



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2016 – 04:47 AM EST

PDB ID : 5GR8
Title : Crystal structure of PEPR1-AtPEP1
Authors : Chai, J.J.; Tang, J.
Deposited on : 2016-08-08
Resolution : 2.59 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

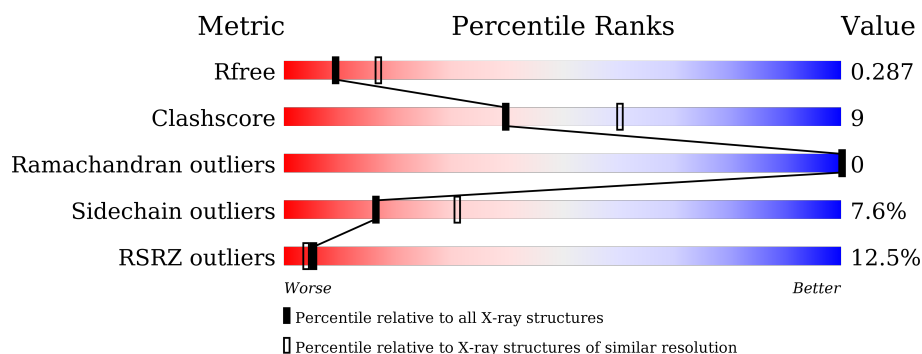
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	710	<div> <div>8%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	D	710	<div> <div>16%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
2	J	17	<div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
2	P	17	<div> <div>24%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11318 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.

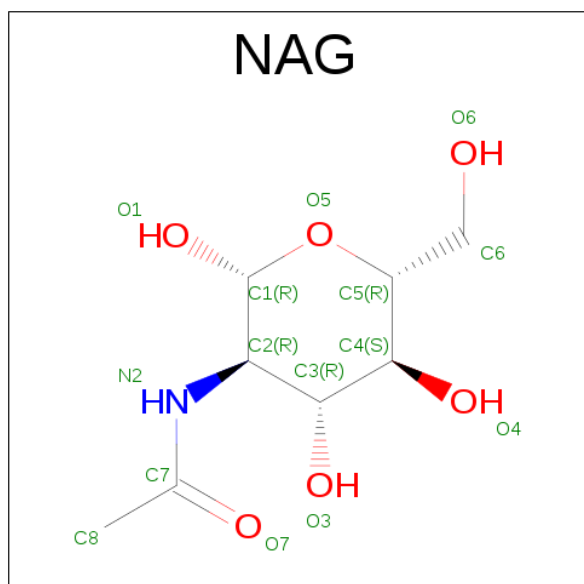
- Molecule 1 is a protein called Leucine-rich repeat receptor-like protein kinase PEPR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5404	3419	915	1054	16			
1	D	710	Total	C	N	O	S	0	0	0
			5404	3419	915	1054	16			

- Molecule 2 is a protein called Elicitor peptide 1.

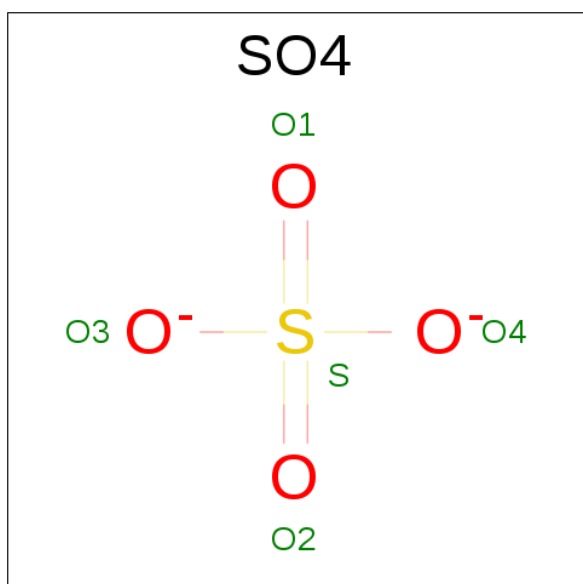
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	17	Total	C	N	O	0	0	0
			133	77	31	25			
2	P	16	Total	C	N	O	0	0	0
			124	71	29	24			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

