



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:23 AM UTC

PDB ID : 5NHU / pdb_00005nhu
Title : HUMAN ALPHA THROMBIN COMPLEXED WITH ANOPHELES GAM-BIAE cE5 ANTICOAGULANT
Authors : Ripoll-Rozada, J.; Pereira, P.J.B.
Deposited on : 2017-03-22
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

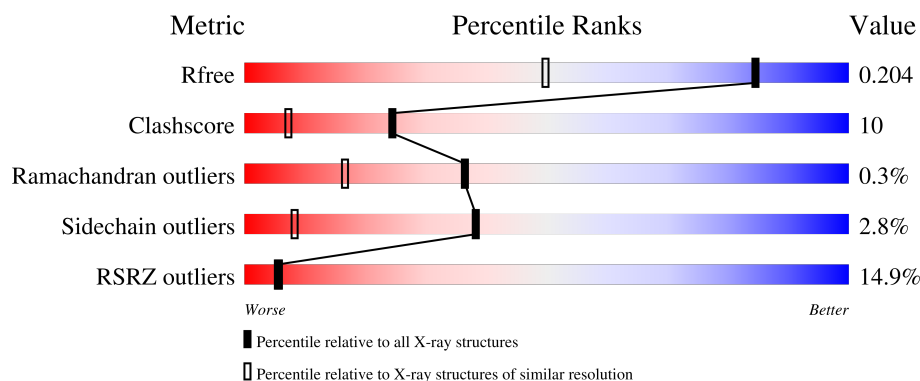
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	36	14% 86% 6% 8%
1	D	36	17% 64% 11% 6% 19%
1	L	36	17% 89% 11%
2	A	259	2% 88% 9% .
2	C	259	36% 53% 40% . .

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Mol	Chain	Length	Quality of chain
2	H	259	
3	I	82	
3	J	82	
3	K	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	601	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9088 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			
1	B	33	Total	C	N	O	S	0	0	0
			265	162	45	57	1			
1	D	29	Total	C	N	O	S	0	1	0
			241	150	39	50	2			

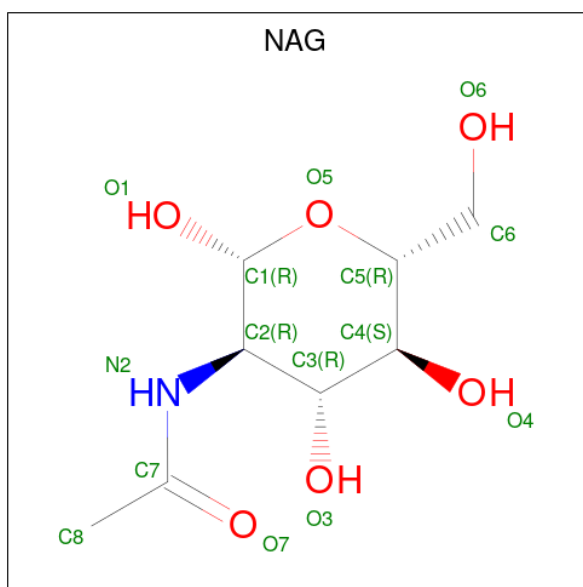
- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	7	0
			2095	1335	373	373	14			
2	A	251	Total	C	N	O	S	0	8	0
			2090	1331	369	376	14			
2	C	249	Total	C	N	O	S	0	99	0
			2828	1814	498	495	21			

- Molecule 3 is a protein called AGAP008004-PA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	24	Total	C	N	O	0	0	0
			189	118	34	37			
3	J	29	Total	C	N	O	0	0	0
			234	143	42	49			
3	K	10	Total	C	N	O	0	0	0
			84	52	17	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	50	Total	O	0	0
			50	50		
6	H	214	Total	O	0	0
			214	214		
6	B	38	Total	O	0	0
			38	38		

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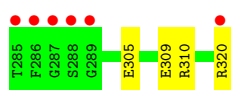
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	242	Total 242	O 242	0	0
6	D	23	Total 23	O 23	0	0
6	C	126	Total 128	O 128	0	6
6	I	12	Total 12	O 12	0	0
6	J	20	Total 20	O 20	0	0
6	K	3	Total 3	O 3	0	0

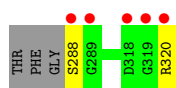
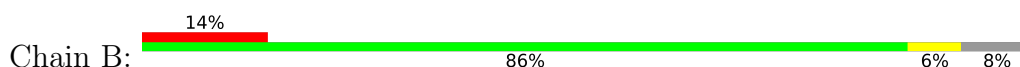
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

