD2	1.41	0.85
2:D:91:ARG:HG2	2:D:430:THR:HB	1.59	0.84
2:F:66:ASP:HA	2:F:86:GLN:NE2	1.91	0.84
1:A:303:ARG:HB2	1:A:335:ARG:HH21	1.43	0.83
2:F:412:LYS:HE2	2:F:413:SER:H	1.43	0.81
4:B:1002:NAG:H61	4:B:1003:NAG:H82	1.63	0.80
2:D:84:SER:HB2	2:D:103:GLN:H	1.44	0.80
1:E:278:HIS:CE1	1:E:339:ALA:HB1	2.17	0.80
2:D:376:ASN:H	2:D:376:ASN:HD22	1.28	0.80
1:A:101:SER:OG	1:A:102:ASP:N	2.15	0.79
2:D:63:VAL:HA	2:D:88:ILE:HG22	1.63	0.79
1:A:264:LEU:O	1:A:282:ALA:HB3	1.84	0.78
2:D:361:ASP:O	2:D:414:PHE:HB3	1.83	0.78
2:D:27:SER:HB3	2:D:438:GLN:HB3	1.66	0.77
1:E:1:LEU:HA	1:E:367:ASP:HB3	1.67	0.77
2:F:84:SER:CB	2:F:85:PRO:CD	2.60	0.77
1:E:264:LEU:O	1:E:282:ALA:HB3	1.85	0.76
2:D:85:PRO:O	2:D:425:LEU:HD13	1.85	0.76
2:D:84:SER:C	2:D:85:PRO:CD	2.52	0.76
1:C:227:ASN:HD21	1:C:229:GLU:HG3	1.51	0.76
1:C:245:ASP:HA	1:C:338:HIS:HE1	1.48	0.76
2:B:365:GLU:HG3	2:B:407:PRO:HG3	1.69	0.75
1:A:163:ASP:OD1	1:A:165:ARG:HD3	1.86	0.74
2:B:412:LYS:HE2	2:B:413:SER:H	1.52	0.74
2:B:85:PRO:O	2:B:425:LEU:HD13	1.86	0.74
2:B:361:ASP:OD2	2:B:414:PHE:HA	1.88	0.74
2:D:85:PRO:N	2:D:85:PRO:CG	2.45	0.73
2:B:91:ARG:HG3	2:B:430:THR:HB	1.68	0.73
1:E:122:ALA:O	1:E:123:GLU:HB2	1.87	0.73
2:B:373:THR:HG22	2:B:379:VAL:HG22	1.71	0.73
1:C:16:GLY:H	1:C:443:ASN:HD21	1.37	0.73
2:F:375:LEU:H	2:F:375:LEU:HD12	1.54	0.73
2:B:84:SER:OG	2:B:103:GLN:HG3	1.88	0.72
1:A:105:VAL:HG22	1:A:132:LEU:HD13	1.71	0.72
2:F:436:ALA:HB3	2:F:438:GLN:NE2	2.03	0.72
2:D:26:CYS:HB2	2:D:44:LEU:HD13	1.72	0.72
2:B:3:ASN:HD21	2:B:5:CYS:HB2	1.54	0.71
2:F:85:PRO:O	2:F:425:LEU:HD13	1.90	0.71
1:A:303:ARG:HD2	1:A:335:ARG:NE	2.02	0.71
2:F:93:ARG:HB2	2:F:94:PRO:HD2	1.72	0.70
2:F:134:LEU:O	2:F:138:LEU:HB2	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:359:ALA:HB3	1:E:377:ALA:HB3	1.74	0.69
1:A:303:ARG:HB2	1:A:335:ARG:NH2	2.07	0.69
2:D:136:THR:HA	2:D:204:ASN:HD21	1.58	0.69
1:E:91:GLN:HG2	1:E:108:ALA:CB	2.19	0.69
4:F:1018:MAN:H3	4:F:1019:BMA:O2	1.91	0.69
1:A:114:ASN:HD22	1:A:115:VAL:H	1.41	0.68
1:A:119:THR:CG2	1:A:119:THR:O	2.40	0.68
2:D:25:TRP:NE1	2:D:27:SER:HB2	2.08	0.68
2:D:215:ASN:HB3	6:D:1302:CAC:C1	2.22	0.68
1:C:395:GLN:HG2	1:C:396:SER:N	2.08	0.68
2:D:8:ARG:HB2	2:D:8:ARG:CZ	2.23	0.68
1:A:1:LEU:HD13	1:A:367:ASP:HB3	1.73	0.68
1:A:312:LEU:HD22	2:B:258:LEU:HD12	1.75	0.68
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.76	0.68
4:F:1016:NAG:H61	4:F:1017:NAG:C8	2.24	0.67
2:B:104:VAL:HG21	2:B:355:VAL:HG11	1.76	0.67
2:B:337:SER:O	2:B:341:LEU:HD23	1.95	0.67
5:D:1008:NAG:C6	5:D:1009:NAG:H82	2.24	0.67
1:A:303:ARG:CD	1:A:335:ARG:HE	2.02	0.67
2:B:82:GLN:NE2	2:B:107:VAL:HG12	2.10	0.66
1:A:332:LEU:O	1:A:334:PRO:HD3	1.95	0.66
2:B:83:VAL:HG22	2:B:104:VAL:HG12	1.78	0.66
2:D:376:ASN:HD22	2:D:376:ASN:N	1.92	0.66
2:B:111:PRO:HB2	2:B:242:ALA:HB2	1.77	0.66
1:E:278:HIS:CE1	1:E:339:ALA:CB	2.78	0.66
1:C:163:ASP:OD1	1:C:165:ARG:HD3	1.96	0.66
2:D:176:PRO:HB2	2:D:214:ARG:HB2	1.78	0.65
1:A:122:ALA:O	1:A:123:GLU:HG3	1.97	0.65
2:B:365:GLU:HG3	2:B:407:PRO:CG	2.25	0.65
2:F:400:GLU:HB2	3:F:1020:NAG:H81	1.78	0.65
2:D:11:SER:O	2:D:12:SER:HB3	1.98	0.64
2:D:85:PRO:CD	2:D:85:PRO:CB	2.66	0.64
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.80	0.64
2:B:63:VAL:HA	2:B:88:ILE:HG22	1.79	0.64
2:D:92:LEU:HD13	2:D:403:VAL:HG11	1.78	0.64
1:E:105:VAL:HG22	1:E:132:LEU:HD13	1.81	0.63
2:F:306:LEU:HB3	2:F:328:THR:HG22	1.81	0.63
2:F:84:SER:HB2	2:F:103:GLN:N	2.02	0.63
2:B:376:ASN:HD22	2:B:376:ASN:N	1.96	0.63
2:F:61:ALA:HA	2:F:89:ALA:O	1.99	0.63
2:D:84:SER:CB	2:D:85:PRO:HD2	2.29	0.63
1:E:338:HIS:ND1	1:E:338:HIS:N	2.47	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:218:ALA:HB3	2:F:219:PRO:HD3	1.80	0.62
2:D:8:ARG:NH1	2:D:8:ARG:HB2	2.14	0.62
1:A:69:LEU:O	1:A:140:ARG:NH1	2.32	0.62
1:E:227:ASN:ND2	1:E:229:GLU:H	1.98	0.62
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.82	0.61
1:C:243:GLU:H	1:C:304:HIS:CD2	2.18	0.61
1:C:317:ARG:HH11	1:C:317:ARG:HG2	1.64	0.61
2:D:61:ALA:HA	2:D:89:ALA:O	2.00	0.61
2:B:122:TYR:HB2	2:B:214:ARG:HG2	1.83	0.61
1:C:16:GLY:H	1:C:443:ASN:ND2	1.98	0.61
5:D:1008:NAG:H62	5:D:1009:NAG:H82	1.80	0.61
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.81	0.61
1:E:180:GLU:HB3	1:E:197:GLN:HE22	1.66	0.61
2:F:215:ASN:HB3	6:F:1303:CAC:C1	2.31	0.61
2:B:436:ALA:HB3	2:B:438:GLN:NE2	2.15	0.60
2:D:94:PRO:HB3	2:D:406:CYS:HB2	1.82	0.60
2:B:31:LEU:HD11	2:B:49:CYS:SG	2.42	0.60
2:B:61:ALA:HA	2:B:89:ALA:O	2.01	0.60
1:C:55:LEU:O	1:C:66:PRO:HD2	2.02	0.60
4:F:1017:NAG:H3	4:F:1018:MAN:O5	2.00	0.60
1:E:69:LEU:O	1:E:140:ARG:NH1	2.35	0.59
2:F:8:ARG:HH11	2:F:8:ARG:HG3	1.67	0.59
1:A:114:ASN:ND2	1:A:115:VAL:H	2.00	0.59
1:A:155:TYR:CE2	1:A:165:ARG:HD2	2.37	0.59
2:B:65:GLU:HG2	2:B:87:ARG:HB3	1.84	0.59
2:F:176:PRO:HB2	2:F:214:ARG:HB2	1.83	0.59
2:F:437:CYS:SG	2:F:437:CYS:O	2.60	0.59
2:D:292:LEU:HA	2:D:295:MET:HE3	1.83	0.59
2:D:361:ASP:O	2:D:414:PHE:CB	2.51	0.59
2:F:436:ALA:HB3	2:F:438:GLN:HE21	1.66	0.59
1:A:317:ARG:HH11	1:A:317:ARG:HG2	1.67	0.59
1:A:119:THR:O	1:A:119:THR:HG22	2.00	0.59
2:F:66:ASP:CG	2:F:85:PRO:HG3	2.23	0.59
1:A:227:ASN:HD22	1:A:227:ASN:C	2.05	0.58
2:B:371:ASN:HB2	2:B:398:SER:HB3	1.85	0.58
1:C:117:GLU:CA	1:C:118:LYS:N	2.61	0.58
2:B:337:SER:HB2	2:B:341:LEU:HD23	1.85	0.58
1:E:303:ARG:HD2	1:E:334:PRO:O	2.03	0.58
2:F:31:LEU:HD21	2:F:49:CYS:SG	2.43	0.58
2:F:354:LYS:HB3	2:F:387:MET:HG2	1.86	0.58
1:A:113:TRP:CE3	1:A:147:ARG:HD2	2.37	0.58
1:E:155:TYR:CE2	1:E:165:ARG:HD2	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:88:LYS:O	1:E:91:GLN:HB2	2.03	0.58
1:A:227:ASN:ND2	1:A:229:GLU:H	2.01	0.58
2:F:5:CYS:HB2	2:F:39:ASP:HA	1.84	0.58
1:E:41:ARG:HH11	1:E:41:ARG:HG2	1.69	0.58
1:A:101:SER:CA	1:A:101:SER:OG	2.50	0.57
2:D:418:PRO:HG2	2:D:421:PHE:HB2	1.87	0.57
1:A:30:HIS:HB3	1:E:429:ASP:OD2	2.04	0.57
2:F:61:ALA:HB2	2:F:90:LEU:HD12	1.87	0.57
