



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 PM GMT

PDB ID : 4KDO
Title : Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus in complex with human receptor analog LSTc
Authors : Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-25
Resolution : 2.40 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

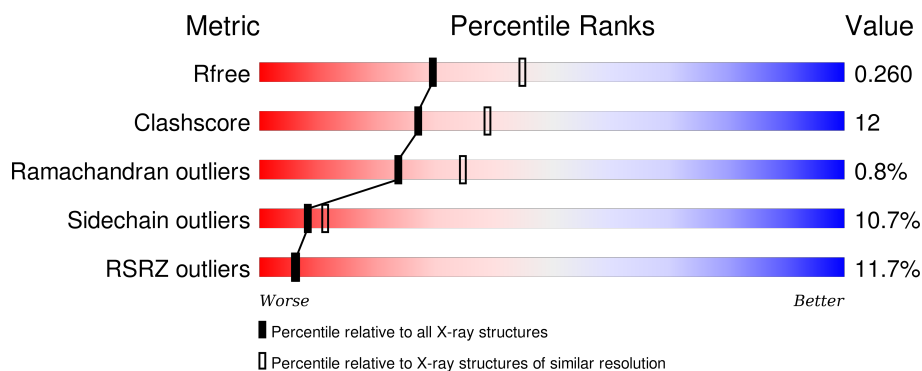
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	322	<div> <div>4%</div> <div>69% 25% 6%</div> </div>
1	C	322	<div> <div>5%</div> <div>70% 24% 7%</div> </div>
1	E	322	<div> <div>7%</div> <div>70% 23% 7%</div> </div>
2	B	175	<div> <div>24%</div> <div>72% 23% 5%</div> </div>
2	D	175	<div> <div>30%</div> <div>73% 25% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	175	<div><div></div><div>18%</div><div>73%</div><div>24%</div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12373 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	C	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	EXPRESSION TAG	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	319	ILE	THR	engineered mutation	UNP Q6DQ33
C	4	GLN	-	EXPRESSION TAG	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	319	ILE	THR	engineered mutation	UNP Q6DQ33
E	4	GLN	-	EXPRESSION TAG	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	319	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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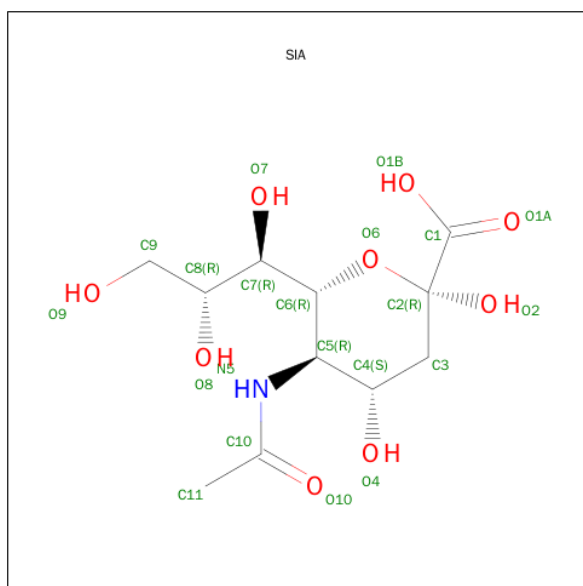
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	3	Total	C	N	O	0	0
			46	25	2	19		

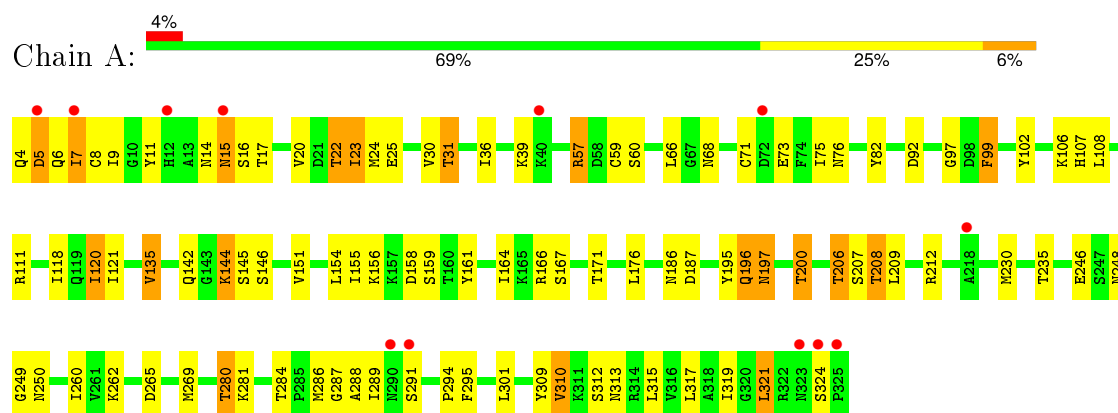
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	80	Total	O	0	0
			80	80		
7	C	80	Total	O	0	0
			80	80		
7	E	64	Total	O	0	0
			64	64		
7	B	24	Total	O	0	0
			24	24		
7	D	22	Total	O	0	0
			22	22		
7	F	13	Total	O	0	0
			13	13		

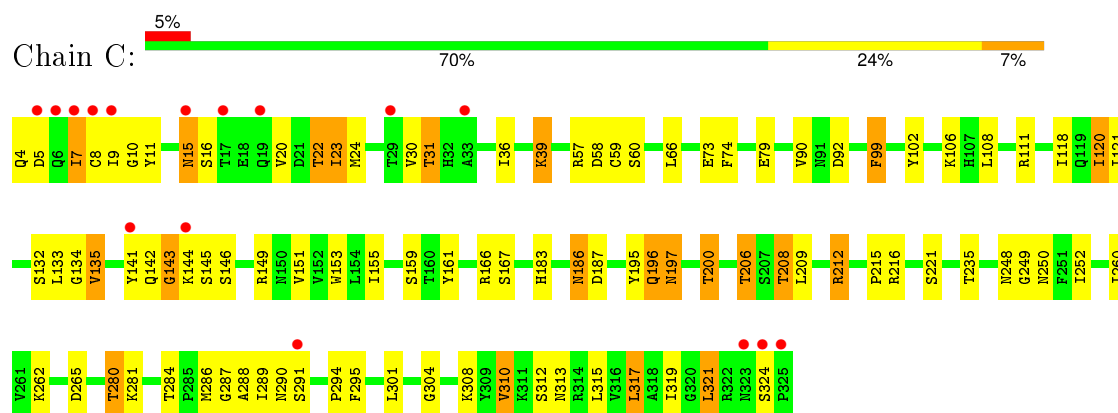
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