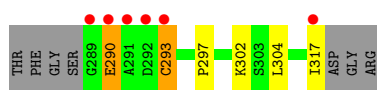
- Molecule 1: Prothrombin



- Molecule 1: Prothrombin



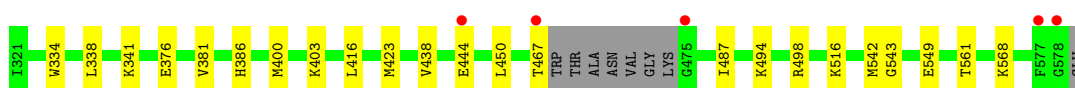
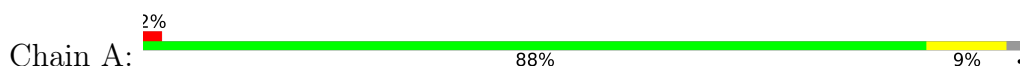
- Molecule 1: Prothrombin



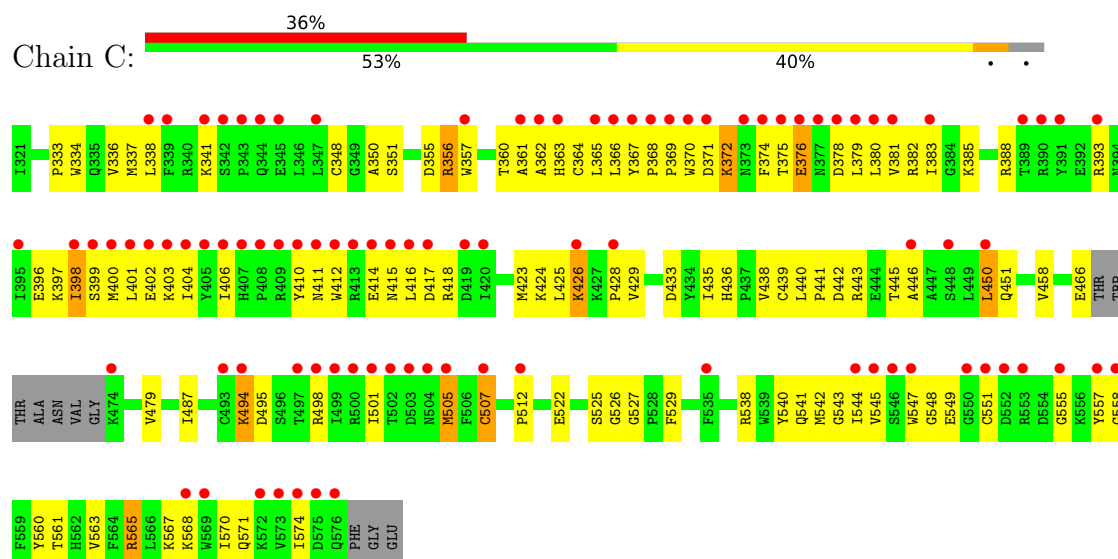
- Molecule 2: Prothrombin



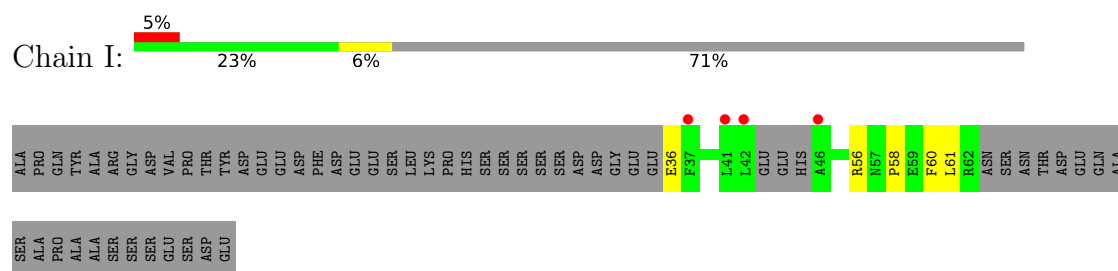
- Molecule 2: Prothrombin



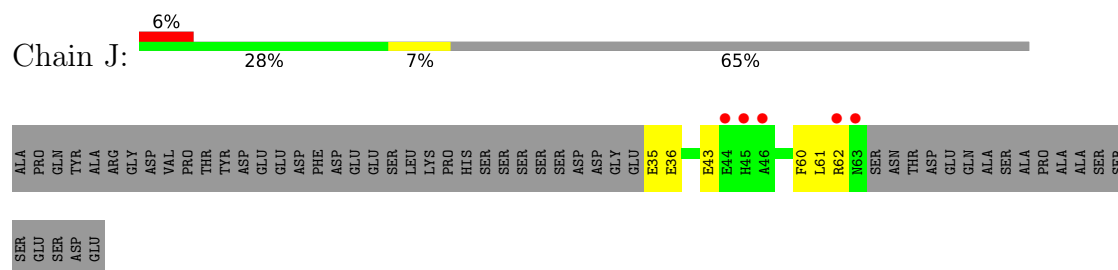
- Molecule 2: Prothrombin



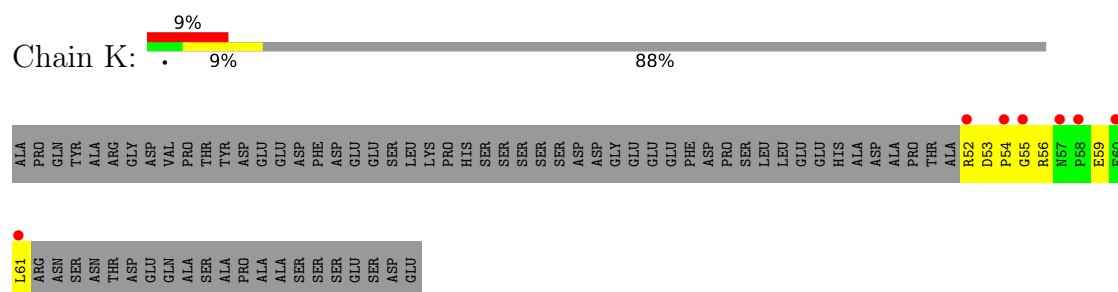
• Molecule 3: AGAP008004-PA



• Molecule 3: AGAP008004-PA



• Molecule 3: AGAP008004-PA



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.71Å 78.64Å 136.11Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	54.18 – 1.45 54.18 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.3 (54.18-1.45) 98.3 (54.18-1.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.179 , 0.203 0.180 , 0.204	Depositor DCC
R_{free} test set	9836 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9088	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.92	0/267	1.05	0/353
1	D	0.91	0/243	1.11	0/323