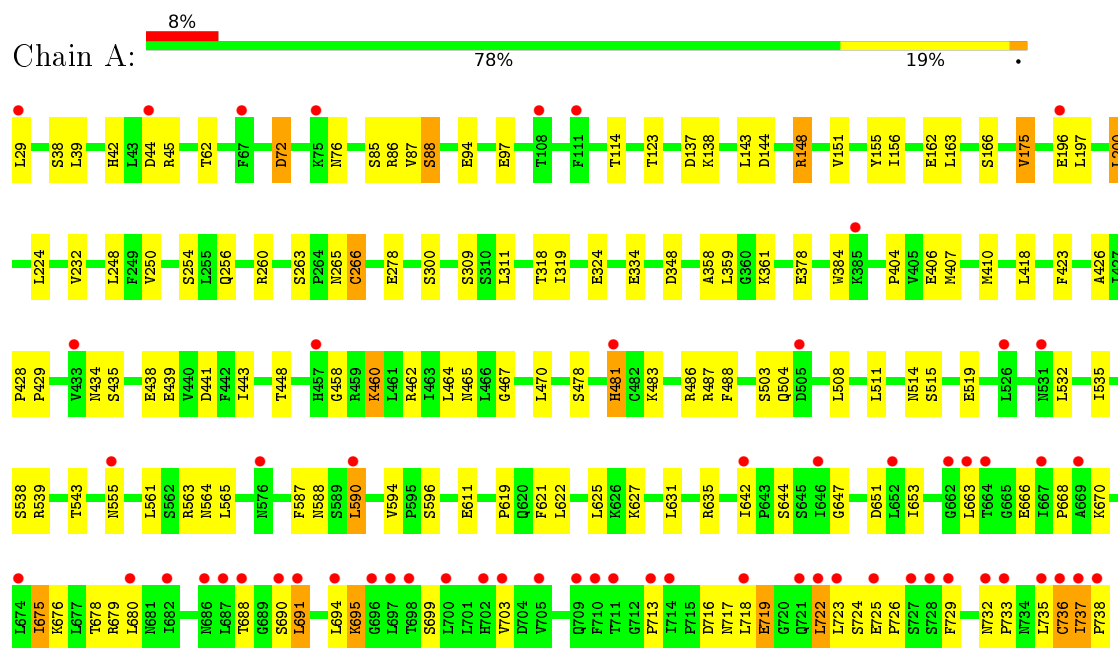
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	47	Total	O		0	0
			47	47			
5	D	13	Total	O		0	0
			13	13			
5	J	4	Total	O		0	0
			4	4			
5	P	2	Total	O		0	0
			2	2			