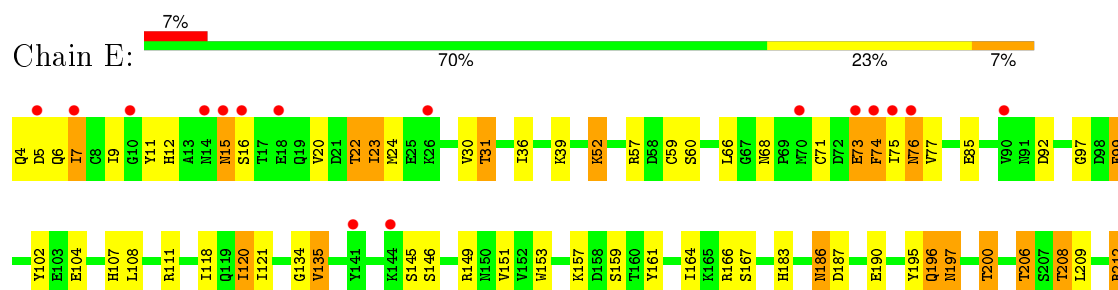
• Molecule 1: Hemagglutinin

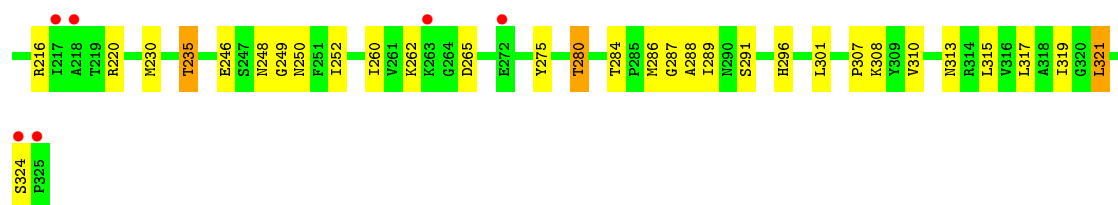


• Molecule 1: Hemagglutinin

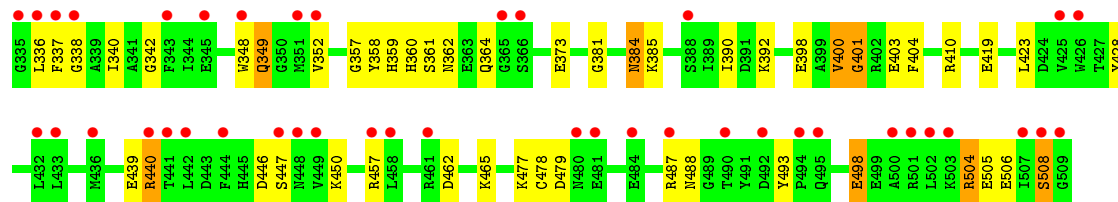


• Molecule 1: Hemagglutinin

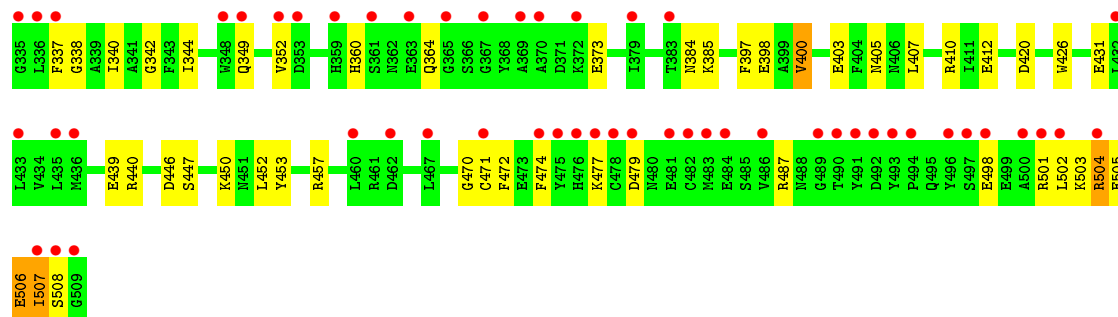
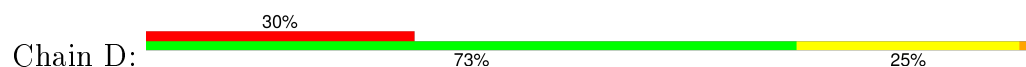