1	L	0.92	0/290	0.95	0/384
2	A	0.96	1/2142 (0.0%)	1.00	0/2893
2	C	0.53	0/2902	0.70	0/3920
2	H	0.89	1/2147 (0.0%)	0.98	0/2898
3	I	0.89	1/193 (0.5%)	0.92	0/261
3	J	0.78	0/240	0.93	0/326
3	K	0.52	0/86	0.74	0/115
All	All	0.80	3/8510 (0.0%)	0.90	0/11473

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
2	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	542	MET	SD-CE	-7.17	1.61	1.79
2	H	542	MET	SD-CE	-5.28	1.66	1.79
3	I	56	ARG	CZ-NH2	-5.18	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	557	TYR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	265	0	256	0	0
1	D	241	0	234	10	0
1	L	287	0	275	3	1
2	A	2090	0	2060	20	0
2	C	2828	0	2805	121	1
2	H	2095	0	2076	14	0
3	I	189	0	176	2	0
3	J	234	0	208	7	0
3	K	84	0	78	10	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	H	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	H	1	0	0	0	0
6	A	242	0	0	5	0
6	B	38	0	0	0	0
6	C	128	0	0	11	0
6	D	23	0	0	0	0
6	H	214	0	0	3	0
6	I	12	0	0	0	0
6	J	20	0	0	2	0
6	K	3	0	0	1	0
6	L	50	0	0	0	0
All	All	9088	0	8207	165	1

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 10.

