



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 AM GMT

PDB ID : 3E7J
Title : HeparinaseII H202A/Y257A double mutant complexed with a heparan sulfate tetrasaccharide substrate
Authors : Shaya, D.; Cygler, M.
Deposited on : 2008-08-18
Resolution : 2.10 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

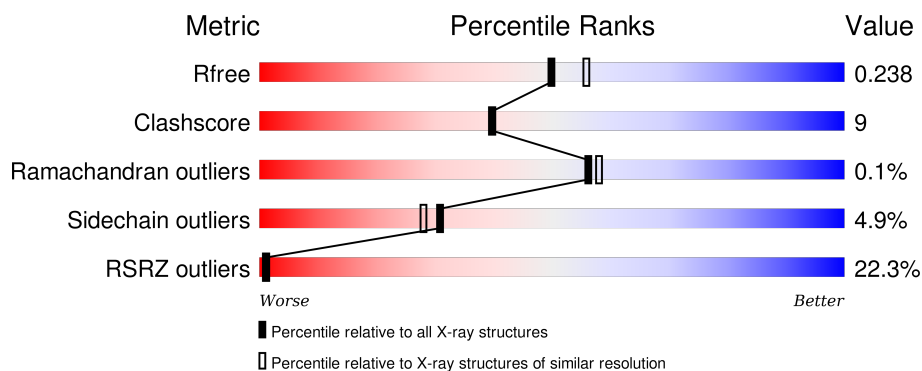
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	749	<div> <div>18%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	B	749	<div> <div>26%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>

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	GCU	A	775	X	-	-	-
4	NAG	A	776	X	-	-	-
4	GCU	B	775	X	-	-	X
4	NAG	B	776	X	-	-	-
4	GCD	B	777	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12784 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 Heparinase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5938	3823	1001	1091	23			
1	B	743	Total	C	N	O	S	0	0	0
			5938	3823	1001	1091	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	HIS	ENGINEERED	UNP Q46080
A	257	ALA	TYR	ENGINEERED	UNP Q46080
A	758	ALA	PRO	SEE REMARK 999	UNP Q46080
B	202	ALA	HIS	ENGINEERED	UNP Q46080
B	257	ALA	TYR	ENGINEERED	UNP Q46080
B	758	ALA	PRO	SEE REMARK 999	UNP Q46080

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			52	28	2	22		
4	B	4	Total	C	N	O	0	0
			52	28	2	22		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	480	Total	O	0	0
			480	480		
5	B	302	Total	O	0	0
			302	302		

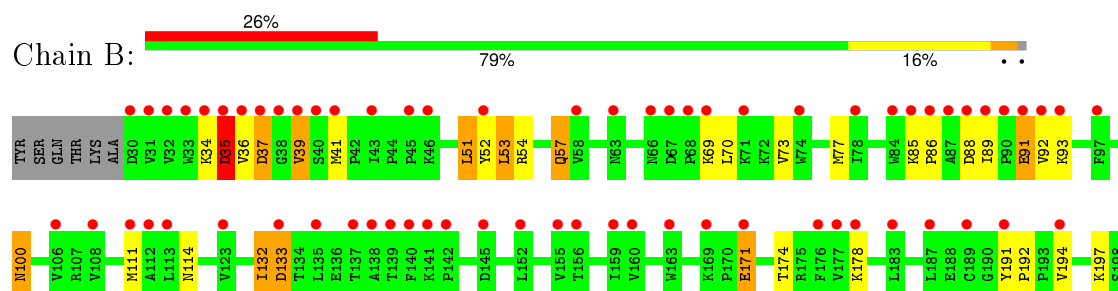
3 Residue-property plots

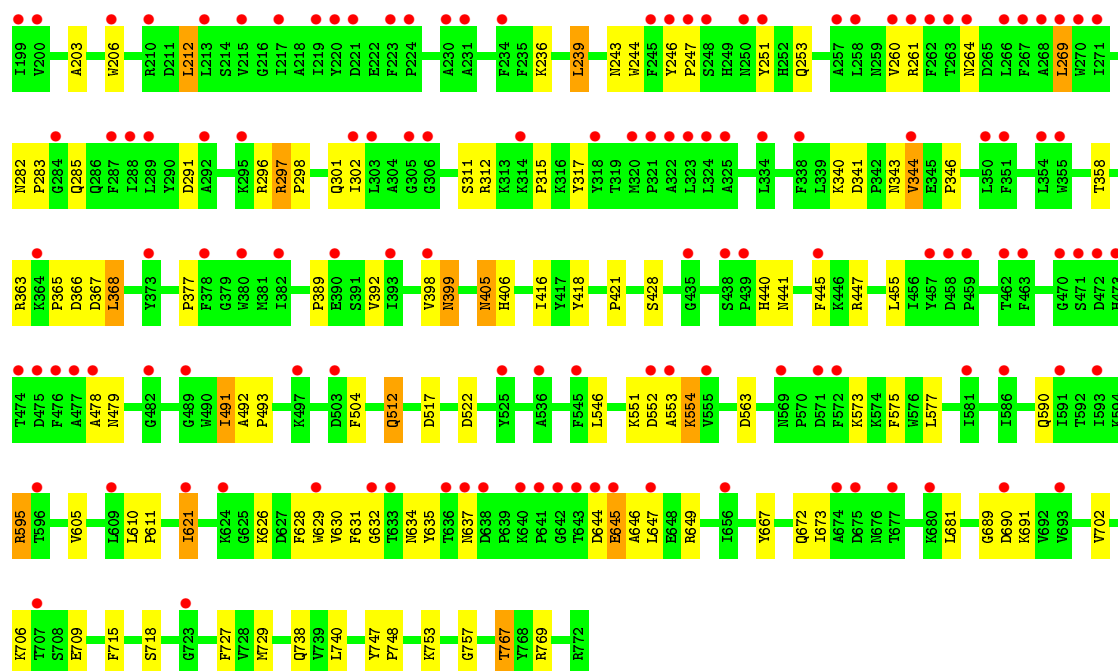
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: Heparinase II protein