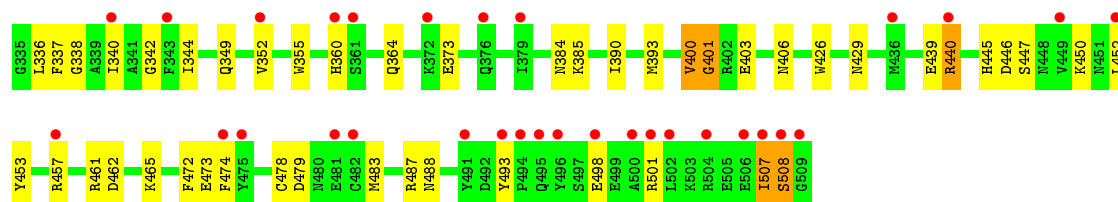
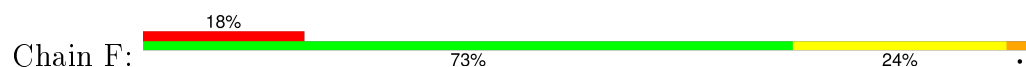
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.26Å 245.91Å 69.57Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	34.18 – 2.40 34.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.18-2.40) 97.2 (34.18-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.237 , 0.269 0.228 , 0.260	Depositor DCC
R_{free} test set	3971 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.5	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78968 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12373	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SIA, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/2621	0.82	9/3558 (0.3%)
1	C	0.59	0/2621	0.98	10/3558 (0.3%)
1	E	0.58	0/2621	0.88	10/3558 (0.3%)
2	B	0.51	0/1443	0.62	0/1939
2	D	0.51	0/1443	0.59	0/1939
2	F	0.54	1/1443 (0.1%)	0.56	0/1939
All	All	0.57	1/12192 (0.0%)	0.80	29/16491 (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
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	429	ASN	CG-ND2	-6.90	1.15	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ARG	NE-CZ-NH1	-18.41	111.10	120.30
1	C	57	ARG	NE-CZ-NH2	17.42	129.01	120.30
1	C	212	ARG	NE-CZ-NH1	-16.97	111.81	120.30
1	C	212	ARG	NE-CZ-NH2	16.17	128.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	ARG	NE-CZ-NH1	-11.93	114.34	120.30
1	E	149	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	E	57	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	E	57	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	A	212	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	E	212	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	57	ARG	CD-NE-CZ	7.38	133.94	123.60
1	A	73	GLU	C-N-CA	-7.34	103.34	121.70
1	C	212	ARG	CD-NE-CZ	7.12	133.57	123.60
1	E	212	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	66	LEU	N-CA-C	-6.80	92.64	111.00
1	C	149	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	66	LEU	N-CA-C	-6.59	93.21	111.00
1	A	212	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	73	GLU	CA-C-N	6.37	131.20	117.20
1	C	66	LEU	N-CA-C	-6.30	93.98	111.00
1	A	73	GLU	O-C-N	-6.12	112.90	122.70
1	A	57	ARG	CB-CG-CD	6.11	127.50	111.60
1	A	57	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	195	TYR	N-CA-C	-5.62	95.81	111.00
1	E	195	TYR	N-CA-C	-5.48	96.19	111.00
1	A	195	TYR	N-CA-C	-5.45	96.29	111.00
1	C	149	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	235	THR	CB-CA-C	-5.09	97.87	111.60
1	E	57	ARG	CD-NE-CZ	5.05	130.67	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ILE	Peptide
1	C	143	GLY	Peptide
1	C	4	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	0	2514	73	1
1	C	2559	0	2513	70	2
1	E	2559	0	2514	79	1
2	B	1416	0	1319	48	0
2	D	1416	0	1319	40	0
2	F	1416	0	1319	52	0
3	A	28	0	25	0	0
3	C	28	0	25	0	0
3	E	28	0	25	0	0
4	A	21	0	18	0	0
5	C	14	0	13	0	0
6	C	46	0	40	2	0
7	A	80	0	0	6	0
7	B	24	0	0	4	0
7	C	80	0	0	10	0
7	D	22	0	0	3	0
7	E	64	0	0	11	0
7	F	13	0	0	3	0
All	All	12373	0	11644	285	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (285) 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:C:7:ILE:HG22	2:D:472:PHE:HB2	1.39	1.04
2:D:398:GLU:OE2	7:D:617:HOH:O	1.81	0.99
1:A:8:CYS:N	2:B:359:HIS:O	2.03	0.91
1:C:206:THR:HG22	1:C:208:THR:H	1.35	0.90
1:E:5:ASP:O	2:F:474:PHE:N	2.02	0.90
1:E:284:THR:HG22	1:E:286:MET:H	1.37	0.90
2:B:498:GLU:OE2	7:B:604:HOH:O	1.92	0.87
1:C:284:THR:HG22	1:C:286:MET:H	1.38	0.85
1:E:206:THR:HG22	1:E:208:THR:H	1.41	0.84
1:C:7:ILE:O	2:D:472:PHE:N	2.10	0.84
1:A:284:THR:HG22	1:A:286:MET:H	1.41	0.83
2:D:503:LYS:O	2:D:507:ILE:N	2.11	0.82
2:B:336:LEU:O	2:F:447:SER:OG	1.98	0.81
1:A:8:CYS:HB2	2:B:359:HIS:HB3	1.61	0.81
1:E:39:LYS:NZ	1:E:313:ASN:O	2.13	0.80
2:F:406:ASN:O	7:F:608:HOH:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:SER:HA	7:C:759:HOH:O	1.81	0.80
1:A:206:THR:HG22	1:A:208:THR:H	1.46	0.79
2:B:488:ASN:ND2	7:B:623:HOH:O	2.13	0.79
1:C:8:CYS:HA	2:D:471:CYS:HA	1.63	0.79
2:D:501:ARG:NH1	2:F:508:SER:OG	2.15	0.79
2:D:403:GLU:OE2	7:D:603:HOH:O	2.02	0.77
1:E:275:TYR:OH	7:E:557:HOH:O	2.01	0.77
1:A:8:CYS:O	2:B:359:HIS:N	2.20	0.75
1:C:186:ASN:O	7:C:726:HOH:O	2.04	0.74
1:A:39:LYS:NZ	1:A:313:ASN:O	2.16	0.74
1:E:11:TYR:OH	2:F:340:ILE:O	2.02	0.74
1:E:6:GLN:HA	2:F:472:PHE:O	1.89	0.73
1:A:200:THR:HG21	1:A:250:ASN:OD1	1.88	0.73
1:E:5:ASP:HB2	2:F:474:PHE:HB2	1.71	0.73
1:C:9:ILE:N	2:D:470:GLY:O	2.22	0.71
2:B:419:GLU:OE2	7:B:622:HOH:O	2.08	0.70
2:D:412:GLU:OE2	7:D:610:HOH:O	2.09	0.70
1:E:206:THR:HB	1:E:209:LEU:HB3	1.74	0.69
1:E:134:GLY:N	7:E:511:HOH:O	2.22	0.69
2:D:360:HIS:HD2	2:D:487:ARG:HH21	1.39	0.69
1:E:200:THR:HG21	1:E:250:ASN:OD1	1.93	0.69
2:B:360:HIS:HD2	2:B:487:ARG:HH21	1.39	0.69
2:B:360:HIS:HD2	2:B:487:ARG:NH2	1.91	0.69
1:E:85:GLU:OE2	7:E:510:HOH:O	2.10	0.68
6:C:605:GAL:O3	7:C:729:HOH:O	2.11	0.68
1:C:22:THR:HG22	1:C:24:MET:H	1.59	0.68
1:E:9:ILE:HD13	2:F:453:TYR:HA	1.75	0.68
1:E:284:THR:HB	1:E:287:GLY:O	1.95	0.67
2:D:504:ARG:O	2:D:508:SER:N	2.19	0.67
1:C:39:LYS:NZ	1:C:313:ASN:O	2.21	0.66
2:D:360:HIS:HD2	2:D:487:ARG:NH2	1.94	0.66
1:A:206:THR:HB	1:A:209:LEU:HB3	1.78	0.66
1:A:6:GLN:N	2:B:361:SER:O	2.25	0.66
1:C:200:THR:HG21	1:C:250:ASN:OD1	1.95	0.66
1:E:22:THR:HG22	1:E:24:MET:H	1.61	0.66
1:A:7:ILE:HD13	2:B:359:HIS:O	1.96	0.65
1:C:290:ASN:ND2	7:C:742:HOH:O	2.29	0.65
1:E:190:GLU:OE1	7:E:527:HOH:O	2.14	0.65