All (165) 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)
2:C:360[B]:THR:HG21	2:C:423[B]:MET:HE3	1.33	1.07
2:C:401:LEU:HD22	2:C:423[B]:MET:HB3	1.51	0.92
2:C:334:TRP:O	2:C:351[B]:SER:HA	1.75	0.87
1:L:320:ARG:NH2	2:H:451[A]:GLN:OE1	2.10	0.85
2:C:370[B]:TRP:O	2:C:372[B]:LYS:N	2.14	0.80
2:C:381[B]:VAL:O	2:C:398:ILE:HA	1.86	0.76
2:C:341:LYS:HB3	2:C:378[B]:ASP:HA	1.68	0.74
2:C:527:GLY:O	2:C:545[B]:VAL:N	2.19	0.72
2:C:443[B]:ARG:NH1	6:C:701:HOH:O	2.16	0.72
2:C:567[B]:LYS:O	2:C:571[B]:GLN:HG2	1.90	0.71
2:C:450:LEU:HD23	2:C:487:ILE:HD13	1.72	0.71
2:C:383[B]:ILE:O	2:C:396:GLU:HA	1.92	0.70
2:C:336:VAL:HG22	2:C:383[A]:ILE:HG23	1.73	0.69
2:C:336:VAL:HB	2:C:350[B]:ALA:HB3	1.74	0.69
2:C:365[B]:LEU:HD11	2:C:423[B]:MET:HE2	1.75	0.67
2:C:501:ILE:HG23	2:C:505:MET:HE2	1.75	0.67
2:C:338:LEU:HD23	2:C:364[B]:CYS:HB3	1.76	0.67
2:C:441[B]:PRO:HA	2:C:540:TYR:CD1	2.29	0.67
2:C:365[B]:LEU:HD13	2:C:404:ILE:HG12	1.76	0.67
3:K:52:ARG:HG2	3:K:53:ASP:H	1.59	0.67
2:C:360[B]:THR:CG2	2:C:423[B]:MET:HE3	2.17	0.66
1:D:293[B]:CYS:C	2:C:439[B]:CYS:SG	2.79	0.65
2:C:376[A]:GLU:HA	2:C:404:ILE:HD12	1.80	0.63
2:C:334:TRP:CD2	2:C:438[B]:VAL:HB	2.33	0.63
2:C:547[B]:TRP:NE1	6:C:703:HOH:O	2.26	0.62
1:D:293[B]:CYS:HB2	2:C:439[B]:CYS:HA	1.80	0.62
2:C:336:VAL:N	2:C:350[B]:ALA:O	2.30	0.62
2:C:334:TRP:HB3	2:C:436[A]:HIS:O	2.00	0.62
2:C:451:GLN:HG3	6:C:722:HOH:O	1.99	0.62
2:A:338[B]:LEU:CD2	2:A:381:VAL:HG12	2.31	0.61
2:A:450[A]:LEU:HD12	2:A:487:ILE:HD13	1.82	0.61
2:C:543[B]:GLY:HA2	2:C:561[B]:THR:O	2.00	0.61
2:C:382[B]:ARG:HA	2:C:397:LYS:O	2.01	0.60
2:C:568[B]:LYS:HB3	6:C:774:HOH:O	2.00	0.60
2:H:338[B]:LEU:HD21	2:H:423:MET:HE1	1.84	0.58
2:C:403:LYS:HG3	2:C:404:ILE:H	1.68	0.58
2:C:401:LEU:C	2:C:426[A]:LYS:HG2	2.28	0.58
2:C:541:GLN:NE2	2:C:544[B]:ILE:HG12	2.19	0.57
2:C:361[B]:ALA:HB2	2:C:526:GLY:HA2	1.85	0.57
2:C:549[B]:GLU:HB2	3:K:61:LEU:HD11	1.87	0.57
2:C:336:VAL:O	2:C:350[B]:ALA:N	2.38	0.57
2:A:400:MET:HE3	6:A:702:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338[B]:LEU:HD21	2:A:423:MET:HE1	1.87	0.55
3:K:56:ARG:NH2	6:K:102:HOH:O	2.40	0.55
2:C:548[B]:GLY:O	3:K:55:GLY:O	2.25	0.55
1:D:302:LYS:HE2	1:D:304:LEU:HD12	1.89	0.54
2:C:567[B]:LYS:HE2	2:C:571[B]:GLN:OE1	2.06	0.54
2:C:341:LYS:N	2:C:378[B]:ASP:O	2.40	0.54
2:C:439[B]:CYS:SG	2:C:538:ARG:HD3	2.47	0.54
2:C:400:MET:HB2	2:C:426[A]:LYS:HG3	1.89	0.54
1:L:310:ARG:NH1	2:A:444:GLU:OE2	2.40	0.54
2:C:439[A]:CYS:HB2	2:C:540:TYR:CD1	2.42	0.54
2:C:360[B]:THR:HG21	2:C:423[B]:MET:CE	2.23	0.54
1:D:293[B]:CYS:HB2	2:C:439[B]:CYS:CA	2.38	0.54