• Molecule 1: Heparinase II protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.95Å 162.21Å 93.84Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	42.52 – 2.10 42.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	82.9 (42.52-2.10) 82.9 (42.53-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.199 , 0.234 0.207 , 0.238	Depositor DCC
R_{free} test set	3630 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.5	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71944 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12784	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, GCU, GCD, ACT

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	0.34	1/6098 (0.0%)	0.55	6/8253 (0.1%)
1	B	0.35	2/6098 (0.0%)	0.57	8/8253 (0.1%)
All	All	0.34	3/12196 (0.0%)	0.56	14/16506 (0.1%)

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
4	A	2	0
4	B	3	0
All	All	5	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	344	VAL	CB-CG2	-7.57	1.36	1.52
1	A	344	VAL	CB-CG2	-7.40	1.37	1.52
1	B	344	VAL	CB-CG1	-7.18	1.37	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ASP	CB-CG-OD2	13.62	130.56	118.30
1	A	133	ASP	CB-CG-OD1	-12.07	107.43	118.30
1	A	133	ASP	CB-CG-OD2	11.43	128.59	118.30
1	A	35	ASP	CB-CG-OD2	10.50	127.75	118.30
1	B	133	ASP	CB-CG-OD1	-10.44	108.91	118.30
1	B	35	ASP	CB-CG-OD2	9.79	127.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	B	344	VAL	CG1-CB-CG2	-9.13	96.29	110.90
1	B	517	ASP	CB-CG-OD2	9.07	126.46	118.30
1	A	35	ASP	CB-CG-OD1	-8.56	110.60	118.30
1	A	517	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	552	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	552	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	91	GLU	CA-CB-CG	5.12	124.66	113.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	775	GCU	C1
4	A	776	NAG	C1
4	B	775	GCU	C1
4	B	776	NAG	C1
4	B	777	GCD	C1

There are no planarity outliers.