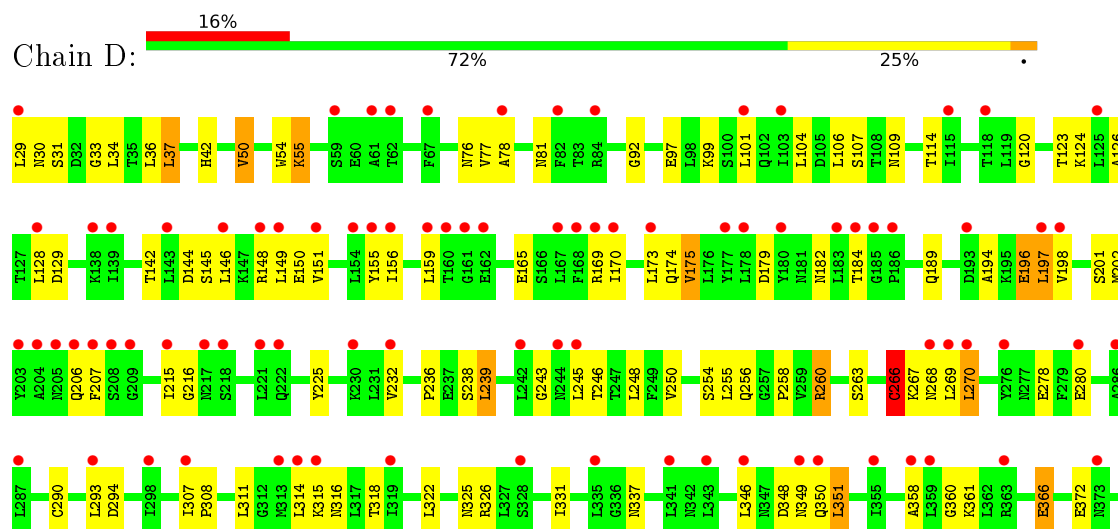
3 Residue-property plots

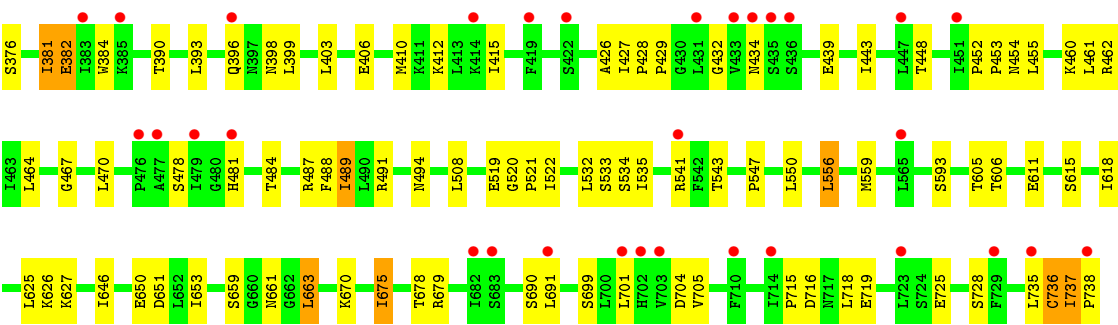
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Leucine-rich repeat receptor-like protein kinase PEPR1

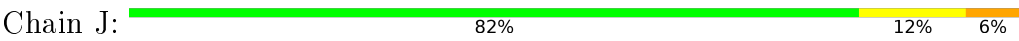


- Molecule 1: Leucine-rich repeat receptor-like protein kinase PEPR1

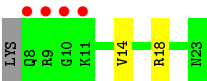
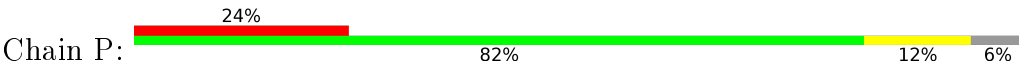