2:C:365[B]:LEU:HD13	2:C:404:ILE:CG1	2.38	0.54
2:C:365[B]:LEU:HD21	2:C:423[B]:MET:CE	2.38	0.54
2:A:498:ARG:NH1	3:J:61:LEU:O	2.42	0.53
2:C:415:ASN:OD1	2:C:417:ASP:HB2	2.08	0.53
2:C:441[A]:PRO:HB2	2:C:446:ALA:HB2	1.90	0.53
2:A:549:GLU:HG2	3:J:61:LEU:HD11	1.89	0.53
2:C:336:VAL:HB	2:C:350[B]:ALA:CB	2.38	0.52
1:D:293[B]:CYS:CB	2:C:439[B]:CYS:HA	2.39	0.52
2:C:350[A]:ALA:HA	2:C:526:GLY:O	2.10	0.52
1:D:293[B]:CYS:HB2	2:C:438[B]:VAL:C	2.36	0.51
3:J:43:GLU:OE2	6:J:101:HOH:O	2.19	0.51
2:C:355[B]:ASP:OD2	2:C:428[B]:PRO:HB3	2.11	0.51
2:C:400:MET:N	6:C:708:HOH:O	2.44	0.51
2:C:441[A]:PRO:HD3	2:C:541:GLN:O	2.11	0.51
2:C:376[A]:GLU:H	2:C:376[A]:GLU:CD	2.18	0.51
2:A:516:LYS:HE3	6:A:851:HOH:O	2.09	0.51
2:C:338:LEU:CD2	2:C:364[B]:CYS:HB3	2.41	0.51
2:C:348[B]:CYS:HB2	2:C:525:SER:O	2.12	0.50
2:H:376:GLU:HG2	2:H:403:LYS:HA	1.91	0.50
2:C:442[A]:ASP:OD1	2:C:445:THR:HB	2.12	0.50
2:A:376[B]:GLU:HG2	2:A:403:LYS:HA	1.92	0.50
2:A:494:LYS:HD2	6:A:730:HOH:O	2.11	0.50
2:C:363[A]:HIS:HB3	2:C:416:LEU:HD21	1.93	0.50
2:H:498:ARG:HG2	6:H:829:HOH:O	2.12	0.49
2:C:526:GLY:N	2:C:545[B]:VAL:O	2.25	0.49
2:C:570[A]:ILE:O	2:C:574[A]:ILE:HG12	2.12	0.49
2:C:527:GLY:O	2:C:545[B]:VAL:HG23	2.12	0.49
2:C:365[B]:LEU:HD21	2:C:423[B]:MET:HE2	1.95	0.49
2:C:363[A]:HIS:HD2	3:K:54:PRO:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:440[B]:LEU:O	6:C:702:HOH:O	2.20	0.49
2:C:406:ILE:HD11	2:C:410:TYR:CD2	2.48	0.48
2:C:529:PHE:HB2	2:C:560[B]:TYR:CD1	2.48	0.48
2:A:450[A]:LEU:HD12	2:A:487:ILE:CD1	2.43	0.48
2:C:375[B]:THR:HA	2:C:404:ILE:HD12	1.96	0.48
2:C:396:GLU:O	2:C:397:LYS:HD2	2.13	0.48
2:C:399:SER:CB	2:C:425[B]:LEU:HD22	2.44	0.48
2:C:402:GLU:N	2:C:426[A]:LYS:HG2	2.29	0.48
2:C:507:CYS:HA	2:C:558[B]:GLY:O	2.14	0.47
2:C:522:GLU:HG3	3:K:53:ASP:HB3	1.96	0.47
2:A:450[B]:LEU:HD22	2:A:450[B]:LEU:HA	1.63	0.47
2:C:336:VAL:HB	2:C:350[B]:ALA:C	2.38	0.47
2:H:393[A]:ARG:O	2:H:394:ASN:HB2	2.14	0.47
2:C:406:ILE:HG23	6:C:783:HOH:O	2.15	0.47
2:C:333:PRO:O	2:C:435[A]:ILE:HA	2.14	0.47
2:C:334:TRP:CG	2:C:438[B]:VAL:HB	2.50	0.47
2:C:400:MET:HG2	6:C:710:HOH:O	2.15	0.47
2:C:544[B]:ILE:HG23	6:C:705:HOH:O	2.15	0.46
2:H:412:TRP:CZ3	2:H:413:ARG:HG2	2.50	0.46
2:C:367[B]:TYR:HD1	2:C:410:TYR:HH	1.61	0.46
2:C:388:ARG:HD3	6:C:770:HOH:O	2.13	0.46
2:H:416:LEU:HG	3:I:60:PHE:HE2	1.81	0.46
2:H:397:LYS:HG2	2:H:429:VAL:HG23	1.98	0.46
1:D:293[B]:CYS:O	2:C:439[B]:CYS:SG	2.74	0.46
2:C:362[A]:ALA:HB1	2:C:406:ILE:CD1	2.46	0.45
2:H:409:ARG:CG	2:H:409:ARG:HH21	2.29	0.45
2:C:466:GLU:HB2	2:C:551[B]:CYS:HB2	1.97	0.45