1:E:12:HIS:HB2	2:F:355:TRP:HA	1.78	0.65
2:D:501:ARG:HH12	2:F:508:SER:CB	2.09	0.65
2:B:465:LYS:NZ	2:F:461:ARG:HH12	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:ND1	2:B:403:GLU:OE1	2.26	0.64
1:A:197:ASN:OD1	1:A:197:ASN:N	2.31	0.64
1:C:301:LEU:HA	2:D:400:VAL:HG22	1.79	0.64
1:E:104:GLU:OE2	2:B:410:ARG:NE	2.26	0.64
1:A:284:THR:HB	1:A:287:GLY:O	1.99	0.63
1:E:52:LYS:HE2	7:E:557:HOH:O	1.99	0.63
2:F:488:ASN:ND2	7:F:612:HOH:O	2.29	0.63
1:E:74:PHE:HZ	1:E:76:ASN:HD22	1.47	0.62
1:C:135:VAL:HG22	1:C:146:SER:HA	1.81	0.62
1:C:284:THR:HB	1:C:287:GLY:O	2.00	0.62
1:C:197:ASN:N	1:C:197:ASN:OD1	2.33	0.62
1:E:12:HIS:N	2:F:355:TRP:O	2.28	0.61
1:A:289:ILE:HG22	1:A:291:SER:HB3	1.82	0.61
1:A:135:VAL:HG22	1:A:146:SER:HA	1.82	0.61
1:C:159:SER:O	1:C:196:GLN:HG3	2.01	0.61
1:E:301:LEU:HA	2:F:400:VAL:HG22	1.83	0.61
2:B:465:LYS:HZ3	2:F:461:ARG:HH12	1.47	0.61
1:C:206:THR:HB	1:C:209:LEU:HB3	1.82	0.60
1:C:289:ILE:HG22	1:C:291:SER:HB3	1.82	0.60
1:A:22:THR:HG22	1:A:24:MET:H	1.67	0.60
1:E:75:ILE:HG12	1:E:77:VAL:HG23	1.85	0.59
2:F:340:ILE:HG13	2:F:446:ASP:HA	1.84	0.59
1:C:24:MET:HA	2:B:384:ASN:HB3	1.84	0.58
1:A:197:ASN:ND2	7:A:519:HOH:O	2.36	0.58
1:A:5:ASP:CG	2:B:362:ASN:HA	2.23	0.58
1:E:289:ILE:HG22	1:E:291:SER:HB3	1.84	0.58
1:C:141:TYR:CG	1:C:142:GLN:N	2.71	0.58
1:A:8:CYS:O	2:B:358:TYR:HA	2.02	0.58
1:C:10:GLY:HA2	2:D:344:ILE:HG21	1.84	0.57
1:A:159:SER:O	1:A:196:GLN:HG3	2.04	0.57
1:C:7:ILE:HB	2:D:474:PHE:HE1	1.70	0.57
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.86	0.57
1:C:215:PRO:O	7:C:775:HOH:O	2.18	0.57
1:E:321:LEU:HB3	2:F:445:HIS:CD2	2.39	0.57
2:D:502:LEU:O	2:D:506:GLU:HB3	2.06	0.56
2:D:340:ILE:HG13	2:D:446:ASP:HA	1.86	0.56
2:B:340:ILE:HG13	2:B:446:ASP:HA	1.86	0.56
7:E:517:HOH:O	2:B:410:ARG:HB2	2.05	0.56
1:E:159:SER:O	1:E:196:GLN:HG3	2.05	0.56
1:E:9:ILE:O	2:F:344:ILE:HD13	2.05	0.56
2:D:364:GLN:OE1	2:D:479:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:PHE:HB3	1:E:102:TYR:HB2	1.87	0.56
1:E:135:VAL:HG22	1:E:146:SER:HA	1.87	0.56
1:C:31:THR:HB	1:C:321:LEU:H	1.71	0.56
1:A:6:GLN:O	2:B:361:SER:N	2.36	0.55
1:E:75:ILE:O	1:E:77:VAL:N	2.38	0.55
1:C:11:TYR:OH	2:D:340:ILE:O	2.13	0.55
1:C:23:ILE:HD12	2:B:385:LYS:HG3	1.89	0.55
1:E:108:LEU:HD12	1:E:262:LYS:HD2	1.89	0.54
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.88	0.54
1:C:135:VAL:HG13	1:C:145:SER:HB3	1.88	0.54
1:C:108:LEU:HD12	1:C:262:LYS:HD2	1.90	0.54
1:C:99:PHE:HB3	1:C:102:TYR:HB2	1.88	0.54
1:E:31:THR:HB	1:E:321:LEU:H	1.73	0.54
1:C:7:ILE:HB	2:D:474:PHE:CE1	2.43	0.54
1:A:23:ILE:HD12	2:F:385:LYS:HG3	1.90	0.54
1:A:57:ARG:O	7:A:525:HOH:O	2.18	0.54
1:A:301:LEU:HA	2:B:400:VAL:HG22	1.89	0.54
1:A:120:ILE:HG22	1:A:121:ILE:HG13	1.89	0.54
1:C:206:THR:HG22	1:C:209:LEU:H	1.73	0.53
1:A:108:LEU:HD12	1:A:262:LYS:HD2	1.91	0.53
1:C:280:THR:HG21	1:C:288:ALA:HB1	1.91	0.53
1:C:24:MET:HB3	2:B:381:GLY:HA2	1.92	0.52
1:E:5:ASP:N	7:E:537:HOH:O	2.35	0.52
1:A:31:THR:HB	1:A:321:LEU:H	1.74	0.52
1:E:74:PHE:CE2	1:E:76:ASN:HB2	2.45	0.52
2:B:398:GLU:OE1	2:D:420:ASP:OD2	2.28	0.52
1:A:135:VAL:HG13	1:A:145:SER:HB3	1.92	0.51
1:E:197:ASN:N	1:E:197:ASN:OD1	2.40	0.51
1:E:6:GLN:HG2	2:F:473:GLU:HA	1.91	0.51
1:E:135:VAL:HG13	1:E:145:SER:HB3	1.92	0.51
1:A:17:THR:O	7:A:575:HOH:O	2.19	0.51
1:A:206:THR:HG22	1:A:209:LEU:H	1.74	0.51
1:E:212:ARG:NH2	7:E:513:HOH:O	2.06	0.51
1:C:308:LYS:HD2	2:D:426:TRP:CE2	2.45	0.51
2:F:364:GLN:OE1	2:F:479:ASP:HB2	2.11	0.51
2:B:462:ASP:OD1	2:B:493:TYR:OH	2.19	0.51
1:A:14:ASN:HA	2:B:349:GLN:NE2	2.26	0.51
1:C:143:GLY:C	1:C:144:LYS:HG3	2.32	0.51
2:B:364:GLN:OE1	2:B:479:ASP:HB2	2.11	0.51
2:B:504:ARG:O	2:B:506:GLU:N	2.44	0.50
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ILE:HB	2:F:474:PHE:CE1	2.47	0.50
1:C:9:ILE:HD13	2:D:453:TYR:CD1	2.45	0.50
2:F:478:CYS:HB3	2:F:483:MET:HE3	1.93	0.50
1:C:15:ASN:N	1:C:15:ASN:OD1	2.39	0.50
1:E:200:THR:OG1	1:E:248:ASN:HB3	2.11	0.49
1:E:216:ARG:O	1:E:220:ARG:NH2	2.46	0.49
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.47	0.49
2:B:337:PHE:CE1	2:B:447:SER:HB2	2.48	0.49
2:D:337:PHE:CE1	2:D:447:SER:HB2	2.48	0.48
1:A:158:ASP:O	7:A:574:HOH:O	2.20	0.48
1:A:280:THR:HG21	1:A:288:ALA:HB1	1.94	0.48
1:C:200:THR:OG1	1:C:248:ASN:HB3	2.13	0.48
1:E:107:HIS:ND1	2:F:403:GLU:OE1	2.42	0.48
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.49	0.48
2:D:504:ARG:C	2:D:506:GLU:H	2.17	0.48
2:D:360:HIS:CD2	2:D:487:ARG:NH2	2.79	0.48
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.49	0.48
1:E:68:ASN:HB3	1:E:71:CYS:SG	2.54	0.48
2:B:337:PHE:CE2	2:F:337:PHE:HE2	2.32	0.48
2:B:360:HIS:CD2	2:B:487:ARG:NH2	2.78	0.48
2:F:452:LEU:HD12	2:F:452:LEU:HA	1.70	0.48
1:C:79:GLU:HB3	7:C:777:HOH:O	2.14	0.48
2:B:384:ASN:OD1	7:B:619:HOH:O	2.19	0.47
1:C:23:ILE:HG22	1:C:24:MET:HG3	1.96	0.47
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.49	0.47
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.49	0.47
1:C:133:LEU:O	6:C:604:SIA:H113	2.14	0.47
1:E:7:ILE:HB	2:F:474:PHE:HE1	1.78	0.47
2:F:462:ASP:OD1	2:F:493:TYR:OH	2.20	0.47
1:E:164:ILE:O	1:E:246:GLU:HA	2.15	0.47
1:E:15:ASN:N	1:E:15:ASN:OD1	2.39	0.47
1:A:164:ILE:O	1:A:246:GLU:HA	2.15	0.47
1:E:23:ILE:HG22	1:E:24:MET:HG3	1.97	0.47
1:A:309:TYR:CD2	2:B:423:LEU:HD13	2.50	0.47
2:F:337:PHE:CE1	2:F:447:SER:HB2	2.50	0.46
1:E:7:ILE:HG22	2:F:472:PHE:HB2	1.97	0.46
1:E:108:LEU:CD1	1:E:262:LYS:HD2	2.46	0.46
1:C:108:LEU:CD1	1:C:262:LYS:HD2	2.46	0.46
1:E:120:ILE:HG22	1:E:121:ILE:HG13	1.97	0.46