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	5938	0	5853	103	0
1	B	5938	0	5853	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	12	1	0
3	B	4	0	3	0	0
4	A	52	0	37	1	0
4	B	52	0	37	0	0
5	A	480	0	0	5	0
5	B	302	0	0	2	0
All	All	12784	0	11795	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 9.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:PHE:H	1:A:634:ASN:HD21	1.05	1.02
1:A:769:ARG:HG2	1:A:769:ARG:HH21	1.23	1.01
1:A:769:ARG:CG	1:A:769:ARG:HH21	1.76	0.98
1:B:522:ASP:OD1	1:B:551:LYS:NZ	2.00	0.95
1:B:628:PHE:H	1:B:634:ASN:HD21	1.06	0.94
1:A:53:LEU:HB2	1:A:57:GLN:HG3	1.46	0.93
1:B:253:GLN:HE22	1:B:405:ASN:HB3	1.34	0.92
1:A:253:GLN:HE22	1:A:405:ASN:HB3	1.34	0.90
1:A:590:GLN:NE2	1:A:607:THR:OG1	2.06	0.88
1:B:261:ARG:HH11	1:B:261:ARG:HG3	1.42	0.83
1:B:398:VAL:O	1:B:399:ASN:HB2	1.79	0.81
1:A:269:LEU:HD23	1:A:285:GLN:HE22	1.46	0.80
1:A:171:GLU:CD	1:A:171:GLU:H	1.86	0.78
1:B:690:ASP:O	1:B:715:PHE:HB2	1.82	0.78
1:B:297:ARG:HB3	1:B:298:PRO:HD2	1.66	0.76
1:A:269:LEU:CD2	1:A:285:GLN:HE22	1.99	0.76
1:A:628:PHE:H	1:A:634:ASN:ND2	1.84	0.75
1:B:628:PHE:H	1:B:634:ASN:ND2	1.84	0.74
1:B:53:LEU:HB2	1:B:57:GLN:HG3	1.68	0.74
1:B:191:TYR:HA	1:B:192:PRO:C	2.08	0.74
1:A:261:ARG:HH11	1:A:261:ARG:HG3	1.52	0.73
1:B:546:LEU:HD22	1:B:702:VAL:HG21	1.70	0.73
1:B:92:VAL:HG13	1:B:92:VAL:O	1.89	0.72
1:A:455:LEU:HD11	1:A:577:LEU:HD11	1.72	0.72
1:B:171:GLU:H	1:B:171:GLU:CD	1.94	0.71
1:A:297:ARG:HB3	1:A:298:PRO:HD2	1.73	0.70
1:A:398:VAL:O	1:A:399:ASN:HB2	1.90	0.70
1:B:86:PRO:HA	1:B:89:ILE:HD12	1.75	0.69
1:A:416:ILE:HG21	1:A:673:ILE:HD12	1.77	0.67
1:A:111:MET:HE2	1:A:126:GLU:HG2	1.77	0.67
1:B:573:LYS:HD3	1:B:575:PHE:CZ	2.30	0.67
1:B:455:LEU:HD11	1:B:577:LEU:HD11	1.76	0.67
1:B:92:VAL:CG1	1:B:92:VAL:O	2.42	0.66
1:A:621:ILE:HD13	1:A:621:ILE:N	2.10	0.66
1:A:628:PHE:N	1:A:634:ASN:HD21	1.87	0.66
1:A:573:LYS:HD3	1:A:575:PHE:CZ	2.31	0.66
1:A:92:VAL:O	1:A:92:VAL:HG13	1.96	0.66
1:B:644:ASP:OD2	1:B:649:ARG:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ASP:OD2	1:A:649:ARG:HD2	1.96	0.65
1:B:269:LEU:HG	1:B:285:GLN:HE22	1.61	0.65
1:B:301:GLN:NE2	1:B:311:SER:O	2.29	0.64
1:A:301:GLN:NE2	1:A:311:SER:O	2.30	0.64
1:A:769:ARG:NH2	1:A:769:ARG:HG2	2.05	0.63
1:B:51:LEU:HD13	1:B:52:TYR:CE1	2.33	0.63
1:A:345:GLU:OE1	5:A:1211:HOH:O	2.16	0.63
1:A:590:GLN:HE21	1:A:607:THR:HG23	1.65	0.62
1:A:610:LEU:HA	1:A:611:PRO:C	2.19	0.61
1:B:261:ARG:NH1	1:B:261:ARG:HG3	2.15	0.61
1:B:365:PRO:HA	1:B:368:LEU:HD12	1.83	0.60
1:A:86:PRO:HA	1:A:89:ILE:HD12	1.84	0.59
1:B:629:TRP:CH2	1:B:632:GLY:O	2.54	0.59
1:A:416:ILE:HG21	1:A:673:ILE:CD1	2.32	0.59
1:A:35:ASP:HB2	5:A:1234:HOH:O	2.03	0.59
1:A:769:ARG:CG	1:A:769:ARG:NH2	2.46	0.59
1:B:610:LEU:HA	1:B:611:PRO:C	2.23	0.58
1:A:365:PRO:HA	1:A:368:LEU:HD12	1.87	0.57
1:A:253:GLN:HE22	1:A:406:HIS:H	1.52	0.57
1:A:92:VAL:O	1:A:92:VAL:CG1	2.52	0.57
1:B:73:VAL:O	1:B:77:MET:HG3	2.05	0.57
1:B:53:LEU:CB	1:B:57:GLN:HG3	2.34	0.57
1:A:590:GLN:NE2	1:A:607:THR:HG23	2.21	0.56
1:A:563:ASP:HB2	1:A:667:TYR:HB2	1.86	0.56
1:B:253:GLN:HE21	1:B:261:ARG:HH12	1.54	0.55
1:A:546:LEU:HD22	1:A:702:VAL:HG21	1.88	0.55
1:A:741:LYS:HA	1:A:767:THR:O	2.07	0.55
1:B:628:PHE:N	1:B:634:ASN:HD21	1.89	0.55
1:A:620:SER:C	1:A:621:ILE:HD13	2.27	0.55
1:A:73:VAL:O	1:A:77:MET:HG3	2.07	0.55
1:B:296:ARG:HE	1:B:302:ILE:HD13	1.72	0.55
1:B:621:ILE:N	1:B:621:ILE:CD1	2.70	0.54
1:B:563:ASP:HB2	1:B:667:TYR:HB2	1.87	0.54
3:A:5:ACT:H3	4:A:775:GCU:H3	1.90	0.54
1:B:260:VAL:HG13	1:B:261:ARG:N	2.23	0.54
1:B:253:GLN:HE22	1:B:406:HIS:H	1.55	0.54
1:A:428:SER:H	1:A:440:HIS:HE1	1.55	0.53
1:A:253:GLN:NE2	1:A:405:ASN:HB3	2.15	0.53
1:A:191:TYR:HA	1:A:192:PRO:C	2.29	0.53
1:B:689:GLY:O	1:B:706:LYS:NZ	2.41	0.53
1:B:260:VAL:CG1	1:B:261:ARG:N	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TRP:CZ3	1:A:377:PRO:HG3	2.44	0.53
1:B:398:VAL:O	1:B:399:ASN:CB	2.54	0.53
1:B:312:ARG:NH1	1:B:646:ALA:HB2	2.23	0.53
1:A:359:GLN:HG3	5:A:1237:HOH:O	2.09	0.52
1:B:312:ARG:HH11	1:B:312:ARG:HG3	1.74	0.52
1:B:672:GLN:OE1	1:B:681:LEU:HB3	2.09	0.52
1:A:261:ARG:NH1	1:A:261:ARG:HG3	2.21	0.52
1:B:769:ARG:HH11	1:B:769:ARG:HG2	1.73	0.52
1:B:34:LYS:NZ	5:B:1311:HOH:O	2.41	0.52
1:A:111:MET:HE2	1:A:126:GLU:CG	2.39	0.52
1:B:296:ARG:HE	1:B:302:ILE:CD1	2.23	0.52
1:A:111:MET:CE	1:A:126:GLU:CD	2.78	0.51
1:B:70:LEU:HG	1:B:358:THR:HG21	1.92	0.51
1:A:246:TYR:N	1:A:247:PRO:CD	2.73	0.51
1:B:428:SER:H	1:B:440:HIS:HE1	1.57	0.51
1:A:39:VAL:HG13	1:A:41:MET:HE3	1.93	0.51
1:B:269:LEU:HG	1:B:285:GLN:NE2	2.26	0.51
1:B:244:TRP:CZ3	1:B:377:PRO:HG3	2.45	0.51
1:B:246:TYR:N	1:B:247:PRO:CD	2.72	0.51
1:A:171:GLU:N	1:A:171:GLU:OE1	2.41	0.51
1:A:35:ASP:HA	1:A:39:VAL:O	2.10	0.51
1:B:416:ILE:HG21	1:B:673:ILE:HD12	1.94	0.50