2:C:458:VAL:HG21	2:C:560[B]:TYR:OH	2.15	0.45
2:C:544[B]:ILE:HB	2:C:561[B]:THR:HB	1.98	0.45
3:I:58:PRO:HG2	3:I:61:LEU:HG	1.98	0.45
2:C:366[B]:LEU:HD11	2:C:406:ILE:HG21	1.99	0.44
2:C:369[A]:PRO:HB3	3:K:59:GLU:HG3	1.99	0.44
2:C:410:TYR:CZ	2:C:412:TRP:HB3	2.52	0.44
2:C:442[A]:ASP:O	2:C:446:ALA:CB	2.66	0.44
2:C:397:LYS:HG2	2:C:429[B]:VAL:HG23	2.00	0.44
2:C:401:LEU:CD1	2:C:423[B]:MET:SD	3.06	0.44
2:C:337[A]:MET:HE1	2:C:385[A]:LYS:HD3	2.00	0.44
2:A:338[B]:LEU:HD23	2:A:381:VAL:HG12	2.00	0.44
2:C:357[A]:TRP:CZ3	2:C:424[A]:LYS:HB2	2.53	0.44
2:C:368[A]:PRO:HG2	2:C:412:TRP:CE2	2.53	0.43
3:K:56:ARG:HA	3:K:56:ARG:HD3	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:565:ARG:NH1	6:H:706:HOH:O	2.40	0.43
2:C:365[B]:LEU:HD22	2:C:404:ILE:HD13	2.00	0.43
3:J:62:ARG:HD2	6:J:106:HOH:O	2.18	0.43
2:A:334:TRP:CG	2:A:438:VAL:HB	2.53	0.43
2:A:568:LYS:HD3	2:A:568:LYS:HA	1.81	0.43
2:H:409:ARG:HH21	2:H:409:ARG:HG2	1.84	0.43
2:A:386:HIS:HE1	6:A:926:HOH:O	2.01	0.43
2:C:512:PRO:HG3	2:C:555:GLY:N	2.33	0.43
2:A:543:GLY:HA2	2:A:561:THR:O	2.19	0.43
2:C:411:ASN:ND2	2:C:414:GLU:HB3	2.34	0.43
2:A:549:GLU:HG2	3:J:61:LEU:CD1	2.48	0.43
2:H:475:GLY:HA3	6:H:864:HOH:O	2.19	0.42
2:C:380[B]:LEU:HA	2:C:399:SER:O	2.19	0.42
3:J:35:GLU:HG3	3:J:36:GLU:N	2.34	0.42
2:C:356[A]:ARG:HE	2:C:428[A]:PRO:HB3	1.84	0.42
2:C:498:ARG:HH12	3:K:61:LEU:C	2.28	0.42
2:C:525:SER:HA	2:C:545[B]:VAL:HG12	2.02	0.42
2:H:356:ARG:NH1	2:H:424:LYS:HE2	2.35	0.42
2:C:541:GLN:HG2	2:C:563[B]:VAL:HG11	2.01	0.42
2:A:416:LEU:HG	3:J:60:PHE:HE2	1.85	0.42
1:D:293[B]:CYS:HB2	2:C:439[B]:CYS:N	2.35	0.42
1:D:297:PRO:HB2	2:C:433[B]:ASP:HA	2.02	0.41
2:C:547[B]:TRP:CD1	6:C:703:HOH:O	2.70	0.41
2:C:494:LYS:HD2	2:C:495:ASP:OD1	2.20	0.41
1:L:305:GLU:HG2	1:L:309:GLU:CD	2.46	0.41
2:C:401:LEU:HD13	2:C:423[B]:MET:SD	2.60	0.41
2:C:336:VAL:HG22	2:C:383[B]:ILE:CD1	2.50	0.41
2:C:374[B]:PHE:HB2	2:C:379[B]:LEU:HD11	2.03	0.41
2:C:404:ILE:HG12	2:C:423[A]:MET:HG2	2.02	0.41
2:C:545[B]:VAL:HG22	2:C:560[B]:TYR:CE1	2.56	0.41
2:C:355[A]:ASP:OD2	2:C:356[A]:ARG:HG2	2.21	0.41
2:C:549[B]:GLU:CB	3:K:61:LEU:HD11	2.51	0.41
2:C:446:ALA:HA	2:C:542[A]:MET:HE1	2.03	0.41
1:D:290:GLU:O	1:D:293[A]:CYS:HB2	2.21	0.40
2:C:376[A]:GLU:CA	2:C:404:ILE:HD12	2.50	0.40
2:C:363[B]:HIS:CE1	2:C:525:SER:HB3	2.57	0.40
2:C:376[A]:GLU:OE2	2:C:403:LYS:HD2	2.22	0.40
2:A:341:LYS:NZ	6:A:702:HOH:O	2.47	0.40
2:C:341:LYS:HB3	2:C:378[B]:ASP:CA	2.45	0.40
2:C:365[B]:LEU:HA	2:C:365[B]:LEU:HD23	1.73	0.40
2:H:395:ILE:HD12	2:H:434:TYR:CE2	2.57	0.40