1:C:7:ILE:HG22	2:D:472:PHE:CB	2.28	0.46
1:C:22:THR:CG2	1:C:24:MET:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:LYS:NZ	7:E:533:HOH:O	2.19	0.46
2:F:465:LYS:NZ	7:F:613:HOH:O	2.28	0.46
1:C:206:THR:HG22	1:C:208:THR:N	2.17	0.46
1:E:5:ASP:CG	7:E:537:HOH:O	2.54	0.46
2:F:338:GLY:O	2:F:342:GLY:HA3	2.16	0.46
1:A:15:ASN:OD1	1:A:15:ASN:N	2.38	0.46
2:B:508:SER:OG	2:F:501:ARG:NH2	2.37	0.46
1:C:5:ASP:O	2:D:474:PHE:N	2.48	0.46
1:A:36:ILE:HG22	1:A:315:LEU:CB	2.46	0.46
1:C:120:ILE:HG22	1:C:121:ILE:HG13	1.97	0.46
2:B:338:GLY:O	2:B:342:GLY:HA3	2.16	0.46
2:D:504:ARG:O	2:D:508:SER:HB3	2.16	0.45
1:A:22:THR:HG22	1:A:25:GLU:H	1.80	0.45
1:E:206:THR:HG22	1:E:208:THR:N	2.20	0.45
1:A:200:THR:OG1	1:A:248:ASN:HB3	2.16	0.45
1:E:296:HIS:CD2	1:E:307:PRO:HG2	2.51	0.45
1:E:22:THR:CG2	1:E:24:MET:H	2.29	0.45
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.99	0.45
1:A:60:SER:OG	1:A:92:ASP:HA	2.16	0.45
1:E:36:ILE:HD11	2:F:390:ILE:CG1	2.47	0.45
2:F:507:ILE:HA	2:F:507:ILE:HD13	1.69	0.45
1:A:9:ILE:C	2:B:348:TRP:CH2	2.90	0.45
2:B:428:TYR:CD1	2:F:393:MET:HA	2.52	0.45
2:B:508:SER:CB	2:F:501:ARG:HH22	2.30	0.45
1:E:6:GLN:O	2:F:483:MET:HE2	2.17	0.45
1:E:7:ILE:O	2:F:472:PHE:N	2.45	0.45
1:A:206:THR:HG22	1:A:208:THR:N	2.23	0.45
1:A:159:SER:HB3	1:A:196:GLN:HE21	1.82	0.45
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.44
1:A:108:LEU:CD1	1:A:262:LYS:HD2	2.46	0.44
1:A:36:ILE:HD11	2:B:390:ILE:HD11	1.99	0.44
1:E:206:THR:HG22	1:E:209:LEU:H	1.82	0.44
1:E:183:HIS:HB2	1:E:252:ILE:HD11	1.99	0.44
1:A:207:SER:HA	1:C:221:SER:HB2	1.99	0.44
1:E:321:LEU:HB3	2:F:445:HIS:CG	2.53	0.44
1:C:216:ARG:NH1	7:C:716:HOH:O	2.49	0.44
1:A:107:HIS:HD1	2:B:403:GLU:CD	2.15	0.44
1:C:141:TYR:HA	7:C:766:HOH:O	2.17	0.44
2:F:393:MET:HE2	2:F:393:MET:HB2	1.88	0.44
1:E:186:ASN:OD1	1:E:186:ASN:N	2.50	0.43
1:A:23:ILE:HG22	1:A:24:MET:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:SER:HA	7:E:508:HOH:O	2.18	0.43
1:C:321:LEU:HB2	7:C:746:HOH:O	2.18	0.43
1:A:8:CYS:C	2:B:348:TRP:HH2	2.22	0.43
1:A:120:ILE:CG2	1:A:121:ILE:HG13	2.48	0.43
1:E:308:LYS:HD2	2:F:426:TRP:CE2	2.54	0.43
1:E:23:ILE:HD12	2:D:385:LYS:HG3	2.00	0.43
2:B:400:VAL:HA	2:B:401:GLY:HA3	1.85	0.43
1:A:144:LYS:HE2	1:A:144:LYS:HB3	1.87	0.43
1:C:317:LEU:HA	1:C:317:LEU:HD12	1.79	0.43
1:A:171:THR:HA	7:A:568:HOH:O	2.19	0.43
1:A:9:ILE:HA	2:B:357:GLY:O	2.19	0.43
1:A:206:THR:CG2	1:A:207:SER:N	2.82	0.43
1:E:11:TYR:CE2	2:F:340:ILE:HA	2.54	0.43
1:A:36:ILE:HG22	1:A:315:LEU:HB3	1.99	0.43
1:E:36:ILE:HG22	1:E:315:LEU:CB	2.49	0.43
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.99	0.43
1:E:120:ILE:CG2	1:E:121:ILE:HG13	2.49	0.43
1:A:280:THR:HG22	1:A:281:LYS:H	1.83	0.42
2:B:392:LYS:HD2	2:D:431:GLU:HB3	2.01	0.42
2:D:338:GLY:O	2:D:342:GLY:HA3	2.19	0.42
2:B:440:ARG:HG3	2:F:440:ARG:NH2	2.34	0.42
2:D:405:ASN:OD1	2:D:407:LEU:N	2.43	0.42
1:A:118:ILE:HG13	1:A:120:ILE:HD13	2.01	0.42
1:C:36:ILE:HG22	1:C:315:LEU:CB	2.50	0.42
1:A:97:GLY:HA3	1:A:230:MET:O	2.20	0.42
2:D:507:ILE:HA	2:D:507:ILE:HD13	1.87	0.42
1:C:141:TYR:CD2	1:C:142:GLN:HB2	2.54	0.42
1:E:22:THR:HG22	1:E:24:MET:N	2.31	0.42
1:A:294:PRO:HG2	1:A:295:PHE:CD1	2.55	0.42
1:C:9:ILE:HD13	2:D:453:TYR:HD1	1.85	0.42
2:F:360:HIS:HD2	2:F:487:ARG:HH21	1.66	0.42
1:A:82:TYR:CE1	1:A:269:MET:HE1	2.54	0.42
1:C:22:THR:HG22	1:C:24:MET:N	2.29	0.42
2:F:400:VAL:HA	2:F:401:GLY:HA3	1.80	0.42
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.54	0.42
1:E:36:ILE:HD11	2:F:390:ILE:HG13	2.02	0.42
1:C:304:GLY:HA2	2:D:397:PHE:CD1	2.54	0.41
1:C:58:ASP:OD1	1:C:90:VAL:HG23	2.20	0.41
2:D:337:PHE:HZ	2:F:336:LEU:HB3	1.85	0.41
1:E:11:TYR:HB2	1:E:321:LEU:HD11	2.03	0.41
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:CB	7:C:746:HOH:O	2.67	0.41
1:A:289:ILE:CG2	1:A:291:SER:HB3	2.50	0.41
1:A:11:TYR:HB2	1:A:321:LEU:HD11	2.03	0.41
1:C:310:VAL:CG1	1:C:312:SER:HB3	2.51	0.41
1:C:7:ILE:HA	1:C:7:ILE:HD13	1.93	0.41
1:A:22:THR:CG2	1:A:24:MET:H	2.33	0.41
2:F:508:SER:OG	2:F:508:SER:O	2.37	0.41
2:B:404:PHE:HA	2:D:410:ARG:NH1	2.35	0.41
1:E:97:GLY:HA3	1:E:230:MET:O	2.21	0.41
1:C:294:PRO:HG2	1:C:295:PHE:CD1	2.55	0.41
1:E:118:ILE:HG13	1:E:120:ILE:HD13	2.03	0.41
1:A:4:GLN:N	7:A:549:HOH:O	2.53	0.41
1:C:281:LYS:HB3	1:C:281:LYS:HE2	1.89	0.41
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.72	0.41
1:C:60:SER:OG	1:C:92:ASP:HA	2.20	0.41
1:A:22:THR:HG22	1:A:24:MET:N	2.34	0.41
2:B:337:PHE:CE2	2:F:337:PHE:CE2	3.09	0.40
1:C:118:ILE:HG13	1:C:120:ILE:HD13	2.02	0.40
1:A:310:VAL:CG1	1:A:312:SER:HB3	2.51	0.40
1:E:9:ILE:CD1	2:F:453:TYR:HA	2.47	0.40
1:E:60:SER:OG	1:E:92:ASP:HA	2.21	0.40
1:A:154:LEU:O	1:A:155:ILE:HD12	2.21	0.40
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.61	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLN:O	1:C:132:SER:OG[1_556]	2.10	0.10
1:C:58:ASP:OD2	1:E:73:GLU:OE1[1_655]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/322 (99%)	300 (94%)	18 (6%)	2 (1%)	30	43
1	C	320/322 (99%)	301 (94%)	18 (6%)	1 (0%)	46	63
1	E	320/322 (99%)	302 (94%)	16 (5%)	2 (1%)	30	43
2	B	173/175 (99%)	160 (92%)	9 (5%)	4 (2%)	8	8
2	D	173/175 (99%)	162 (94%)	9 (5%)	2 (1%)	16	23
2	F	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	30	43
All	All	1479/1491 (99%)	1389 (94%)	78 (5%)	12 (1%)	24	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	E	74	PHE
2	B	504	ARG
2	B	508	SER
2	D	505	GLU
1	C	74	PHE
1	A	5	ASP
1	E	76	ASN
2	B	505	GLU
2	D	504	ARG
2	F	401	GLY
2	B	401	GLY