1:A:760:TYR:HE1	5:A:1212:HOH:O	1.95	0.50
1:A:728:VAL:HG22	1:A:760:TYR:HD1	1.76	0.50
1:B:341:ASP:OD1	1:B:343:ASN:ND2	2.43	0.50
1:B:491:ILE:HD12	1:B:492:ALA:H	1.76	0.50
1:A:590:GLN:NE2	1:A:607:THR:CB	2.75	0.49
1:A:373:TYR:CD2	1:A:512:GLN:NE2	2.80	0.49
1:B:37:ASP:HB3	1:B:236:LYS:NZ	2.28	0.49
1:A:253:GLN:NE2	1:A:406:HIS:H	2.10	0.49
1:A:70:LEU:HG	1:A:358:THR:HG21	1.94	0.49
1:A:171:GLU:CD	1:A:171:GLU:N	2.61	0.48
1:A:605:VAL:HG21	1:A:681:LEU:HD11	1.94	0.48
1:A:421:PRO:HD2	1:A:595:ARG:HD2	1.95	0.48
1:B:645:GLU:H	1:B:645:GLU:CD	2.17	0.48
1:B:191:TYR:CA	1:B:192:PRO:C	2.81	0.48
1:A:690:ASP:O	1:A:715:PHE:HB2	2.13	0.48
1:A:714:PRO:HA	1:A:770:PHE:O	2.13	0.48
1:B:718:SER:OG	1:B:767:THR:HG22	2.14	0.48
1:A:440:HIS:HD2	1:A:635:TYR:O	1.97	0.47
1:A:590:GLN:NE2	1:A:607:THR:CG2	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PRO:HB2	1:B:317:TYR:CZ	2.49	0.47
1:A:344:VAL:HG12	1:A:349:LYS:HD3	1.96	0.47
1:B:174:THR:O	1:B:178:LYS:HG3	2.15	0.47
1:B:296:ARG:HH12	1:B:340:LYS:HE2	1.79	0.47
1:B:440:HIS:HD2	1:B:635:TYR:O	1.97	0.47
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.40	0.47
1:B:421:PRO:HD2	1:B:595:ARG:HD2	1.96	0.47
1:A:398:VAL:O	1:A:399:ASN:CB	2.60	0.46
1:A:253:GLN:HE21	1:A:261:ARG:HH12	1.61	0.46
1:A:455:LEU:CD1	1:A:577:LEU:HD11	2.45	0.46
1:A:260:VAL:HG13	1:A:261:ARG:N	2.30	0.46
1:B:253:GLN:NE2	1:B:406:HIS:H	2.14	0.46
1:B:171:GLU:N	1:B:171:GLU:CD	2.67	0.46
1:A:296:ARG:HE	1:A:302:ILE:CD1	2.29	0.46
1:A:260:VAL:CG1	1:A:261:ARG:N	2.79	0.45
1:B:192:PRO:HB2	1:B:194:VAL:HG13	1.97	0.45
1:A:39:VAL:HG11	1:A:236:LYS:HD2	1.98	0.45
1:B:206:TRP:HA	1:B:264:ASN:OD1	2.16	0.45
1:B:621:ILE:HG22	1:B:626:LYS:HB3	1.97	0.45
1:A:690:ASP:O	1:A:691:LYS:HB2	2.16	0.45
1:A:493:PRO:HD3	1:A:504:PHE:CE2	2.52	0.45
1:B:296:ARG:NH1	1:B:340:LYS:HE2	2.32	0.45
1:A:680:LYS:HD3	1:A:681:LEU:O	2.17	0.45
1:B:605:VAL:HG21	1:B:681:LEU:HD11	1.99	0.45
1:B:553:ALA:O	1:B:554:LYS:C	2.52	0.45
1:B:54:ARG:O	1:B:57:GLN:HG2	2.16	0.45
1:B:738:GLN:HE21	1:B:740:LEU:HD11	1.82	0.45
1:A:312:ARG:NH1	1:A:646:ALA:HB2	2.31	0.45
1:B:690:ASP:O	1:B:691:LYS:HB2	2.17	0.44
1:B:239:LEU:HD22	1:B:243:ASN:ND2	2.32	0.44
1:A:54:ARG:O	1:A:57:GLN:HG2	2.16	0.44
1:B:36:VAL:O	1:B:37:ASP:HB2	2.17	0.44
1:A:769:ARG:HA	1:A:769:ARG:HD2	1.81	0.44
1:A:769:ARG:HG3	1:A:769:ARG:HH21	1.74	0.44
1:B:253:GLN:NE2	1:B:405:ASN:HB3	2.16	0.44
1:A:111:MET:CE	1:A:126:GLU:OE1	2.66	0.44
1:A:96:ARG:HD2	5:A:1209:HOH:O	2.18	0.44
1:B:197:LYS:O	1:B:203:ALA:HB3	2.17	0.44
1:A:647:LEU:HD12	1:A:649:ARG:HD3	2.00	0.43
1:A:296:ARG:HE	1:A:302:ILE:HD13	1.83	0.43
1:A:206:TRP:HA	1:A:264:ASN:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.90	0.43
1:B:416:ILE:HG21	1:B:673:ILE:CD1	2.48	0.43
1:B:455:LEU:HB2	1:B:575:PHE:HB2	2.00	0.43
1:B:35:ASP:HA	1:B:39:VAL:O	2.18	0.43
1:A:111:MET:CE	1:A:126:GLU:CG	2.97	0.43
1:B:100:ASN:HD22	1:B:346:PRO:HG2	1.83	0.43
1:B:512:GLN:OE1	1:B:512:GLN:C	2.57	0.43
1:B:37:ASP:HB3	1:B:236:LYS:HZ1	1.84	0.43
1:A:197:LYS:O	1:A:203:ALA:HB3	2.18	0.43
1:A:296:ARG:NH1	1:A:340:LYS:HE2	2.33	0.43
1:B:621:ILE:N	1:B:621:ILE:HD12	2.33	0.43
1:A:479:ASN:C	1:A:479:ASN:HD22	2.21	0.43
1:B:647:LEU:HD12	1:B:649:ARG:HD3	1.99	0.42
1:A:52:TYR:O	1:A:53:LEU:HB3	2.19	0.42
1:A:192:PRO:HB3	1:A:229:LEU:HD13	2.01	0.42
1:B:769:ARG:NH1	1:B:769:ARG:HG2	2.34	0.42
1:A:363:ARG:NH1	1:A:367:ASP:OD2	2.52	0.42
1:B:447:ARG:NH2	1:B:478:ALA:O	2.45	0.42
1:B:493:PRO:HD3	1:B:504:PHE:CE2	2.55	0.42
1:B:392:VAL:HG22	1:B:418:TYR:CD1	2.54	0.42
1:A:100:ASN:HA	1:A:346:PRO:HG2	2.01	0.42
1:A:174:THR:O	1:A:178:LYS:HG3	2.19	0.42
1:B:132:ILE:O	1:B:132:ILE:HD13	2.19	0.42
1:A:769:ARG:NH2	1:A:769:ARG:HG3	2.32	0.42
1:B:298:PRO:CB	1:B:389:PRO:HA	2.50	0.42
1:A:392:VAL:HG22	1:A:418:TYR:CD1	2.55	0.42
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.46	0.42
1:B:85:LYS:O	1:B:88:ASP:N	2.45	0.42
1:A:455:LEU:HB2	1:A:575:PHE:HB2	2.02	0.41
1:A:739:VAL:HG22	1:A:770:PHE:CD2	2.55	0.41
1:A:312:ARG:HG3	1:A:312:ARG:HH11	1.86	0.41
1:B:440:HIS:CD2	1:B:637:ASN:HB2	2.55	0.41
1:A:315:PRO:HB2	1:A:317:TYR:CZ	2.55	0.41
1:A:41:MET:HB3	1:A:41:MET:HE3	1.52	0.41
1:A:605:VAL:HG21	1:A:681:LEU:CD1	2.51	0.41
1:B:753:LYS:O	1:B:757:GLY:N	2.52	0.41
1:B:291:ASP:HB3	5:B:1352:HOH:O	2.21	0.41
1:B:57:GLN:HB3	1:B:57:GLN:HE21	1.65	0.41
1:A:441:ASN:HA	1:A:445:PHE:HB3	2.03	0.41
1:B:630:VAL:O	1:B:631:PHE:C	2.60	0.41
1:B:747:TYR:HA	1:B:748:PRO:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:CD1	1:B:577:LEU:HD11	2.48	0.40
1:B:709:GLU:HA	1:B:709:GLU:OE1	2.20	0.40
1:B:441:ASN:HA	1:B:445:PHE:HB3	2.03	0.40
1:B:39:VAL:HG13	1:B:41:MET:HG2	2.03	0.40
1:B:282:ASN:HA	1:B:283:PRO:HD3	1.94	0.40
1:B:53:LEU:HB2	1:B:57:GLN:CG	2.45	0.40
1:B:727:PHE:HB3	1:B:729:MET:HE3	2.03	0.40
1:B:363:ARG:NH1	1:B:367:ASP:OD2	2.53	0.40