All (1) 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:L:320:ARG:OXT	2:C:565[A]:ARG:NH2[4_544]	2.12	0.08

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	B	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
1	D	28/36 (78%)	27 (96%)	1 (4%)	0	100	100
1	L	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
2	A	255/259 (98%)	247 (97%)	8 (3%)	0	100	100
2	C	343/259 (132%)	321 (94%)	18 (5%)	4 (1%)	10	1
2	H	255/259 (98%)	247 (97%)	7 (3%)	1 (0%)	30	11
3	I	20/82 (24%)	20 (100%)	0	0	100	100
3	J	27/82 (33%)	25 (93%)	2 (7%)	0	100	100
3	K	8/82 (10%)	8 (100%)	0	0	100	100
All	All	1001/1131 (88%)	958 (96%)	38 (4%)	5 (0%)	36	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	371[A]	ASP
2	C	371[B]	ASP
2	C	418[A]	ARG
2	C	418[B]	ARG
2	H	394	ASN

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	B	29/31 (94%)	27 (93%)	2 (7%)	14	1
1	D	27/31 (87%)	23 (85%)	4 (15%)	3	0
1	L	31/31 (100%)	31 (100%)	0	100	100
2	A	227/225 (101%)	226 (100%)	1 (0%)	84	70
2	C	306/225 (136%)	289 (94%)	17 (6%)	19	1
2	H	227/225 (101%)	224 (99%)	3 (1%)	61	31
3	I	20/70 (29%)	19 (95%)	1 (5%)	22	2
3	J	25/70 (36%)	25 (100%)	0	100	100
3	K	9/70 (13%)	9 (100%)	0	100	100
All	All	901/978 (92%)	873 (97%)	28 (3%)	38	7

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	409	ARG
2	H	445	THR
2	H	467	THR
1	B	288	SER
1	B	320	ARG
2	A	467	THR
1	D	290	GLU
1	D	293[A]	CYS
1	D	293[B]	CYS
1	D	317	ILE
2	C	356[A]	ARG
2	C	356[B]	ARG
2	C	372[A]	LYS
2	C	372[B]	LYS
2	C	376[A]	GLU
2	C	376[B]	GLU
2	C	393	ARG
2	C	398	ILE

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Mol	Chain	Res	Type
2	C	426[A]	LYS
2	C	426[B]	LYS
2	C	450	LEU
2	C	479	VAL
2	C	494	LYS
2	C	505	MET
2	C	507	CYS
2	C	565[A]	ARG
2	C	565[B]	ARG
3	I	36	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	504	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
4	NAG	H	601	2	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
4	NAG	C	601	2	14,14,15	2.51	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	A	601	2	14,14,15	0.47	0	17,19,21	1.12	1 (5%)