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	290/290 (100%)	257 (89%)	33 (11%)	7	9
1	C	290/290 (100%)	254 (88%)	36 (12%)	6	7
1	E	290/290 (100%)	255 (88%)	35 (12%)	6	8
2	B	149/149 (100%)	137 (92%)	12 (8%)	15	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	149/149 (100%)	136 (91%)	13 (9%)	13	19
2	F	149/149 (100%)	137 (92%)	12 (8%)	15	22
All	All	1317/1317 (100%)	1176 (89%)	141 (11%)	8	11

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	15	ASN
1	A	16	SER
1	A	20	VAL
1	A	22	THR
1	A	23	ILE
1	A	30	VAL
1	A	31	THR
1	A	59	CYS
1	A	99	PHE
1	A	111	ARG
1	A	120	ILE
1	A	135	VAL
1	A	144	LYS
1	A	151	VAL
1	A	166	ARG
1	A	167	SER
1	A	186	ASN
1	A	187	ASP
1	A	196	GLN
1	A	197	ASN
1	A	200	THR
1	A	206	THR
1	A	208	THR
1	A	235	THR
1	A	260	ILE
1	A	265	ASP
1	A	280	THR
1	A	310	VAL
1	A	317	LEU
1	A	319	ILE
1	A	321	LEU
1	A	324	SER
1	C	7	ILE