There are no symmetry-related clashes.

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	741/749 (99%)	710 (96%)	30 (4%)	1 (0%)	56	58
1	B	741/749 (99%)	707 (95%)	33 (4%)	1 (0%)	56	58
All	All	1482/1498 (99%)	1417 (96%)	63 (4%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	ASN
1	A	399	ASN

5.3.2 Protein sidechains [i](#)

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	628/633 (99%)	599 (95%)	29 (5%)	33	31
1	B	628/633 (99%)	595 (95%)	33 (5%)	28	25
All	All	1256/1266 (99%)	1194 (95%)	62 (5%)	31	28

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	53	LEU
1	A	57	GLN
1	A	69	LYS
1	A	91	GLU
1	A	93	LYS
1	A	100	ASN
1	A	111	MET
1	A	114	ASN
1	A	132	ILE
1	A	133	ASP
1	A	171	GLU
1	A	212	LEU
1	A	236	LYS
1	A	239	LEU
1	A	251	TYR
1	A	297	ARG
1	A	344	VAL
1	A	368	LEU
1	A	405	ASN
1	A	479	ASN
1	A	491	ILE
1	A	512	GLN
1	A	546	LEU
1	A	595	ARG
1	A	621	ILE
1	A	709	GLU
1	A	729	MET
1	A	769	ARG
1	B	35	ASP
1	B	37	ASP
1	B	39	VAL
1	B	51	LEU
1	B	53	LEU