1:E:3:LEU:O	1:E:5:PRO:HD3	2.03	0.57
1:C:330:LEU:HD22	1:C:399:LEU:HD12	1.85	0.57
1:C:334:PRO:HB2	1:C:338:HIS:HA	1.87	0.57
1:E:317:ARG:HG2	1:E:317:ARG:HH11	1.69	0.57
2:F:17:LEU:HD13	2:F:57:PRO:HG2	1.87	0.57
4:B:1003:NAG:O3	4:B:1004:MAN:H5	2.03	0.57
1:C:245:ASP:HA	1:C:338:HIS:CE1	2.36	0.57
2:D:219:PRO:HG3	2:D:253:LYS:HG3	1.86	0.57
2:F:122:TYR:HB2	2:F:214:ARG:HG2	1.87	0.57
2:F:27:SER:O	2:F:53:SER:HB2	2.05	0.57
1:E:180:GLU:HB3	1:E:197:GLN:NE2	2.20	0.57
1:E:41:ARG:CG	1:E:41:ARG:HH11	2.18	0.56
2:D:407:PRO:HB2	2:D:431:PHE:CE2	2.40	0.56
1:C:19:PHE:CE1	1:C:445:VAL:HG23	2.41	0.56
4:B:1004:MAN:H3	4:B:1005:BMA:O2	2.05	0.56
2:B:84:SER:HB2	2:B:103:GLN:H	1.69	0.56
2:D:136:THR:HA	2:D:204:ASN:ND2	2.21	0.56
4:F:1017:NAG:C3	4:F:1018:MAN:O5	2.54	0.56
2:B:82:GLN:HB2	2:B:105:ARG:O	2.05	0.56
2:D:28:ASP:CG	2:D:29:GLU:H	2.09	0.56
1:E:227:ASN:C	1:E:227:ASN:HD22	2.08	0.56
2:F:10:VAL:HB	2:F:15:GLN:NE2	2.21	0.56
2:B:8:ARG:O	2:B:10:VAL:HG23	2.06	0.56
1:C:264:LEU:O	1:C:282:ALA:HB3	2.07	0.55
2:B:161:VAL:HG23	2:B:285:THR:HG22	1.88	0.55
1:A:216:VAL:O	1:A:219:GLN:HB3	2.05	0.55
2:B:400:GLU:HB2	3:B:1006:NAG:H83	1.87	0.55
1:C:340:LEU:H	1:C:340:LEU:HD12	1.71	0.55
2:B:436:ALA:C	2:B:438:GLN:HE21	2.10	0.55
1:C:13:GLY:HA3	1:C:19:PHE:CD2	2.40	0.55
1:C:404:SER:O	1:C:405:GLN:HB2	2.05	0.55
2:D:82:GLN:NE2	2:D:107:VAL:HG12	2.20	0.55
1:E:166:TYR:O	1:E:187:GLY:HA3	2.05	0.55
5:D:1010:MAN:H3	5:D:1011:BMA:O2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:2:ASN:HD22	1:E:2:ASN:N	2.05	0.55
1:C:243:GLU:H	1:C:304:HIS:HD2	1.55	0.55
2:B:158:ASP:O	2:B:189:GLY:HA2	2.06	0.55
1:C:114:ASN:ND2	1:C:115:VAL:H	2.05	0.55
1:C:243:GLU:HB2	1:C:304:HIS:HD2	1.72	0.55
2:D:102:ILE:HG22	2:D:397:PHE:HB2	1.89	0.55
1:A:18:GLN:H	1:A:443:ASN:HD21	1.54	0.54
1:C:197:GLN:NE2	1:C:220:SER:HB3	2.20	0.54
2:D:70:SER:OG	2:D:80:VAL:HG22	2.07	0.54
2:B:390:LYS:H	2:B:390:LYS:HD2	1.73	0.54
1:C:69:LEU:O	1:C:140:ARG:NH1	2.39	0.54
1:C:390:LEU:HG	1:C:406:VAL:HG22	1.90	0.54
2:B:161:VAL:CG2	2:B:285:THR:HG22	2.38	0.54
1:E:2:ASN:HD22	1:E:2:ASN:H	1.56	0.54
1:E:395:GLN:HG2	1:E:397:GLU:N	2.19	0.54
1:A:303:ARG:CB	1:A:335:ARG:HH21	2.18	0.54
1:E:244:PHE:HB2	1:E:252:GLU:HG3	1.90	0.54
2:F:10:VAL:HB	2:F:15:GLN:HE22	1.71	0.54
2:D:82:GLN:HB2	2:D:105:ARG:O	2.08	0.54
1:E:124:LYS:N	2:F:168:SER:HG	2.05	0.54
1:E:2:ASN:HB2	1:E:405:GLN:OE1	2.08	0.54
1:C:117:GLU:N	1:C:117:GLU:C	2.58	0.53
2:F:361:ASP:O	2:F:414:PHE:HB3	2.08	0.53
2:B:257:ALA:O	2:B:258:LEU:HB2	2.09	0.53
1:C:3:LEU:H	1:C:405:GLN:HE22	1.56	0.53
1:C:379:PRO:HA	1:C:417:PHE:O	2.09	0.53
2:B:16:CYS:SG	2:B:24:ALA:O	2.66	0.53
2:D:66:ASP:HB2	2:D:85:PRO:HD3	1.90	0.53
1:E:177:GLN:NE2	1:E:177:GLN:HA	2.24	0.53
1:E:227:ASN:HD22	1:E:228:PRO:N	2.06	0.53
2:B:161:VAL:HG12	2:B:162:SER:O	2.09	0.53
1:E:426:ASP:CG	1:E:429:ASP:HA	2.28	0.53
2:F:7:THR:HG22	2:F:8:ARG:HG3	1.91	0.53
1:A:395:GLN:CD	1:A:396:SER:H	2.13	0.53
1:A:262:TRP:CD1	2:B:317:LEU:HD12	2.44	0.53
2:D:122:TYR:HB2	2:D:213:SER:O	2.09	0.52
2:D:157:VAL:O	2:D:220:GLU:HB3	2.10	0.52
1:E:174:VAL:HG23	1:E:239:VAL:HG23	1.92	0.52
1:C:166:TYR:O	1:C:187:GLY:HA3	2.09	0.52
2:D:27:SER:CB	2:D:438:GLN:HB3	2.39	0.52
4:F:1016:NAG:H61	4:F:1017:NAG:H82	1.91	0.52
2:B:157:VAL:O	2:B:220:GLU:HB3	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:191:LYS:HD3	2:B:280:HIS:NE2	2.25	0.52
1:E:143:TYR:OH	1:E:219:GLN:HG3	2.09	0.52
2:B:69:LEU:HB2	2:B:105:ARG:NH1	2.24	0.52
2:D:376:ASN:H	2:D:376:ASN:ND2	2.04	0.52
1:E:332:LEU:O	1:E:334:PRO:HD3	2.10	0.52
1:C:3:LEU:O	1:C:5:PRO:HD3	2.10	0.52
1:E:227:ASN:HD21	1:E:229:GLU:HG3	1.74	0.52
2:D:84:SER:HB3	2:D:85:PRO:HD2	1.91	0.51
2:F:82:GLN:HB2	2:F:105:ARG:O	2.10	0.51
2:B:111:PRO:HB2	2:B:242:ALA:CB	2.39	0.51
1:C:15:ASN:HA	1:C:443:ASN:ND2	2.25	0.51
2:D:60:GLU:O	2:D:98:LYS:HE2	2.09	0.51
1:E:342:ALA:HB1	1:E:343:PRO:HD2	1.91	0.51
1:E:282:ALA:HB2	1:E:289:PHE:CG	2.45	0.51
2:F:103:GLN:HG2	2:F:396:SER:HB3	1.91	0.51
2:F:25:TRP:HE1	2:F:27:SER:HB2	1.76	0.51
2:D:371:ASN:HB2	2:D:398:SER:HB3	1.92	0.51
1:A:227:ASN:HD21	1:A:229:GLU:HG3	1.76	0.51
2:B:28:ASP:HB2	2:B:53:SER:OG	2.10	0.51
1:E:163:ASP:OD1	1:E:165:ARG:HD3	2.11	0.51
2:B:119:ASP:O	2:B:124:MET:HG3	2.10	0.51
2:F:5:CYS:CB	2:F:39:ASP:HA	2.41	0.51
5:D:1009:NAG:C3	5:D:1010:MAN:O5	2.59	0.50
1:C:113:TRP:CE3	1:C:147:ARG:HD2	2.45	0.50
2:F:100:PHE:HA	3:F:1015:NAG:H83	1.94	0.50
1:A:262:TRP:HD1	2:B:317:LEU:HD12	1.75	0.50
2:F:16:CYS:SG	2:F:24:ALA:O	2.69	0.50
1:A:395:GLN:OE1	1:A:397:GLU:HB2	2.11	0.50
1:C:114:ASN:HD22	1:C:115:VAL:H	1.58	0.50
2:D:374:CYS:HB2	2:D:376:ASN:ND2	2.27	0.50
2:F:278:ASP:O	2:F:279:ASN:HB2	2.12	0.50
2:F:66:ASP:CB	2:F:85:PRO:HG3	2.42	0.50
2:B:143:ARG:NH1	2:B:147:SER:HA	2.27	0.50
2:F:39:ASP:OD2	2:F:43:ASN:HB2	2.12	0.50
4:B:1003:NAG:O3	4:B:1004:MAN:C5	2.59	0.49
1:C:395:GLN:HG2	1:C:396:SER:H	1.75	0.49
2:D:7:THR:HG22	2:D:8:ARG:HG3	1.94	0.49
2:F:160:PRO:HA	2:F:187:MET:HE2	1.95	0.49
1:A:101:SER:CB	1:A:101:SER:HG	2.14	0.49
2:D:132:GLN:HE21	2:D:208:LYS:HA	1.77	0.49
1:C:2:ASN:N	1:C:2:ASN:HD22	2.10	0.49
2:D:67:ARG:HG2	2:D:86:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:282:ALA:HB2	1:E:289:PHE:CB	2.42	0.49
1:C:167:CYS:HB3	1:C:185:ALA:HB1	1.94	0.49
2:D:195:THR:HG22	2:D:196:LEU:N	2.28	0.49
2:D:50:ALA:HB3	2:D:53:SER:OG	2.11	0.49
1:E:8:LEU:H	1:E:8:LEU:HD23	1.78	0.49
2:F:203:PHE:HD2	2:F:204:ASN:ND2	2.10	0.49
2:D:230:THR:HG23	2:D:304:ILE:HD12	1.94	0.49
1:E:87:PHE:CD1	1:E:124:LYS:HE3	2.47	0.49
1:E:282:ALA:HB2	1:E:289:PHE:HB3	1.95	0.49
2:F:92:LEU:O	2:F:92:LEU:HD12	2.13	0.49
1:E:113:TRP:CE3	1:E:147:ARG:HD2	2.47	0.49
2:B:376:ASN:N	2:B:376:ASN:ND2	2.61	0.48
1:E:101:SER:OG	1:E:102:ASP:N	2.44	0.48
1:E:330:LEU:HD22	1:E:399:LEU:HD12	1.96	0.48
2:B:3:ASN:ND2	2:B:5:CYS:H	2.11	0.48
1:A:105:VAL:HG22	1:A:132:LEU:CD1	2.42	0.48