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Mol	Chain	Res	Type
1	C	15	ASN
1	C	16	SER
1	C	20	VAL
1	C	22	THR
1	C	23	ILE
1	C	30	VAL
1	C	31	THR
1	C	39	LYS
1	C	59	CYS
1	C	73	GLU
1	C	99	PHE
1	C	111	ARG
1	C	120	ILE
1	C	135	VAL
1	C	151	VAL
1	C	155	ILE
1	C	166	ARG
1	C	167	SER
1	C	186	ASN
1	C	187	ASP
1	C	196	GLN
1	C	197	ASN
1	C	200	THR
1	C	206	THR
1	C	208	THR
1	C	212	ARG
1	C	235	THR
1	C	260	ILE
1	C	265	ASP
1	C	280	THR
1	C	310	VAL
1	C	317	LEU
1	C	319	ILE
1	C	321	LEU
1	C	324	SER
1	E	4	GLN
1	E	7	ILE
1	E	15	ASN
1	E	16	SER
1	E	20	VAL
1	E	22	THR
1	E	23	ILE

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Mol	Chain	Res	Type
1	E	30	VAL
1	E	31	THR
1	E	52	LYS
1	E	59	CYS
1	E	73	GLU
1	E	99	PHE
1	E	111	ARG
1	E	120	ILE
1	E	135	VAL
1	E	151	VAL
1	E	166	ARG
1	E	167	SER
1	E	186	ASN
1	E	187	ASP
1	E	196	GLN
1	E	197	ASN
1	E	200	THR
1	E	206	THR
1	E	208	THR
1	E	235	THR
1	E	260	ILE
1	E	265	ASP
1	E	280	THR
1	E	310	VAL
1	E	317	LEU
1	E	319	ILE
1	E	321	LEU
1	E	324	SER
2	B	349	GLN
2	B	352	VAL
2	B	373	GLU
2	B	384	ASN
2	B	400	VAL
2	B	439	GLU
2	B	440	ARG
2	B	450	LYS
2	B	457	ARG
2	B	477	LYS
2	B	478	CYS
2	B	498	GLU
2	D	349	GLN
2	D	352	VAL

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Mol	Chain	Res	Type
2	D	373	GLU
2	D	384	ASN
2	D	400	VAL
2	D	439	GLU
2	D	440	ARG
2	D	450	LYS
2	D	457	ARG
2	D	477	LYS
2	D	498	GLU
2	D	506	GLU
2	D	507	ILE
2	F	349	GLN
2	F	352	VAL
2	F	373	GLU
2	F	384	ASN
2	F	400	VAL
2	F	439	GLU
2	F	440	ARG
2	F	450	LYS
2	F	457	ARG
2	F	498	GLU
2	F	507	ILE
2	F	508	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	E	76	ASN
2	B	360	HIS
2	B	396	GLN
2	B	495	GLN
2	D	360	HIS
2	D	429	ASN
2	D	495	GLN
2	F	360	HIS
2	F	396	GLN
2	F	429	ASN
2	F	495	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 ⓘ

9 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	401	1,3	14,14,15	0.64	0	15,19,21	1.22	2 (13%)
3	NAG	A	402	3	14,14,15	0.66	0	15,19,21	1.28	2 (13%)
3	NAG	C	602	1,3	14,14,15	0.50	0	15,19,21	1.17	1 (6%)
3	NAG	C	603	3	14,14,15	0.54	0	15,19,21	1.03	0
6	SIA	C	604	6	16,20,21	3.69	7 (43%)	18,28,31	2.70	7 (38%)
6	GAL	C	605	6	11,11,12	1.04	1 (9%)	14,15,17	1.44	3 (21%)
6	NAG	C	606	6	15,15,15	0.40	0	17,21,21	1.61	2 (11%)
3	NAG	E	401	1,3	14,14,15	0.49	0	15,19,21	1.23	2 (13%)
3	NAG	E	402	3	14,14,15	0.56	0	15,19,21	1.57	2 (13%)

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	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	NAG	C	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	603	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SIA	C	604	6	-	0/14/34/38	0/1/1/1
6	GAL	C	605	6	-	0/2/19/22	0/1/1/1
6	NAG	C	606	6	-	0/6/26/26	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	604	SIA	C7-C6	-9.84	1.40	1.52
6	C	604	SIA	C3-C4	-7.86	1.40	1.52
6	C	604	SIA	C3-C2	-3.87	1.46	1.52
6	C	604	SIA	O8-C8	-2.47	1.37	1.43
6	C	605	GAL	O5-C1	-2.23	1.40	1.43
6	C	604	SIA	C11-C10	2.19	1.54	1.50
6	C	604	SIA	O6-C6	3.01	1.48	1.43
6	C	604	SIA	O4-C4	3.99	1.52	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	604	SIA	O6-C2-C3	-7.71	95.04	109.86
3	E	402	NAG	C2-N2-C7	-4.88	116.76	123.04
6	C	604	SIA	O6-C6-C5	-4.87	100.51	108.48
3	A	402	NAG	C2-N2-C7	-3.58	118.44	123.04
6	C	605	GAL	C1-O5-C5	-2.95	108.50	112.25
6	C	604	SIA	C5-N5-C10	-2.59	116.45	123.10
3	E	401	NAG	C2-N2-C7	-2.33	120.04	123.04
6	C	605	GAL	O5-C1-C2	-2.28	107.17	110.86
3	C	602	NAG	C1-O5-C5	-2.25	109.39	112.25
3	A	401	NAG	O4-C4-C3	-2.10	105.61	110.34
6	C	604	SIA	C11-C10-N5	2.17	120.25	116.11
6	C	604	SIA	C3-C4-C5	2.22	113.95	111.47
3	E	402	NAG	O5-C5-C6	2.23	112.17	107.35
3	A	402	NAG	C3-C4-C5	2.46	114.48	110.20
6	C	605	GAL	C1-C2-C3	2.49	112.49	109.54
3	E	401	NAG	C1-O5-C5	2.50	115.42	112.25
6	C	604	SIA	C7-C6-C5	2.66	118.34	114.32
3	A	401	NAG	C1-O5-C5	2.81	115.81	112.25
6	C	606	NAG	O5-C5-C4	3.47	116.19	109.68
6	C	604	SIA	O9-C9-C8	3.94	119.66	111.10
6	C	606	NAG	C1-O5-C5	4.39	121.59	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	604	SIA	1	0
6	C	605	GAL	1	0

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SIA	A	403	-	17,21,21	3.90	6 (35%)	19,31,31	1.88	5 (26%)
5	NAG	C	601	1	14,14,15	0.42	0	15,19,21	1.60	1 (6%)