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	69	LYS
1	B	91	GLU
1	B	93	LYS
1	B	100	ASN
1	B	111	MET
1	B	114	ASN
1	B	132	ILE
1	B	133	ASP
1	B	171	GLU
1	B	212	LEU
1	B	239	LEU
1	B	251	TYR
1	B	269	LEU
1	B	297	ARG
1	B	344	VAL
1	B	366	ASP
1	B	368	LEU
1	B	405	ASN
1	B	479	ASN
1	B	491	ILE
1	B	512	GLN
1	B	554	LYS
1	B	590	GLN
1	B	595	ARG
1	B	621	ILE
1	B	645	GLU
1	B	767	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	66	ASN
1	A	100	ASN
1	A	114	ASN
1	A	253	GLN
1	A	285	GLN
1	A	335	ASN
1	A	440	HIS
1	A	479	ASN
1	A	590	GLN

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Mol	Chain	Res	Type
1	A	634	ASN
1	B	63	ASN
1	B	66	ASN
1	B	100	ASN
1	B	114	ASN
1	B	253	GLN
1	B	285	GLN
1	B	335	ASN
1	B	440	HIS
1	B	590	GLN
1	B	634	ASN
1	B	738	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 ⓘ

8 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	A	774	4	15,15,15	0.52	0	17,21,21	0.91	0
4	GCU	A	775	4	9,12,13	0.94	1 (11%)	13,17,19	0.73	0
4	NAG	A	776	4	14,14,15	0.45	0	15,19,21	0.98	0
4	GCD	A	777	4	7,11,12	1.51	1 (14%)	8,15,17	0.85	0
4	NAG	B	774	4	15,15,15	0.56	0	17,21,21	0.95	1 (5%)
4	GCU	B	775	4	9,12,13	0.94	1 (11%)	13,17,19	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	776	4	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
4	GCD	B	777	4	7,11,12	1.53	1 (14%)	8,15,17	0.81	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	A	774	4	-	0/6/26/26	0/1/1/1
4	GCU	A	775	4	1/1/5/6	0/0/21/24	0/1/1/1
4	NAG	A	776	4	1/1/5/7	0/6/23/26	0/1/1/1
4	GCD	A	777	4	-	0/0/17/20	0/1/1/1
4	NAG	B	774	4	-	0/6/26/26	0/1/1/1
4	GCU	B	775	4	1/1/5/6	0/0/21/24	0/1/1/1
4	NAG	B	776	4	1/1/5/7	0/6/23/26	0/1/1/1
4	GCD	B	777	4	1/1/4/6	0/0/17/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	775	GCU	O5-C5	-2.14	1.41	1.43
4	A	775	GCU	O5-C5	-2.07	1.41	1.43
4	A	777	GCD	O5-C5	3.71	1.43	1.37
4	B	777	GCD	O5-C5	3.73	1.43	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	774	NAG	C3-C4-C5	2.01	113.69	110.20
4	B	776	NAG	C2-N2-C7	2.48	126.22	123.04

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	776	NAG	C1
4	A	776	NAG	C1
4	A	775	GCU	C1
4	B	775	GCU	C1
4	B	777	GCD	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	775	GCU	1	0

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	ACT	A	3	-	1,3,3	1.26	0	0,3,3	0.00	-
3	ACT	A	4	-	1,3,3	1.46	0	0,3,3	0.00	-
3	ACT	A	5	-	1,3,3	0.86	0	0,3,3	0.00	-
3	ACT	A	773	-	1,3,3	1.27	0	0,3,3	0.00	-
3	ACT	B	773	-	1,3,3	1.27	0	0,3,3	0.00	-

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	ACT	A	3	-	-	0/0/0/0	0/0/0/0
3	ACT	A	4	-	-	0/0/0/0	0/0/0/0
3	ACT	A	5	-	-	0/0/0/0	0/0/0/0
3	ACT	A	773	-	-	0/0/0/0	0/0/0/0
3	ACT	B	773	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5	ACT	1	0