1:A:227:ASN:HD22	1:A:228:PRO:N	2.12	0.48
2:B:114:ILE:HD11	2:B:142:MET:HG3	1.96	0.48
1:C:282:ALA:HB2	1:C:289:PHE:HB3	1.96	0.48
1:A:427:ILE:HG22	1:A:434:ASP:OD2	2.14	0.48
2:F:120:LEU:HD22	2:F:155:ALA:CB	2.43	0.48
1:C:1:LEU:HA	1:C:367:ASP:HB3	1.94	0.48
4:F:1016:NAG:H61	4:F:1017:NAG:H81	1.93	0.48
2:F:361:ASP:O	2:F:414:PHE:CB	2.61	0.48
1:C:227:ASN:ND2	1:C:229:GLU:H	2.11	0.48
4:F:1016:NAG:C6	4:F:1017:NAG:H82	2.44	0.48
2:F:119:ASP:O	2:F:124:MET:HG3	2.14	0.48
2:F:418:PRO:HG2	2:F:421:PHE:HB2	1.95	0.48
1:A:359:ALA:HB3	1:A:377:ALA:HB3	1.95	0.48
2:B:376:ASN:ND2	2:B:376:ASN:H	2.12	0.48
1:C:317:ARG:NH1	1:C:317:ARG:HG2	2.28	0.48
2:D:257:ALA:O	2:D:258:LEU:HB2	2.14	0.47
2:D:84:SER:O	2:D:85:PRO:C	2.52	0.47
1:A:19:PHE:O	1:A:440:TYR:HA	2.15	0.47
1:A:195:LEU:HD11	1:A:239:VAL:HG11	1.96	0.47
2:B:116:TYR:HB3	2:B:153:PHE:HB2	1.95	0.47
2:B:3:ASN:HD21	2:B:5:CYS:CB	2.25	0.47
1:C:395:GLN:NE2	1:C:400:ARG:HH12	2.13	0.47
1:E:23:LEU:HG	1:E:420:SER:OG	2.14	0.47
2:F:435:CYS:HB2	2:F:436:ALA:O	2.15	0.47
1:A:18:GLN:H	1:A:443:ASN:ND2	2.13	0.47
2:B:120:LEU:HD22	2:B:155:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:319:GLN:O	2:B:322:SER:HB3	2.14	0.47
1:C:174:VAL:HG11	1:C:240:ALA:HA	1.96	0.47
2:D:7:THR:HG22	2:D:8:ARG:N	2.30	0.47
2:B:82:GLN:HB3	2:B:107:VAL:HG12	1.97	0.47
2:B:50:ALA:C	2:B:52:GLU:H	2.18	0.47
9:C:1434:HOH:O	2:D:216:ARG:HD3	2.13	0.47
1:C:166:TYR:CE1	2:D:216:ARG:HD2	2.49	0.47
1:A:303:ARG:CZ	1:A:336:GLY:H	2.27	0.47
1:A:395:GLN:CG	1:A:396:SER:H	2.28	0.47
2:D:376:ASN:ND2	2:D:376:ASN:N	2.63	0.47
2:B:102:ILE:HD12	2:B:425:LEU:HD23	1.97	0.46
2:D:90:LEU:HD23	2:D:429:VAL:HG12	1.97	0.46
1:A:421:LEU:CD2	1:A:437:VAL:HG22	2.45	0.46
2:B:337:SER:HB2	2:B:341:LEU:CD2	2.45	0.46
1:A:117:GLU:O	1:A:118:LYS:HB2	2.16	0.46
1:A:73:ARG:NH1	1:C:73:ARG:HB2	2.31	0.46
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.97	0.46
1:C:155:TYR:CZ	1:C:165:ARG:HD2	2.51	0.46
2:B:223:PHE:HD1	2:B:226:ILE:HD12	1.81	0.46
1:A:395:GLN:CD	1:A:397:GLU:H	2.18	0.46
1:A:84:LEU:HD12	1:A:115:VAL:HG13	1.98	0.46
1:A:327:ARG:HH21	1:A:348:THR:HG21	1.80	0.46
2:B:361:ASP:O	2:B:414:PHE:HB3	2.15	0.46
1:E:393:LEU:HG	1:E:404:SER:HB3	1.98	0.46
1:C:283:GLU:HG2	1:C:329:TYR:OH	2.15	0.46
2:D:105:ARG:HB3	2:D:394:THR:HG23	1.98	0.46
1:E:395:GLN:HB2	1:E:400:ARG:HH11	1.81	0.46
1:A:114:ASN:HD22	1:A:115:VAL:N	2.11	0.46
1:C:103:VAL:HG21	1:C:200:VAL:HG11	1.98	0.46
1:C:235:TRP:HZ2	1:C:270:LEU:HD21	1.80	0.46
1:E:243:GLU:H	1:E:304:HIS:CD2	2.34	0.46
2:F:86:GLN:H	2:F:86:GLN:CD	2.19	0.46
1:A:258:PRO:HB2	1:A:288:TYR:CD2	2.50	0.46
1:A:432:TYR:HA	1:A:433:PRO:HD3	1.82	0.46
2:B:121:SER:O	2:B:124:MET:HB2	2.15	0.46
1:C:132:LEU:N	1:C:132:LEU:HD22	2.31	0.46
2:D:132:GLN:NE2	2:D:208:LYS:HA	2.31	0.46
2:F:102:ILE:HD12	2:F:425:LEU:CD2	2.46	0.45
2:B:389:LEU:H	2:B:389:LEU:HD23	1.81	0.45
2:D:407:PRO:HB2	2:D:431:PHE:HE2	1.81	0.45
1:E:332:LEU:O	1:E:334:PRO:CD	2.65	0.45
1:C:19:PHE:HE1	1:C:445:VAL:HG23	1.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:67:ARG:H	2:D:86:GLN:HE22	1.62	0.45
2:F:98:LYS:HA	2:F:98:LYS:HD2	1.78	0.45
1:A:282:ALA:HB2	1:A:289:PHE:CG	2.50	0.45
1:C:132:LEU:HB2	1:C:141:ALA:HB3	1.98	0.45
2:F:319:GLN:HA	2:F:330:VAL:HG21	1.98	0.45
1:A:291:HIS:HD2	2:B:258:LEU:HD13	1.81	0.45
1:E:317:ARG:NH1	1:E:317:ARG:HG2	2.32	0.45
1:E:395:GLN:HG2	1:E:396:SER:N	2.30	0.45
1:C:254:VAL:HG22	1:C:269:ILE:CD1	2.47	0.45
1:A:313:TYR:HE1	1:A:315:GLU:HA	1.82	0.45
1:C:327:ARG:HG2	1:C:329:TYR:CE1	2.52	0.45
1:C:329:TYR:N	1:C:329:TYR:CD1	2.85	0.45
2:B:376:ASN:HD22	2:B:376:ASN:H	1.62	0.45
1:C:264:LEU:HD22	1:C:282:ALA:HB3	1.97	0.45
1:E:270:LEU:HD13	1:E:276:ARG:HA	1.98	0.45
1:A:176:THR:OG1	1:A:180:GLU:HG2	2.17	0.44
1:A:3:LEU:O	1:A:5:PRO:HD3	2.17	0.44
2:B:176:PRO:HB2	2:B:214:ARG:HB2	1.99	0.44
2:D:92:LEU:CD1	2:D:403:VAL:HG11	2.44	0.44
1:E:14:PRO:HG2	1:E:17:SER:HB3	1.98	0.44
2:F:94:PRO:HB3	2:F:406:CYS:HB2	1.98	0.44
1:A:29:SER:HB3	1:A:102:ASP:OD1	2.17	0.44
2:B:308:PHE:HB2	2:B:330:VAL:HG22	1.99	0.44
2:D:360:ARG:HG2	2:D:360:ARG:HH11	1.83	0.44
2:D:35:SER:HA	2:D:36:PRO:HD3	1.84	0.44
2:F:317:LEU:HA	4:F:1016:NAG:H81	2.00	0.44
2:F:84:SER:OG	2:F:103:GLN:HB2	2.18	0.44
2:F:71:ASP:O	2:F:107:VAL:HG22	2.17	0.44
2:B:112:VAL:O	2:B:149:LEU:HD12	2.17	0.44
2:F:115:TYR:HH	2:F:192:HIS:HD1	1.66	0.44
1:C:59:ARG:HG3	1:C:62:GLY:H	1.82	0.44
2:B:249:THR:HG22	2:B:309:ALA:HB3	2.00	0.44
2:B:88:ILE:HG13	2:B:427:VAL:HG13	2.00	0.44
1:C:241:VAL:HG12	1:C:253:TYR:HD1	1.81	0.44
1:E:338:HIS:HB2	1:E:339:ALA:H	1.43	0.44
1:A:317:ARG:NH1	1:A:317:ARG:HG2	2.31	0.44
2:D:119:ASP:O	2:D:124:MET:HG3	2.18	0.44
1:A:354:GLY:HA2	1:A:380:TYR:C	2.38	0.44
1:A:284:GLN:OE1	1:A:314:MET:HB2	2.18	0.44
1:C:296:THR:O	1:C:305:ASP:HB2	2.17	0.44
1:A:400:ARG:NH1	1:A:400:ARG:HG3	2.33	0.43
1:A:379:PRO:HA	1:A:417:PHE:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:220:GLU:OE1	6:B:1301:CAC:C1	2.66	0.43
1:C:155:TYR:CE2	1:C:165:ARG:HD2	2.53	0.43
2:B:240:ASN:N	2:B:240:ASN:ND2	2.66	0.43
2:D:159:LYS:HE2	2:D:289:TYR:CE1	2.53	0.43
2:F:57:PRO:O	2:F:93:ARG:HD2	2.17	0.43
1:E:231:PHE:CD1	1:E:231:PHE:N	2.85	0.43
1:A:195:LEU:HD11	1:A:239:VAL:CG1	2.49	0.43
2:B:164:TYR:HB3	2:B:215:ASN:HD21	1.84	0.43
2:D:84:SER:HB3	2:D:85:PRO:CD	2.48	0.43
2:F:223:PHE:CZ	2:F:254:THR:HG21	2.53	0.43
1:A:400:ARG:HH11	1:A:400:ARG:HG3	1.82	0.43
2:B:120:LEU:HD22	2:B:155:ALA:CB	2.48	0.43
2:B:98:LYS:HA	2:B:98:LYS:HD2	1.80	0.43
2:D:128:LEU:HD12	2:D:128:LEU:HA	1.85	0.43
1:E:103:VAL:HG23	1:E:104:ILE:N	2.33	0.43
1:E:112:HIS:NE2	1:E:126:PRO:HG3	2.34	0.43
2:B:373:THR:CG2	2:B:379:VAL:HG22	2.44	0.43
2:B:25:TRP:CG	2:B:26:CYS:N	2.86	0.43
2:D:82:GLN:HB3	2:D:107:VAL:HG12	2.01	0.43
2:D:84:SER:CB	2:D:85:PRO:CD	2.97	0.43
2:F:65:GLU:HG3	2:F:87:ARG:HB3	2.00	0.43
9:A:1429:HOH:O	2:B:216:ARG:HD3	2.18	0.43
2:D:70:SER:HB2	2:D:107:VAL:HG21	2.01	0.43