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	H	601	2	-	0/6/23/26	0/1/1/1
4	NAG	C	601	2	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	A	601	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	NAG	O5-C1	-8.70	1.29	1.43
4	C	601	NAG	C1-C2	-3.38	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	4.01	117.56	112.19
4	H	601	NAG	C1-O5-C5	2.70	115.80	112.19
4	C	601	NAG	C3-C4-C5	2.68	115.10	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	601	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2
4	C	601	NAG	C4-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	B	33/36 (91%)	0.37	5 (15%) 5 5	16, 24, 63, 76	0
1	D	29/36 (80%)	0.63	6 (20%) 2 3	19, 29, 51, 60	1 (3%)
1	L	36/36 (100%)	0.38	6 (16%) 4 4	17, 27, 63, 75	0
2	A	251/259 (96%)	-0.25	5 (1%) 65 67	7, 20, 40, 56	8 (3%)
2	C	249/259 (96%)	1.70	94 (37%) 1 1	9, 29, 76, 90	99 (39%)
2	H	252/259 (97%)	-0.08	4 (1%) 70 73	8, 23, 43, 63	7 (2%)
3	I	24/82 (29%)	1.07	4 (16%) 4 4	19, 35, 66, 100	0
3	J	29/82 (35%)	0.95	5 (17%) 4 4	18, 32, 84, 94	0
3	K	10/82 (12%)	2.57	7 (70%) 0 0	63, 69, 75, 92	0
All	All	913/1131 (80%)	0.51	136 (14%) 5 6	7, 24, 67, 100	115 (12%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	406	ILE	8.3
2	C	404	ILE	7.6
2	C	410	TYR	7.3
2	C	412	TRP	6.8
3	I	46	ALA	6.6
2	C	405	TYR	6.1
2	H	467	THR	5.4
2	C	407	HIS	5.3
2	C	408	PRO	5.1
2	C	374[A]	PHE	5.1
2	C	569[A]	TRP	5.0
2	C	398	ILE	4.7
2	C	416	LEU	4.7
2	C	401	LEU	4.6
2	C	378[A]	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	501	ILE	4.5
2	C	499	ILE	4.5
2	C	369[A]	PRO	4.3
2	C	381[A]	VAL	4.3
2	C	535	PHE	4.2
2	C	389	THR	4.2
1	D	293[A]	CYS	4.2
2	C	366[A]	LEU	4.0
3	J	46	ALA	3.9
2	C	411	ASN	3.8
1	B	288	SER	3.7
2	C	399	SER	3.7
2	C	415	ASN	3.7
2	C	413	ARG	3.7
3	J	45	HIS	3.6
2	C	547[A]	TRP	3.6
2	C	390	ARG	3.6
1	L	285	THR	3.5
2	C	575[A]	ASP	3.5
3	K	61	LEU	3.5
3	K	60	PHE	3.5
2	A	467	THR	3.5
1	L	286	PHE	3.4
2	C	373[A]	ASN	3.4
1	B	320	ARG	3.4
2	C	379[A]	LEU	3.4
2	C	572[A]	LYS	3.3
3	K	52	ARG	3.3
2	H	578	GLY	3.3
2	C	450	LEU	3.2
2	C	375[A]	THR	3.2
2	C	370[A]	TRP	3.2
2	C	428[A]	PRO	3.2
2	C	341	LYS	3.2
2	C	383[A]	ILE	3.2
2	C	568[A]	LYS	3.1
2	C	357[A]	TRP	3.1
1	D	289	GLY	3.1
2	C	557	TYR	3.1
2	C	409	ARG	3.1
1	D	317	ILE	3.1
2	A	578	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	380[A]	LEU	3.0
2	C	417	ASP	3.0
3	J	63	ASN	3.0
2	C	368[A]	PRO	3.0
1	L	287	GLY	3.0
3	I	42	LEU	3.0
2	C	400	MET	3.0
2	C	546[A]	SER	3.0
2	A	577	PHE	3.0
2	C	339[A]	PHE	2.9
3	I	37	PHE	2.9
2	C	576[A]	GLN	2.9
2	C	426[A]	LYS	2.9
2	C	377[A]	ASN	2.9
2	C	497	THR	2.9
2	C	551[A]	CYS	2.9
1	D	290	GLU	2.8
2	C	544[A]	ILE	2.8
2	C	367[A]	TYR	2.8
1	L	289	GLY	2.8
2	C	362[A]	ALA	2.7
2	C	371[A]	ASP	2.7
2	C	502	THR	2.7
2	C	343	PRO	2.7
3	K	54	PRO	2.7
2	C	504	ASN	2.7
2	C	550[A]	GLY	2.6
3	J	44	GLU	2.6
2	C	414	GLU	2.6
2	C	574[A]	ILE	2.6
3	K	58	PRO	2.6
2	C	403	LYS	2.5
1	D	291	ALA	2.5
2	C	402	GLU	2.5
2	C	573[A]	VAL	2.5
2	C	446	ALA	2.5
1	B	289	GLY	2.4
3	K	55	GLY	2.4
2	C	338	LEU	2.4
1	D	292	ASP	2.4
2	C	493	CYS	2.4
2	C	494	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	391	TYR	2.4
2	C	365[A]	LEU	2.4
2	C	393	ARG	2.4
2	C	558[A]	GLY	2.4
2	C	419[A]	ASP	2.3
2	A	444	GLU	2.3
2	C	420[A]	ILE	2.3
2	C	500	ARG	2.3
2	C	342	SER	2.3
2	C	361[A]	ALA	2.2
3	K	57	ASN	2.2
2	C	498	ARG	2.2
2	A	475	GLY	2.2
3	I	41	LEU	2.2
2	C	512	PRO	2.2
2	C	505	MET	2.2
2	H	515	GLY	2.2
2	H	577	PHE	2.2
2	C	376[A]	GLU	2.2
2	C	555	GLY	2.1
2	C	345[A]	GLU	2.1
1	B	318	ASP	2.1
2	C	395	ILE	2.1
2	C	363[A]	HIS	2.1
2	C	553	ARG	2.1
2	C	347	LEU	2.1
2	C	474	LYS	2.1
2	C	507	CYS	2.1
1	L	320	ARG	2.1
1	L	288	SER	2.1
2	C	448	SER	2.1
2	C	552	ASP	2.1
2	C	503	ASP	2.0
1	B	319	GLY	2.0
3	J	62	ARG	2.0
2	C	344[A]	GLN	2.0
2	C	545[A]	VAL	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	601	14/15	0.66	0.31	43,63,71,72	14
4	NAG	H	601	14/15	0.77	0.14	45,56,62,64	0
4	NAG	A	601	14/15	0.83	0.13	35,48,58,61	0
5	NA	C	602	1/1	0.96	0.14	32,32,32,32	0
5	NA	A	602	1/1	0.99	0.03	17,17,17,17	0
5	NA	H	602	1/1	0.99	0.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.