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	743/749 (99%)	1.16	137 (18%)	2 2	47, 50, 50, 53	0
1	B	743/749 (99%)	1.54	195 (26%)	1 1	47, 50, 50, 53	0
All	All	1486/1498 (99%)	1.35	332 (22%)	1 1	47, 50, 50, 53	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	ALA	10.9
1	B	36	VAL	10.2
1	B	37	ASP	8.3
1	B	39	VAL	8.1
1	B	470	GLY	7.7
1	A	36	VAL	7.3
1	B	471	SER	7.2
1	A	37	ASP	7.2
1	B	35	ASP	7.1
1	B	472	ASP	7.0
1	B	473	HIS	6.8
1	B	34	LYS	6.7
1	B	92	VAL	6.6
1	B	133	ASP	6.4
1	B	139	THR	5.8
1	B	267	PHE	5.7
1	B	324	LEU	5.6
1	B	258	LEU	5.6
1	B	640	LYS	5.6
1	A	133	ASP	5.5
1	B	32	VAL	5.5
1	A	472	ASP	5.5
1	B	641	PRO	5.4
1	B	91	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	TRP	5.3
1	B	643	THR	5.3
1	A	38	GLY	5.3
1	B	141	LYS	5.2
1	B	90	PRO	5.1
1	B	88	ASP	5.1
1	B	474	THR	5.0
1	B	68	PRO	4.9
1	A	30	ASP	4.9
1	B	262	PHE	4.9
1	B	266	LEU	4.9
1	B	288	ILE	4.8
1	B	553	ALA	4.7
1	A	91	GLU	4.7
1	B	351	PHE	4.7
1	B	33	TRP	4.6
1	B	633	THR	4.5
1	A	258	LEU	4.4
1	B	89	ILE	4.4
1	B	66	ASN	4.4
1	B	38	GLY	4.3
1	A	471	SER	4.3
1	A	40	SER	4.3
1	A	288	ILE	4.3
1	B	40	SER	4.2
1	B	477	ALA	4.1
1	B	459	PRO	4.1
1	B	41	MET	4.1
1	A	34	LYS	4.0
1	A	31	VAL	4.0
1	B	260	VAL	4.0
1	A	305	GLY	4.0
1	B	85	LYS	4.0
1	B	220	TYR	3.9
1	B	140	PHE	3.9
1	B	269	LEU	3.9
1	B	263	THR	3.9
1	B	31	VAL	3.9
1	A	35	ASP	3.9
1	A	545	PHE	3.9
1	A	292	ALA	3.9
1	B	289	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	251	TYR	3.8
1	B	489	GLY	3.8
1	B	63	ASN	3.7
1	B	245	PHE	3.7
1	A	63	ASN	3.7
1	A	251	TYR	3.7
1	B	478	ALA	3.7
1	B	142	PRO	3.7
1	A	470	GLY	3.6
1	A	39	VAL	3.5
1	A	74	TRP	3.5
1	B	364	LYS	3.5
1	B	292	ALA	3.5
1	A	526	LEU	3.5
1	B	435	GLY	3.5
1	B	723	GLY	3.5
1	B	106	VAL	3.5
1	B	321	PRO	3.5
1	B	199	ILE	3.5
1	B	438	SER	3.4
1	B	135	LEU	3.4
1	A	266	LEU	3.4
1	A	303	LEU	3.4
1	A	324	LEU	3.4
1	B	178	LYS	3.4
1	B	642	GLY	3.4
1	A	586	ILE	3.4
1	A	591	ILE	3.4
1	A	293	ILE	3.3
1	A	87	ALA	3.3
1	B	302	ILE	3.3
1	B	123	VAL	3.3
1	A	609	LEU	3.3
1	B	536	ALA	3.3
1	B	572	PHE	3.3
1	B	97	PHE	3.2
1	B	71	LYS	3.2
1	A	306	GLY	3.2
1	B	552	ASP	3.2
1	A	304	ALA	3.2
1	A	383	ALA	3.2
1	A	66	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	159	ILE	3.1
1	B	690	ASP	3.1
1	B	177	VAL	3.1
1	A	382	ILE	3.1
1	B	187	LEU	3.1
1	A	68	PRO	3.1
1	A	290	TYR	3.1
1	B	270	TRP	3.1
1	A	308	VAL	3.1
1	B	74	TRP	3.1
1	B	629	TRP	3.1
1	B	137	THR	3.1
1	B	571	ASP	3.0
1	B	284	GLY	3.0
1	B	318	TYR	3.0
1	B	350	LEU	3.0
1	B	680	LYS	3.0
1	B	138	ALA	3.0
1	A	262	PHE	3.0
1	A	46	LYS	3.0
1	B	320	MET	3.0
1	A	220	TYR	3.0
1	B	246	TYR	3.0
1	A	245	PHE	3.0
1	A	398	VAL	3.0
1	B	250	ASN	3.0
1	B	482	GLY	2.9
1	A	142	PRO	2.9
1	A	370	LEU	2.9
1	A	396	MET	2.9
1	A	763	GLY	2.9
1	A	71	LYS	2.9
1	B	462	THR	2.9
1	B	636	THR	2.9
1	B	189	CYS	2.9
1	B	354	LEU	2.9
1	B	693	VAL	2.9
1	B	268	ALA	2.9
1	B	163	TRP	2.9
1	A	92	VAL	2.9
1	B	624	LYS	2.9
1	A	89	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	560	ILE	2.9
1	B	323	LEU	2.9
1	B	215	VAL	2.9
1	A	525	TYR	2.9
1	A	693	VAL	2.9
1	B	398	VAL	2.9
1	B	439	PRO	2.9
1	B	171	GLU	2.9
1	B	86	PRO	2.8
1	B	231	ALA	2.8
1	A	524	THR	2.8
1	B	176	PHE	2.8
1	A	41	MET	2.8
1	B	46	LYS	2.8
1	B	271	ILE	2.8
1	B	476	PHE	2.8
1	B	113	LEU	2.8
1	B	43	ILE	2.8
1	A	559	MET	2.7
1	A	189	CYS	2.7
1	A	416	ILE	2.7
1	A	671	ILE	2.7
1	B	111	MET	2.7
1	A	131	ILE	2.7
1	A	393	ILE	2.7
1	B	591	ILE	2.7
1	B	30	ASP	2.7
1	A	82	GLU	2.7
1	B	638	ASP	2.6
1	B	108	VAL	2.6
1	B	257	ALA	2.6
1	B	355	TRP	2.6
1	A	56	GLN	2.6
1	B	210	ARG	2.6