2:D:84:SER:HB2	2:D:103:GLN:N	2.23	0.43
1:A:227:ASN:ND2	1:A:227:ASN:C	2.71	0.43
1:A:298:VAL:HG11	1:A:399:LEU:HD11	2.00	0.43
2:B:104:VAL:HG21	2:B:355:VAL:CG1	2.45	0.43
2:B:136:THR:HA	2:B:204:ASN:HD21	1.84	0.43
2:B:341:LEU:HD13	2:B:341:LEU:HA	1.82	0.43
1:C:415:SER:HB2	1:C:442:ALA:HB2	2.01	0.43
2:D:390:LYS:HE3	2:D:390:LYS:HB2	1.86	0.43
1:E:327:ARG:NH1	1:E:346:LEU:HD23	2.34	0.43
1:E:91:GLN:HG3	1:E:111:GLN:HB2	2.01	0.43
1:E:94:GLY:C	1:E:96:SER:H	2.22	0.43
1:A:123:GLU:CD	1:A:165:ARG:NH2	2.72	0.42
2:B:84:SER:HG	2:B:103:GLN:HG3	1.82	0.42
1:C:94:GLY:C	1:C:96:SER:H	2.22	0.42
1:E:227:ASN:C	1:E:227:ASN:ND2	2.71	0.42
4:F:1016:NAG:O6	4:F:1017:NAG:H82	2.18	0.42
2:F:102:ILE:CG2	2:F:397:PHE:HB2	2.49	0.42
2:F:60:GLU:HG3	2:F:61:ALA:H	1.83	0.42
2:F:91:ARG:HG2	2:F:430:THR:HB	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:243:GLU:N	1:C:304:HIS:HD2	2.16	0.42
2:F:257:ALA:O	2:F:258:LEU:HB2	2.19	0.42
1:A:356:PHE:CZ	1:A:376:VAL:HG11	2.53	0.42
1:C:258:PRO:HA	1:C:289:PHE:O	2.19	0.42
1:C:363:LEU:HD21	1:C:435:LEU:HD13	2.02	0.42
2:F:71:ASP:O	2:F:107:VAL:CG2	2.67	0.42
2:F:34:GLY:O	2:F:36:PRO:HD3	2.19	0.42
1:A:3:LEU:HA	1:A:449:ARG:O	2.20	0.42
1:C:227:ASN:C	1:C:227:ASN:HD22	2.21	0.42
1:C:269:ILE:O	1:C:277:LEU:HB2	2.20	0.42
2:D:122:TYR:HB2	2:D:214:ARG:HG2	2.01	0.42
1:E:311:PRO:HA	1:E:356:PHE:O	2.18	0.42
1:A:28:ASP:O	1:A:30:HIS:N	2.53	0.42
1:A:417:PHE:CE1	1:A:437:VAL:HG11	2.54	0.42
4:B:1003:NAG:H3	4:B:1004:MAN:O5	2.19	0.42
2:B:110:TYR:HA	2:B:111:PRO:HD3	1.91	0.42
1:A:119:THR:O	1:A:119:THR:HG23	2.19	0.42
1:C:112:HIS:NE2	1:C:126:PRO:HG3	2.35	0.42
2:B:46:LYS:NZ	2:B:46:LYS:HB3	2.34	0.42
1:C:1:LEU:H1	1:C:367:ASP:HA	1.84	0.42
2:B:3:ASN:ND2	2:B:5:CYS:HB2	2.29	0.42
1:E:18:GLN:H	1:E:443:ASN:ND2	2.18	0.42
1:E:197:GLN:HG3	1:E:220:SER:HB3	2.02	0.42
1:C:407:LEU:HD13	1:C:448:TYR:CD2	2.54	0.42
2:F:281:TYR:CE1	2:F:283:ALA:HB3	2.54	0.42
2:B:82:GLN:NE2	2:B:107:VAL:H	2.17	0.42
1:C:231:PHE:CD1	1:C:231:PHE:N	2.87	0.42
2:D:65:GLU:HG2	2:D:87:ARG:HB3	2.01	0.42
1:A:333:GLN:O	1:A:335:ARG:NH2	2.54	0.41
1:A:433:PRO:O	1:A:450:ALA:HB2	2.20	0.41
2:B:400:GLU:CB	3:B:1006:NAG:H83	2.50	0.41
2:B:141:GLN:HG2	2:B:341:LEU:HD12	2.02	0.41
2:B:249:THR:HA	2:B:309:ALA:O	2.19	0.41
2:D:139:ALA:O	2:D:143:ARG:HB2	2.19	0.41
1:E:325:VAL:O	1:E:356:PHE:HB3	2.20	0.41
1:E:335:ARG:HG2	1:E:335:ARG:HH11	1.84	0.41
1:C:340:LEU:H	1:C:340:LEU:CD1	2.33	0.41
1:E:297:ASP:O	1:E:372:ASN:HB2	2.20	0.41
1:A:377:ALA:HB2	1:A:421:LEU:HD11	2.02	0.41
1:A:430:ASN:O	1:A:432:TYR:HD1	2.03	0.41
2:B:390:LYS:HD2	2:B:390:LYS:N	2.35	0.41
1:E:181:LEU:O	1:E:197:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:409:SER:HB2	1:E:417:PHE:CD2	2.55	0.41
2:F:121:SER:O	2:F:124:MET:HB2	2.20	0.41
2:F:70:SER:OG	2:F:80:VAL:HG23	2.19	0.41
2:B:82:GLN:HE21	2:B:107:VAL:H	1.68	0.41
2:F:354:LYS:HE3	2:F:354:LYS:HB2	1.89	0.41
1:A:174:VAL:HG23	1:A:182:VAL:HB	2.02	0.41
1:A:87:PHE:CG	1:A:124:LYS:HE3	2.56	0.41
2:B:351:ILE:C	2:B:352:ARG:HD2	2.40	0.41
2:D:44:LEU:O	2:D:49:CYS:HB2	2.21	0.41
1:E:174:VAL:CG2	1:E:239:VAL:HG23	2.49	0.41
2:F:161:VAL:HG12	2:F:162:SER:N	2.35	0.41
2:D:116:TYR:HB3	2:D:153:PHE:CB	2.50	0.41
1:E:198:ALA:HA	1:E:199:PRO:HD3	1.91	0.41
2:F:400:GLU:HB2	3:F:1020:NAG:C8	2.46	0.41
1:A:113:TRP:O	1:A:124:LYS:HA	2.20	0.41
4:B:1003:NAG:C3	4:B:1004:MAN:O5	2.68	0.41
2:B:103:GLN:HB3	2:B:396:SER:HB3	2.02	0.41
1:C:198:ALA:HA	1:C:199:PRO:HD3	1.93	0.41
2:D:117:LEU:HA	2:D:117:LEU:HD12	1.89	0.41
2:F:60:GLU:O	2:F:98:LYS:HE2	2.19	0.41
2:B:87:ARG:HA	2:B:426:ILE:O	2.20	0.41
2:B:245:LEU:HD23	2:B:305:ASN:HB2	2.02	0.41
2:B:97:SER:OG	2:B:402:LYS:HG3	2.19	0.41
1:E:174:VAL:HG12	1:E:175:VAL:N	2.35	0.41
1:E:175:VAL:HA	1:E:180:GLU:O	2.21	0.41
1:E:395:GLN:CG	1:E:396:SER:N	2.84	0.41
1:E:83:THR:HB	1:E:116:LEU:HB2	2.03	0.41
2:F:112:VAL:O	2:F:149:LEU:HD12	2.21	0.41
2:F:84:SER:CB	2:F:85:PRO:HD3	2.49	0.41
2:B:93:ARG:HG3	2:B:96:ASP:HB2	2.02	0.41
1:C:432:TYR:HA	1:C:433:PRO:HD3	1.89	0.41
1:E:440:TYR:CD1	1:E:440:TYR:C	2.94	0.41
2:F:219:PRO:HA	2:F:253:LYS:O	2.21	0.41
2:F:312:GLU:HA	2:F:315:VAL:HG23	2.03	0.41
2:F:410:LYS:HA	2:F:431:PHE:HB2	2.03	0.41
1:A:303:ARG:NH2	1:A:336:GLY:H	2.19	0.41
2:B:136:THR:HA	2:B:204:ASN:ND2	2.36	0.41
2:B:159:LYS:HA	2:B:160:PRO:HD3	1.87	0.41
2:D:60:GLU:HG3	2:D:61:ALA:H	1.85	0.41
1:E:314:MET:HB2	1:E:314:MET:HE3	1.98	0.41
2:B:269:ASN:ND2	2:B:290:PRO:HB3	2.35	0.40
1:C:410:PRO:HG2	1:C:411:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:D:1009:NAG:O3	5:D:1010:MAN:C5	2.69	0.40
2:D:119:ASP:HB2	2:D:249:THR:O	2.20	0.40
2:F:117:LEU:HD12	2:F:117:LEU:HA	1.89	0.40
1:A:244:PHE:HB2	1:A:252:GLU:HG3	2.02	0.40
2:B:377:ASN:N	2:B:377:ASN:HD22	2.19	0.40
2:B:399:ILE:HD13	2:B:416:ILE:HD13	2.03	0.40
2:B:436:ALA:O	2:B:437:CYS:HB2	2.21	0.40
2:D:120:LEU:HD12	2:D:120:LEU:HA	1.72	0.40
1:E:324:GLU:HG2	9:E:1442:HOH:O	2.21	0.40
1:A:114:ASN:ND2	1:A:115:VAL:N	2.68	0.40
2:B:223:PHE:CD1	2:B:226:ILE:HD12	2.56	0.40
2:B:417:LYS:HB3	2:B:424:SER:CB	2.52	0.40
2:B:42:GLU:CD	2:B:42:GLU:H	2.23	0.40
2:D:362:LEU:O	2:D:363:PRO:C	2.60	0.40
2:B:288:ASP:OD1	2:B:289:TYR:N	2.52	0.40
1:C:103:VAL:HG11	1:C:204:PHE:CE2	2.56	0.40
1:E:77:ARG:HA	1:E:77:ARG:HD3	1.86	0.40
1:E:77:ARG:HG2	1:E:212:LEU:HD22	2.04	0.40
2:F:253:LYS:H	2:F:253:LYS:HG2	1.58	0.40
2:F:70:SER:CB	2:F:80:VAL:HG23	2.52	0.40
2:D:308:PHE:HB2	2:D:330:VAL:HG22	2.03	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	450/452 (100%)	404 (90%)	40 (9%)	6 (1%)	18	54
1	C	450/452 (100%)	409 (91%)	34 (8%)	7 (2%)	14	47
1	E	450/452 (100%)	414 (92%)	33 (7%)	3 (1%)	30	72
2	B	438/440 (100%)	390 (89%)	39 (9%)	9 (2%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	438/440 (100%)	387 (88%)	43 (10%)	8 (2%)	13	44
2	F	438/440 (100%)	386 (88%)	45 (10%)	7 (2%)	14	47
All	All	2664/2676 (100%)	2390 (90%)	234 (9%)	40 (2%)	15	50