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	SIA	A	403	-	-	0/14/38/38	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	SIA	C7-C6	-9.01	1.41	1.52
4	A	403	SIA	C3-C4	-8.55	1.39	1.53
4	A	403	SIA	C3-C2	-4.44	1.46	1.51
4	A	403	SIA	O4-C4	3.68	1.51	1.43
4	A	403	SIA	O6-C6	5.27	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	SIA	O6-C2	5.43	1.47	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	SIA	C6-C5-N5	-3.77	104.50	111.07
4	A	403	SIA	C8-C7-C6	-2.80	107.39	113.01
4	A	403	SIA	O7-C7-C6	2.02	114.09	109.43
4	A	403	SIA	O4-C4-C3	2.50	115.93	109.92
4	A	403	SIA	O6-C6-C7	4.51	114.09	107.26
5	C	601	NAG	C1-O5-C5	5.36	119.06	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	322/322 (100%)	0.30	12 (3%)	45	46	24, 48, 89, 162	0
1	C	322/322 (100%)	0.38	16 (4%)	32	33	26, 51, 96, 150	0
1	E	322/322 (100%)	0.52	22 (6%)	20	20	27, 54, 103, 167	0
2	B	175/175 (100%)	1.36	42 (24%)	1	1	34, 78, 126, 170	0
2	D	175/175 (100%)	1.57	52 (29%)	1	1	31, 92, 147, 183	0
2	F	175/175 (100%)	1.07	31 (17%)	2	2	32, 90, 143, 205	0
All	All	1491/1491 (100%)	0.73	175 (11%)	6	6	24, 58, 126, 205	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	PRO	9.7
2	D	509	GLY	8.9
1	E	141	TYR	7.4
2	D	507	ILE	7.2
1	C	141	TYR	6.8
2	B	501	ARG	6.3
2	D	508	SER	6.0
1	A	325	PRO	6.0
2	F	501	ARG	5.7
2	D	370	ALA	5.7
1	E	325	PRO	5.6
2	F	474	PHE	5.6
2	D	337	PHE	5.5
1	E	7	ILE	5.2
2	F	496	TYR	5.1
2	D	353	ASP	4.9
2	F	372	LYS	4.9
2	D	483	MET	4.8
2	D	493	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	507	ILE	4.6
2	B	336	LEU	4.4
1	C	144	LYS	4.3
1	A	15	ASN	4.2
2	F	502	LEU	4.2
2	D	363	GLU	4.1
1	E	5	ASP	4.1
1	E	74	PHE	4.1
2	F	352	VAL	4.1
2	B	481	GLU	4.0
2	B	352	VAL	3.9
2	F	504	ARG	3.9
2	D	481	GLU	3.9
1	A	7	ILE	3.9
2	F	494	PRO	3.8
2	B	337	PHE	3.8
2	D	502	LEU	3.8
2	B	502	LEU	3.7
2	F	360	HIS	3.7
2	D	475	TYR	3.7
2	D	494	PRO	3.6
2	B	366	SER	3.6
2	D	349	GLN	3.6
2	D	365	GLY	3.6
2	F	482	CYS	3.5
1	A	291	SER	3.5
1	A	290	ASN	3.5
2	D	336	LEU	3.5
2	F	507	ILE	3.5
2	F	493	TYR	3.4
1	A	72	ASP	3.4
2	D	504	ARG	3.4
2	B	351	MET	3.4
2	B	508	SER	3.4
2	D	482	CYS	3.4
2	B	433	LEU	3.3
2	D	348	TRP	3.3
1	E	90	VAL	3.3
1	C	324	SER	3.3
2	D	497	SER	3.3
2	D	369	ALA	3.3
1	C	9	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	481	GLU	3.2
1	E	70	MET	3.2
2	B	436	MET	3.2
2	D	496	TYR	3.2
2	B	440	ARG	3.1
2	F	495	GLN	3.1
1	C	7	ILE	3.1
2	D	460	LEU	3.1
2	D	486	VAL	3.1
1	A	324	SER	3.1
1	E	18	GLU	3.1
2	D	361	SER	3.1
1	C	5	ASP	3.0
2	D	489	GLY	3.0
1	E	217	ILE	3.0
2	D	490	THR	3.0
2	B	461	ARG	3.0
2	B	335	GLY	3.0
2	B	492	ASP	3.0
2	F	361	SER	3.0
2	D	478	CYS	2.9
1	A	323	ASN	2.9
1	C	33	ALA	2.9
2	D	372	LYS	2.9
2	B	494	PRO	2.9
2	F	376	GLN	2.9
2	F	343	PHE	2.8
1	C	15	ASN	2.8
1	E	16	SER	2.8
2	D	477	LYS	2.8
1	E	73	GLU	2.8
2	B	484	GLU	2.8
2	F	498	GLU	2.8
2	F	449	VAL	2.7
2	D	436	MET	2.7
2	D	352	VAL	2.7
1	C	17	THR	2.7
2	B	490	THR	2.7
2	D	484	GLU	2.7
2	B	432	LEU	2.7
1	A	218	ALA	2.7
2	B	503	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	19	GLN	2.6
1	E	14	ASN	2.6
1	E	324	SER	2.6
1	A	40	LYS	2.6
1	A	5	ASP	2.6
2	B	457	ARG	2.6
1	C	6	GLN	2.6
2	D	432	LEU	2.6
1	E	15	ASN	2.6
2	D	467	LEU	2.5
2	B	425	VAL	2.5
2	B	388	SER	2.5
2	D	367	GLY	2.5
2	F	440	ARG	2.5
2	F	506	GLU	2.5
1	C	29	THR	2.5
2	D	435	LEU	2.5
2	D	498	GLU	2.5
2	B	444	PHE	2.5
2	B	338	GLY	2.4
2	D	500	ALA	2.4
2	B	458	LEU	2.4
2	D	479	ASP	2.4
2	D	383	THR	2.4
2	B	348	TRP	2.4
2	D	379	ILE	2.4
2	B	447	SER	2.4
1	E	75	ILE	2.4
2	D	492	ASP	2.4
2	F	340	ILE	2.4
2	F	508	SER	2.4
2	D	335	GLY	2.4
2	F	457	ARG	2.4
2	F	509	GLY	2.3
2	F	500	ALA	2.3
2	B	345	GLU	2.3
2	B	441	THR	2.3
2	D	491	TYR	2.3
1	C	323	ASN	2.3
2	B	480	ASN	2.3
2	F	436	MET	2.2
1	E	218	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	26	LYS	2.2
2	B	449	VAL	2.2
1	E	76	ASN	2.2
2	D	476	HIS	2.2
2	F	379	ILE	2.2
2	B	448	ASN	2.2
2	B	426	TRP	2.2
2	F	491	TYR	2.2
1	A	12	HIS	2.1
1	E	144	LYS	2.1
2	D	433	LEU	2.1
2	B	495	GLN	2.1
2	B	500	ALA	2.1
1	C	291	SER	2.1
2	D	462	ASP	2.1
2	D	501	ARG	2.1
1	E	263	LYS	2.1
2	B	343	PHE	2.1
2	B	365	GLY	2.1
2	D	471	CYS	2.1
1	E	272	GLU	2.1
2	D	474	PHE	2.0
2	B	442	LEU	2.0
2	F	452	LEU	2.0
2	B	487	ARG	2.0
1	C	8	CYS	2.0
2	D	359	HIS	2.0
1	E	10	GLY	2.0
2	B	509	GLY	2.0
2	F	475	TYR	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	E	401	14/15	0.93	0.19	1.06	45,58,69,75	0
6	SIA	C	604	20/21	0.93	0.15	0.43	46,60,74,74	0
3	NAG	C	602	14/15	0.90	0.14	0.20	55,68,85,86	0
3	NAG	A	401	14/15	0.93	0.12	-0.35	37,50,65,67	0
6	NAG	C	606	15/15	0.76	0.28	-	119,129,140,147	0
3	NAG	A	402	14/15	0.86	0.28	-	65,79,88,93	0
3	NAG	C	603	14/15	0.84	0.32	-	86,97,111,112	0
6	GAL	C	605	11/12	0.91	0.11	-	81,96,111,112	0
3	NAG	E	402	14/15	0.91	0.32	-	85,107,117,122	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SIA	A	403	21/21	0.91	0.13	-0.22	51,57,68,69	0
5	NAG	C	601	14/15	0.83	0.22	-	98,114,123,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.