1	B	593	ILE	2.6
1	B	155	VAL	2.6
1	A	413	ALA	2.6
1	A	380	TRP	2.6
1	A	373	TYR	2.6
1	B	305	GLY	2.6
1	A	267	PHE	2.6
1	B	497	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	248	SER	2.6
1	A	608	ALA	2.6
1	A	670	VAL	2.6
1	B	344	VAL	2.6
1	B	169	LYS	2.6
1	A	294	TYR	2.6
1	B	221	ASP	2.6
1	A	284	GLY	2.6
1	B	303	LEU	2.6
1	B	609	LEU	2.6
1	A	381	MET	2.6
1	B	393	ILE	2.6
1	A	254	GLY	2.5
1	B	84	TRP	2.5
1	B	206	TRP	2.5
1	A	257	ALA	2.5
1	B	325	ALA	2.5
1	A	200	VAL	2.5
1	B	569	ASN	2.5
1	A	253	GLN	2.5
1	B	457	TYR	2.5
1	A	287	PHE	2.5
1	A	546	LEU	2.5
1	A	260	VAL	2.5
1	A	424	ILE	2.5
1	B	160	VAL	2.5
1	B	219	ILE	2.5
1	A	473	HIS	2.5
1	A	135	LEU	2.5
1	A	414	PHE	2.5
1	B	69	LYS	2.5
1	B	224	PRO	2.5
1	B	555	VAL	2.5
1	B	67	ASP	2.5
1	B	586	ILE	2.5
1	B	380	TRP	2.5
1	A	201	GLY	2.4
1	B	458	ASP	2.4
1	B	334	LEU	2.4
1	A	578	LEU	2.4
1	A	732	LEU	2.4
1	B	637	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	240	VAL	2.4
1	B	382	ILE	2.4
1	A	334	LEU	2.4
1	B	213	LEU	2.4
1	B	445	PHE	2.4
1	B	675	ASP	2.4
1	A	141	LYS	2.4
1	B	58	VAL	2.4
1	A	394	ALA	2.4
1	B	581	ILE	2.4
1	A	314	LYS	2.4
1	A	372	ARG	2.4
1	A	449	ILE	2.4
1	A	140	PHE	2.4
1	A	397	LYS	2.4
1	B	264	ASN	2.4
1	A	656	ILE	2.3
1	B	295	LYS	2.3
1	A	548	LEU	2.3
1	A	514	PHE	2.3
1	A	704	PHE	2.3
1	B	463	PHE	2.3
1	A	263	THR	2.3
1	A	368	LEU	2.3
1	A	295	LYS	2.3
1	A	553	ALA	2.3
1	B	112	ALA	2.3
1	A	217	ILE	2.3
1	B	261	ARG	2.3
1	B	621	ILE	2.3
1	B	503	ASP	2.3
1	B	52	TYR	2.2
1	A	137	THR	2.2
1	A	171	GLU	2.2
1	A	374	SER	2.2
1	A	577	LEU	2.2
1	B	152	LEU	2.2
1	A	747	TYR	2.2
1	B	644	ASP	2.2
1	B	194	VAL	2.2
1	A	321	PRO	2.2
1	A	73	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	2.2
1	A	640	LYS	2.2
1	B	234	PHE	2.2
1	B	287	PHE	2.2
1	A	199	ILE	2.2
1	A	289	LEU	2.2
1	A	351	PHE	2.2
1	B	390	GLU	2.2
1	B	314	LYS	2.2
1	B	475	ASP	2.1
1	B	191	TYR	2.1
1	A	561	VAL	2.1
1	B	247	PRO	2.1
1	B	217	ILE	2.1
1	B	306	GLY	2.1
1	B	645	GLU	2.1
1	A	223	PHE	2.1
1	B	338	PHE	2.1
1	B	378	PHE	2.1
1	B	545	PHE	2.1
1	B	674	ALA	2.1
1	A	325	ALA	2.1
1	B	632	GLY	2.1
1	A	261	ARG	2.1
1	B	525	TYR	2.1
1	B	677	THR	2.1
1	A	291	ASP	2.1
1	B	78	ILE	2.1
1	A	170	PRO	2.1
1	A	348	CYS	2.1
1	A	392	VAL	2.1
1	A	406	HIS	2.0
1	B	656	ILE	2.0
1	A	722	LYS	2.0
1	B	45	PRO	2.0
1	B	93	LYS	2.0
1	A	668	LEU	2.0
1	B	183	LEU	2.0
1	B	230	ALA	2.0
1	A	215	VAL	2.0
1	A	333	TYR	2.0
1	B	200	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	373	TYR	2.0
1	B	707	THR	2.0
1	A	250	ASN	2.0
1	A	152	LEU	2.0
1	B	647	LEU	2.0
1	A	511	ALA	2.0
1	B	145	ASP	2.0
1	B	322	ALA	2.0
1	A	47	THR	2.0
1	A	99	PHE	2.0
1	B	156	THR	2.0
1	B	223	PHE	2.0
1	B	596	THR	2.0
1	A	728	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
4	GCU	B	775	12/13	0.88	0.29	2.31	64,64,65,65	0
4	NAG	B	776	14/15	0.75	0.27	1.08	76,77,79,80	0
4	NAG	A	776	14/15	0.79	0.19	0.28	62,64,67,67	0
4	NAG	B	774	15/15	0.83	0.24	-0.04	58,60,61,62	0
4	GCU	A	775	12/13	0.90	0.20	-0.05	53,54,55,55	0
4	NAG	A	774	15/15	0.91	0.15	-0.83	49,49,50,51	0
4	GCD	A	777	11/12	0.83	0.21	-	88,89,89,89	0
4	GCD	B	777	11/12	0.81	0.32	-	97,97,97,97	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	B	773	4/4	0.83	0.19	0.24	67,67,67,67	0
3	ACT	A	3	4/4	0.92	0.17	0.20	61,61,61,61	0
3	ACT	A	773	4/4	0.93	0.15	-0.10	64,64,64,64	0
2	ZN	A	1	1/1	1.00	0.03	-2.82	42,42,42,42	0
2	ZN	B	2	1/1	0.99	0.05	-4.24	55,55,55,55	0
3	ACT	A	5	4/4	0.88	0.14	-	58,58,58,58	0
3	ACT	A	4	4/4	0.64	0.26	-	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.