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
2	B	85	PRO
1	C	101	SER
1	C	102	ASP
1	C	123	GLU
2	D	12	SER
2	D	49	CYS
2	D	84	SER
1	E	123	GLU
2	F	85	PRO
2	F	361	ASP
2	B	240	ASN
1	C	336	GLY
1	C	339	ALA
2	D	7	THR
2	D	72	LYS
1	E	101	SER
2	F	11	SER
1	A	31	GLY
2	B	11	SER
2	B	436	ALA
2	D	64	LEU
1	E	319	ASP
2	F	70	SER
1	A	319	ASP
1	C	319	ASP
2	D	361	ASP
2	B	34	GLY
2	B	51	PRO
2	B	73	GLY
2	B	233	ASP
2	B	374	CYS
1	C	334	PRO
2	F	199	GLN

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Mol	Chain	Res	Type
1	A	60	ALA
1	A	222	SER
2	D	50	ALA
2	F	374	CYS
2	F	75	GLY
1	A	337	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	360/360 (100%)	329 (91%)	31 (9%)	15	41
1	C	360/360 (100%)	327 (91%)	33 (9%)	13	38
1	E	360/360 (100%)	328 (91%)	32 (9%)	14	40
2	B	392/392 (100%)	361 (92%)	31 (8%)	18	46
2	D	392/392 (100%)	358 (91%)	34 (9%)	15	41
2	F	392/392 (100%)	365 (93%)	27 (7%)	22	54
All	All	2256/2256 (100%)	2068 (92%)	188 (8%)	16	43

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

Mol	Chain	Res	Type
1	A	8	LEU
1	A	23	LEU
1	A	28	ASP
1	A	43	LEU
1	A	59	ARG
1	A	64	GLN
1	A	72	LEU
1	A	84	LEU
1	A	96	SER
1	A	114	ASN
1	A	119	THR
1	A	132	LEU
1	A	136	GLU

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Mol	Chain	Res	Type
1	A	159	ASP
1	A	166	TYR
1	A	180	GLU
1	A	183	LEU
1	A	195	LEU
1	A	197	GLN
1	A	227	ASN
1	A	252	GLU
1	A	264	LEU
1	A	270	LEU
1	A	277	LEU
1	A	288	TYR
1	A	312	LEU
1	A	317	ARG
1	A	337	PRO
1	A	348	THR
1	A	373	ASP
1	A	452	PRO
2	B	3	ASN
2	B	27	SER
2	B	49	CYS
2	B	67	ARG
2	B	79	GLN
2	B	92	LEU
2	B	120	LEU
2	B	137	LYS
2	B	140	THR
2	B	145	LEU
2	B	187	MET
2	B	193	VAL
2	B	202	ARG
2	B	214	ARG
2	B	234	GLU
2	B	239	ARG
2	B	240	ASN
2	B	246	LEU
2	B	294	LEU
2	B	314	VAL
2	B	332	VAL
2	B	342	GLN
2	B	354	LYS
2	B	362	LEU

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Mol	Chain	Res	Type
2	B	364	GLU
2	B	376	ASN
2	B	406	CYS
2	B	407	PRO
2	B	409	GLU
2	B	425	LEU
2	B	437	CYS
1	C	2	ASN
1	C	23	LEU
1	C	64	GLN
1	C	72	LEU
1	C	103	VAL
1	C	114	ASN
1	C	132	LEU
1	C	140	ARG
1	C	147	ARG
1	C	158	ASN
1	C	162	TRP
1	C	166	TYR
1	C	183	LEU
1	C	190	TYR
1	C	197	GLN
1	C	212	LEU
1	C	227	ASN
1	C	243	GLU
1	C	251	THR
1	C	252	GLU
1	C	264	LEU
1	C	270	LEU
1	C	280	LEU
1	C	288	TYR
1	C	312	LEU
1	C	317	ARG
1	C	329	TYR
1	C	334	PRO
1	C	337	PRO
1	C	338	HIS
1	C	348	THR
1	C	400	ARG
1	C	408	ASP
2	D	46	LYS
2	D	49	CYS

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Mol	Chain	Res	Type
2	D	80	VAL
2	D	84	SER
2	D	86	GLN
2	D	92	LEU
2	D	105	ARG
2	D	120	LEU
2	D	137	LYS
2	D	138	LEU
2	D	174	GLU
2	D	193	VAL
2	D	202	ARG
2	D	206	GLU
2	D	214	ARG
2	D	224	ASP
2	D	239	ARG
2	D	246	LEU
2	D	249	THR
2	D	294	LEU
2	D	314	VAL
2	D	322	SER
2	D	339	ASN
2	D	341	LEU
2	D	342	GLN
2	D	352	ARG
2	D	361	ASP
2	D	362	LEU
2	D	365	GLU
2	D	376	ASN
2	D	406	CYS
2	D	407	PRO
2	D	409	GLU
2	D	437	CYS
1	E	1	LEU
1	E	2	ASN
1	E	8	LEU
1	E	23	LEU
1	E	72	LEU
1	E	76	THR
1	E	77	ARG
1	E	103	VAL
1	E	132	LEU
1	E	135	PRO

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Mol	Chain	Res	Type
1	E	147	ARG
1	E	158	ASN
1	E	166	TYR
1	E	183	LEU
1	E	190	TYR
1	E	197	GLN
1	E	212	LEU
1	E	227	ASN
1	E	252	GLU
1	E	277	LEU
1	E	288	TYR
1	E	307	LEU
1	E	312	LEU
1	E	317	ARG
1	E	334	PRO
1	E	335	ARG
1	E	337	PRO
1	E	338	HIS
1	E	348	THR
1	E	366	LEU
1	E	395	GLN
1	E	440	TYR
2	F	10	VAL
2	F	40	LEU
2	F	49	CYS
2	F	66	ASP
2	F	67	ARG
2	F	71	ASP
2	F	77	SER
2	F	85	PRO
2	F	86	GLN
2	F	179	ASP
2	F	198	ASP
2	F	202	ARG
2	F	206	GLU
2	F	214	ARG
2	F	224	ASP
2	F	239	ARG
2	F	246	LEU
2	F	294	LEU
2	F	312	GLU
2	F	319	GLN

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Mol	Chain	Res	Type
2	F	323	GLU
2	F	354	LYS
2	F	361	ASP
2	F	407	PRO
2	F	412	LYS
2	F	433	CYS
2	F	437	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	114	ASN
1	A	158	ASN
1	A	197	GLN
1	A	227	ASN
1	A	372	ASN
1	A	388	GLN
1	A	443	ASN
2	B	3	ASN
2	B	15	GLN
2	B	82	GLN
2	B	141	GLN
2	B	204	ASN
2	B	240	ASN
2	B	319	GLN
2	B	342	GLN
2	B	376	ASN
2	B	377	ASN
2	B	408	GLN
2	B	438	GLN
1	C	2	ASN
1	C	114	ASN
1	C	134	GLN
1	C	227	ASN
1	C	304	HIS
1	C	338	HIS
1	C	388	GLN
1	C	395	GLN
1	C	443	ASN
1	C	444	GLN
2	D	15	GLN

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Mol	Chain	Res	Type
2	D	82	GLN
2	D	132	GLN
2	D	199	GLN
2	D	204	ASN
2	D	319	GLN
2	D	376	ASN
2	D	440	GLN
1	E	2	ASN
1	E	18	GLN
1	E	85	GLN
1	E	158	ASN
1	E	177	GLN
1	E	197	GLN
1	E	227	ASN
1	E	278	HIS
1	E	304	HIS
1	E	351	GLN
1	E	372	ASN
2	F	15	GLN
2	F	82	GLN
2	F	86	GLN
2	F	199	GLN
2	F	204	ASN
2	F	440	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

13 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
4	NAG	B	1002	2,4	12,14,15	0.48	0	15,19,21	0.95	1 (6%)
4	NAG	B	1003	4	12,14,15	0.54	0	15,19,21	1.02	1 (6%)
4	MAN	B	1004	4	10,11,12	0.65	0	11,15,17	1.60	2 (18%)
4	BMA	B	1005	4	10,11,12	0.48	0	11,15,17	0.28	0
5	NAG	D	1008	2,5	12,14,15	0.46	0	15,19,21	0.93	1 (6%)
5	NAG	D	1009	5	12,14,15	0.66	0	15,19,21	1.18	2 (13%)
5	MAN	D	1010	5	10,11,12	0.65	0	11,15,17	1.14	2 (18%)
5	BMA	D	1011	5	10,11,12	0.49	0	11,15,17	0.33	0
5	MAN	D	1012	5	10,11,12	0.48	0	11,15,17	0.27	0
4	NAG	F	1016	2,4	12,14,15	0.56	0	15,19,21	0.85	1 (6%)
4	NAG	F	1017	4	12,14,15	0.69	0	15,19,21	1.13	1 (6%)
4	MAN	F	1018	4	10,11,12	0.54	0	11,15,17	0.73	0
4	BMA	F	1019	4	10,11,12	0.51	0	11,15,17	0.33	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
4	NAG	B	1002	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	4	-	0/6/23/26	0/1/1/1
4	MAN	B	1004	4	-	0/2/19/22	0/1/1/1
4	BMA	B	1005	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1008	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1009	5	-	0/6/23/26	0/1/1/1
5	MAN	D	1010	5	-	0/2/19/22	0/1/1/1
5	BMA	D	1011	5	-	0/2/19/22	0/1/1/1
5	MAN	D	1012	5	-	0/2/19/22	0/1/1/1
4	NAG	F	1016	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	1017	4	-	0/6/23/26	0/1/1/1
4	MAN	F	1018	4	-	0/2/19/22	0/1/1/1
4	BMA	F	1019	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	MAN	C3-C4-C5	3.59	116.61	110.17
4	B	1004	MAN	C4-C3-C2	3.01	113.97	110.61
4	B	1003	NAG	C2-N2-C7	-2.98	119.79	123.39
4	B	1002	NAG	C2-N2-C7	-2.87	119.92	123.39
4	F	1017	NAG	C3-C2-N2	-2.79	107.44	111.62
5	D	1008	NAG	C2-N2-C7	-2.78	120.03	123.39
5	D	1010	MAN	C4-C3-C2	2.47	113.37	110.61
4	F	1016	NAG	C2-N2-C7	-2.36	120.53	123.39
5	D	1009	NAG	C2-N2-C7	-2.36	120.54	123.39
5	D	1009	NAG	C3-C2-N2	-2.32	108.14	111.62
5	D	1010	MAN	C3-C4-C5	2.11	113.95	110.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 21 are monoatomic - leaving 10 for Mogul analysis.

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	B	1001	2	12,14,15	0.60	0	15,19,21	0.92	1 (6%)
3	NAG	B	1006	2	12,14,15	0.45	0	15,19,21	0.88	1 (6%)
6	CAC	B	1301	7	4,4,4	4.46	4 (100%)	6,6,6	7.11	3 (50%)
3	NAG	D	1007	2	12,14,15	0.59	0	15,19,21	0.84	0
3	NAG	D	1013	2	12,14,15	0.58	0	15,19,21	1.00	1 (6%)
6	CAC	D	1302	7	4,4,4	4.33	4 (100%)	6,6,6	5.36	3 (50%)
3	NAG	E	1014	1	12,14,15	0.57	0	15,19,21	0.80	0
3	NAG	F	1015	2	12,14,15	0.55	0	15,19,21	0.82	1 (6%)
3	NAG	F	1020	2	12,14,15	0.45	0	15,19,21	0.93	1 (6%)
6	CAC	F	1303	7	4,4,4	4.32	4 (100%)	6,6,6	5.62	3 (50%)

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	B	1001	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1006	2	-	0/6/23/26	0/1/1/1
6	CAC	B	1301	7	-	0/0/0/0	0/0/0/0
3	NAG	D	1007	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1013	2	-	0/6/23/26	0/1/1/1
6	CAC	D	1302	7	-	0/0/0/0	0/0/0/0
3	NAG	E	1014	1	-	1/6/23/26	0/1/1/1
3	NAG	F	1015	2	-	1/6/23/26	0/1/1/1
3	NAG	F	1020	2	-	0/6/23/26	0/1/1/1
6	CAC	F	1303	7	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1301	CAC	O2-AS	7.29	1.76	1.68
6	F	1303	CAC	O2-AS	7.23	1.76	1.68
6	D	1302	CAC	O2-AS	7.05	1.76	1.68
6	D	1302	CAC	AS-C1	3.98	1.96	1.91
6	B	1301	CAC	AS-C1	3.85	1.96	1.91
6	F	1303	CAC	AS-C1	3.52	1.95	1.91
6	B	1301	CAC	AS-C2	-2.61	1.87	1.91
6	F	1303	CAC	AS-C2	-2.37	1.88	1.91
6	D	1302	CAC	AS-C2	-2.28	1.88	1.91
6	B	1301	CAC	O1-AS	2.16	1.75	1.67
6	F	1303	CAC	O1-AS	2.12	1.75	1.67
6	D	1302	CAC	O1-AS	2.09	1.75	1.67

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1301	CAC	O2-AS-O1	-16.42	108.99	112.54
6	F	1303	CAC	O2-AS-O1	-12.49	109.84	112.54
6	D	1302	CAC	O2-AS-O1	-11.72	110.01	112.54
6	B	1301	CAC	O1-AS-C2	3.91	122.50	109.18
6	F	1303	CAC	O1-AS-C2	3.91	122.50	109.18
6	D	1302	CAC	C2-AS-C1	-3.88	100.57	109.43
6	D	1302	CAC	O1-AS-C2	3.87	122.38	109.18
6	B	1301	CAC	C2-AS-C1	-3.62	101.15	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1303	CAC	C2-AS-C1	-3.53	101.37	109.43
3	D	1013	NAG	C2-N2-C7	-3.47	119.20	123.39
3	F	1020	NAG	C2-N2-C7	-2.90	119.89	123.39
3	B	1006	NAG	C2-N2-C7	-2.68	120.15	123.39
3	F	1015	NAG	C2-N2-C7	-2.37	120.52	123.39
3	B	1001	NAG	C2-N2-C7	-2.33	120.58	123.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1014	NAG	C8-C7-N2-C2
3	F	1015	NAG	O7-C7-N2-C2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	452/452 (100%)	0.17	12 (2%) 52 61	19, 52, 91, 113	2 (0%)
1	C	452/452 (100%)	-0.01	6 (1%) 74 82	24, 47, 87, 108	2 (0%)
1	E	452/452 (100%)	0.01	6 (1%) 74 82	26, 45, 79, 107	2 (0%)
2	B	440/440 (100%)	0.63	52 (11%) 5 7	31, 75, 118, 120	8 (1%)
2	D	440/440 (100%)	0.43	28 (6%) 19 23	27, 67, 108, 120	8 (1%)
2	F	440/440 (100%)	0.77	68 (15%) 3 4	36, 97, 120, 120	8 (1%)
All	All	2676/2676 (100%)	0.33	172 (6%) 19 23	19, 58, 117, 120	30 (1%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	76	ASP	19.0
2	D	75	GLY	16.5
2	D	76	ASP	14.3
2	D	73	GLY	13.9
2	B	75	GLY	13.3
2	D	74	SER	9.4
2	F	75	GLY	9.4
2	B	77	SER	9.3
2	F	11	SER	8.7
2	B	74	SER	8.6
2	F	79	GLN	8.3
1	C	1	LEU	7.0
2	B	79	GLN	6.1
1	A	1	LEU	5.9
2	B	11	SER	5.7
2	F	78	SER	5.6
2	B	78	SER	5.4
2	D	72	LYS	5.3
2	F	74	SER	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	77	SER	5.0
2	F	34	GLY	5.0
1	A	336	GLY	4.9
2	B	73	GLY	4.8
1	E	1	LEU	4.8
2	F	30	ALA	4.8
1	A	29	SER	4.7
2	F	375	LEU	4.7
2	F	48	ASN	4.7
2	F	88	ILE	4.5
1	A	320	ARG	4.5
2	B	408	GLN	4.4
1	A	6	VAL	4.4
2	B	31	LEU	4.4
2	D	408	GLN	4.4
2	B	33	LEU	4.4
2	F	31	LEU	4.4
2	F	435	CYS	4.2
1	C	338	HIS	4.2
2	F	407	PRO	4.2
2	B	41	LYS	4.2
2	F	10	VAL	4.2
2	F	426	ILE	4.0
2	D	107	VAL	4.0
2	B	10	VAL	3.9
2	F	408	GLN	3.9
2	B	9	GLY	3.9
2	B	80	VAL	3.8
2	F	35	SER	3.8
2	F	33	LEU	3.8
1	A	30	HIS	3.8
2	B	81	THR	3.8
2	F	73	GLY	3.8
2	F	36	PRO	3.7
2	F	6	THR	3.7
2	B	71	ASP	3.6
2	B	410	LYS	3.6
2	B	383	LEU	3.6
2	D	77	SER	3.6
2	D	78	SER	3.6
2	D	355	VAL	3.6
2	B	390	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	410	LYS	3.4
1	E	319	ASP	3.4
2	F	90	LEU	3.3
2	F	430	THR	3.3
2	F	425	LEU	3.3
2	F	76	ASP	3.3
2	B	30	ALA	3.2
2	F	26	CYS	3.2
2	B	69	LEU	3.2
2	F	436	ALA	3.2
2	F	58	VAL	3.2
2	B	47	ASP	3.2
2	F	46	LYS	3.1
2	D	79	GLN	3.1
2	D	108	GLU	3.1
1	E	320	ARG	3.0
2	F	80	VAL	3.0
2	D	407	PRO	3.0
2	B	435	CYS	3.0
1	A	452	PRO	3.0
2	F	392	GLY	3.0
2	F	37	ARG	3.0
2	F	395	VAL	2.9
2	F	383	LEU	2.9
2	B	24	ALA	2.9
2	F	414	PHE	2.9
1	A	303	ARG	2.9
2	F	28	ASP	2.9
2	F	409	GLU	2.9
2	B	409	GLU	2.8
2	F	83	VAL	2.8
2	F	107	VAL	2.8
2	F	64	LEU	2.8
2	F	374	CYS	2.8
2	F	32	PRO	2.8
2	F	50	ALA	2.8
2	F	52	GLU	2.8
2	F	422	LYS	2.8
2	F	9	GLY	2.8
2	B	438	GLN	2.8
2	B	25	TRP	2.8
2	F	49	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	409	GLU	2.7
2	B	429	VAL	2.7
1	E	337	PRO	2.7
2	B	55	GLU	2.7
2	F	8	ARG	2.7
2	D	375	LEU	2.6
2	D	378	GLU	2.6
2	B	35	SER	2.6
2	F	439	ALA	2.6
2	B	40	LEU	2.6
2	B	72	LYS	2.6
2	B	426	ILE	2.6
1	C	337	PRO	2.6
2	F	7	THR	2.6
2	F	438	GLN	2.6
2	F	427	VAL	2.5
2	B	70	SER	2.5
2	F	411	GLU	2.5
2	F	397	PHE	2.5
2	B	437	CYS	2.5
2	B	420	GLY	2.5
2	D	82	GLN	2.5
2	B	440	GLN	2.5
2	F	437	CYS	2.5
2	F	428	GLN	2.5
2	B	394	THR	2.5
2	F	429	VAL	2.5
2	F	389	LEU	2.4
2	F	47	ASP	2.4
2	D	241	ASP	2.4
1	A	337	PRO	2.4
2	D	423	ASP	2.4
2	B	56	PHE	2.3
2	F	62	ARG	2.3
2	B	34	GLY	2.3
2	B	424	SER	2.3
1	C	452	PRO	2.3
2	F	376	ASN	2.3
2	F	69	LEU	2.3
2	D	10	VAL	2.3
2	D	29	GLU	2.3
2	B	42	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	2.2
2	B	54	ILE	2.2
1	C	339	ALA	2.2
2	F	87	ARG	2.2
2	B	36	PRO	2.2
1	E	321	LYS	2.2
2	B	46	LYS	2.2
1	A	7	GLN	2.2
2	B	406	CYS	2.1
2	B	375	LEU	2.1
1	C	319	ASP	2.1
2	F	364	GLU	2.1
2	D	360	ARG	2.1
2	B	142	MET	2.1
2	B	378	GLU	2.1
2	F	410	LYS	2.1
2	F	14	GLN	2.1
1	A	398	GLY	2.1
2	D	372	ALA	2.1
2	B	425	LEU	2.1
2	D	383	LEU	2.1
2	D	13	CYS	2.1
1	E	318	ALA	2.0
2	D	380	ILE	2.0
2	B	8	ARG	2.0
2	F	54	ILE	2.0
2	D	31	LEU	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	F	1016	14/15	0.21	1.02	53,59,66,69	0
5	NAG	D	1009	14/15	0.21	0.54	77,81,87,95	0
4	BMA	F	1019	11/12	0.21	-0.05	102,103,104,104	0
4	NAG	B	1002	14/15	0.16	-0.64	53,59,61,69	0
5	NAG	D	1008	14/15	0.13	-3.00	48,52,58,68	0
5	MAN	D	1012	11/12	0.41	-	117,118,119,119	0
4	NAG	B	1003	14/15	0.26	-	77,82,88,96	0
4	MAN	B	1004	11/12	0.37	-	103,107,108,111	0
4	NAG	F	1017	14/15	0.29	-	77,81,86,91	0
4	MAN	F	1018	11/12	0.30	-	97,101,102,103	0
5	MAN	D	1010	11/12	0.34	-	103,110,113,116	0
5	BMA	D	1011	11/12	0.44	-	115,116,117,117	0
4	BMA	B	1005	11/12	0.25	-	112,113,114,115	0

6.4 Ligands

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	F	1015	14/15	0.43	5.31	118,119,120,120	0
8	CA	B	1403	1/1	0.20	3.21	28,28,28,28	0
3	NAG	D	1007	14/15	0.28	2.46	101,104,105,105	0
3	NAG	B	1006	14/15	0.29	2.35	102,103,103,103	0
6	CAC	B	1301	5/5	0.21	1.61	100,101,102,102	0
8	CA	D	1410	1/1	0.21	1.20	24,24,24,24	0
6	CAC	F	1303	5/5	0.19	1.08	114,114,115,115	0
3	NAG	B	1001	14/15	0.26	0.90	109,111,113,114	0
8	CA	F	1417	1/1	0.20	0.79	42,42,42,42	0
3	NAG	E	1014	14/15	0.32	0.68	87,92,95,95	0
3	NAG	F	1020	14/15	0.24	0.34	109,112,113,114	0
8	CA	B	1402	1/1	0.14	0.08	48,48,48,48	0
3	NAG	D	1013	14/15	0.17	-0.14	92,94,96,96	0
6	CAC	D	1302	5/5	0.16	-0.52	96,96,98,98	0
8	CA	C	1412	1/1	0.12	-0.80	46,46,46,46	0
8	CA	E	1419	1/1	0.12	-0.87	35,35,35,35	0
7	MG	F	1415	1/1	0.13	-0.97	32,32,32,32	0
7	MG	D	1408	1/1	0.14	-1.26	18,18,18,18	0
7	MG	B	1401	1/1	0.12	-1.26	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CA	D	1409	1/1	0.14	-1.48	54,54,54,54	0
8	CA	C	1411	1/1	0.09	-1.49	58,58,58,58	0
8	CA	E	1418	1/1	0.09	-1.54	48,48,48,48	0
8	CA	C	1414	1/1	0.06	-1.63	68,68,68,68	0
8	CA	A	1405	1/1	0.07	-1.75	75,75,75,75	0
8	CA	E	1420	1/1	0.08	-1.98	51,51,51,51	0
8	CA	E	1421	1/1	0.09	-2.04	65,65,65,65	0
8	CA	A	1407	1/1	0.07	-2.13	68,68,68,68	0
8	CA	A	1404	1/1	0.06	-2.37	61,61,61,61	0
8	CA	F	1416	1/1	0.06	-2.42	63,63,63,63	0
8	CA	C	1413	1/1	0.08	-2.56	70,70,70,70	0
8	CA	A	1406	1/1	0.07	-3.05	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.