● Molecule 2: Elicitor peptide 1



● Molecule 2: Elicitor peptide 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.49 Å 96.97 Å 106.01 Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	49.55 – 2.59 49.56 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.55-2.59) 99.1 (49.56-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.58 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.234 , 0.288 0.232 , 0.287	Depositor DCC
R_{free} test set	2963 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11318	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.48	0/5500	0.74	0/7470
1	D	0.42	0/5500	0.73	1/7470 (0.0%)
2	J	0.60	0/134	0.87	1/173 (0.6%)
2	P	0.40	0/125	0.65	0/162
All	All	0.45	0/11259	0.74	2/15275 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	CYS	N-CA-C	-5.91	95.04	111.00
2	J	8	GLN	N-CA-C	5.22	125.11	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	ASN	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	5404	0	5464	88	0
1	D	5404	0	5463	109	0
2	J	133	0	134	2	0
2	P	124	0	121	1	0
3	A	84	0	77	0	0
3	D	98	0	89	0	0
4	A	5	0	0	0	0
5	A	47	0	0	5	0
5	D	13	0	0	1	0
5	J	4	0	0	1	0
5	P	2	0	0	0	0
All	All	11318	0	11348	198	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 (198) 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:148:ARG:HG2	1:A:148:ARG:HH11	1.40	0.87
1:D:372:GLU:OE1	1:D:396:GLN:NE2	2.08	0.86
1:A:438:GLU:OE2	1:A:462:ARG:NH1	2.15	0.80
1:D:243:GLY:O	1:D:268:ASN:ND2	2.16	0.79
1:A:45:ARG:HH12	1:A:86:ARG:HH21	1.30	0.78
1:D:194:ALA:HB3	1:D:197:LEU:HD12	1.64	0.78
1:D:81:ASN:ND2	5:D:901:HOH:O	2.16	0.77
1:A:486:ARG:HG3	1:A:487:ARG:HG3	1.65	0.76
1:A:695:LYS:HA	1:A:717:ASN:HD21	1.52	0.74
1:A:736:CYS:SG	1:A:737:ILE:N	2.60	0.73
1:A:666:GLU:HG2	1:A:688:THR:O	1.89	0.73
1:D:155:TYR:HD1	1:D:156:ILE:HG13	1.54	0.72
1:A:197:LEU:HD21	1:A:200:LEU:HG	1.70	0.72
1:A:588:ASN:HB2	1:A:590:LEU:HD22	1.72	0.71
1:D:184:THR:HG22	1:D:206:GLN:HB2	1.73	0.70
1:A:611:GLU:OE2	1:A:635:ARG:NE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:SER:HA	1:D:398:ASN:O	1.92	0.69
1:D:151:VAL:HG12	1:D:175:VAL:HG13	1.73	0.69
1:A:378:GLU:OE2	5:A:901:HOH:O	2.11	0.69
1:D:124:LYS:HD2	1:D:148:ARG:HD2	1.75	0.68
1:D:448:THR:HG22	1:D:470:LEU:HB2	1.78	0.66
1:D:678:THR:HG22	1:D:679:ARG:HG3	1.76	0.66
1:D:439:GLU:OE1	1:D:462:ARG:NH2	2.27	0.66
1:A:44:ASP:HB3	1:A:88:SER:HB2	1.75	0.66
1:A:726:PRO:O	5:A:902:HOH:O	2.12	0.66
1:D:381:ILE:HA	1:D:384:TRP:HD1	1.63	0.64
1:A:675:ILE:O	1:A:699:SER:OG	2.11	0.64
1:A:94:GLU:O	1:A:97:GLU:HG2	1.98	0.64
1:D:453:PRO:O	1:D:478:SER:OG	2.12	0.63
1:A:318:THR:HG23	1:A:319:ILE:HG13	1.81	0.63
1:D:165:GLU:OE2	1:D:169:ARG:NH2	2.32	0.62
1:A:407:MET:HG3	1:A:410:MET:HE3	1.84	0.60
1:D:704:ASP:HA	1:D:728:SER:HB2	1.83	0.60
1:D:322:LEU:O	1:D:325:ASN:ND2	2.33	0.59
1:A:441:ASP:HA	1:A:465:ASN:HB2	1.85	0.59
1:D:690:SER:O	1:D:691:LEU:HB2	2.03	0.59
1:A:519:GLU:OE2	5:A:903:HOH:O	2.17	0.59
1:A:155:TYR:HD1	1:A:156:ILE:HG13	1.67	0.58
1:D:216:GLY:HA3	1:D:238:SER:HB2	1.85	0.58
1:D:294:ASP:HA	1:D:316:ASN:O	2.03	0.58
1:A:151:VAL:HG12	1:A:175:VAL:HG13	1.84	0.58
1:A:678:THR:HG22	1:A:679:ARG:HG3	1.86	0.57
1:D:736:CYS:SG	1:D:737:ILE:N	2.77	0.57
2:J:7:LYS:NZ	5:J:101:HOH:O	2.36	0.57
1:A:358:ALA:O	1:A:361:LYS:HB3	2.04	0.57
1:A:622:LEU:HD13	1:A:631:LEU:HD11	1.85	0.57
1:A:435:SER:HB3	1:A:458:GLY:HA3	1.85	0.57
1:D:358:ALA:O	1:D:361:LYS:HB3	2.05	0.56
1:D:366:GLU:OE1	1:D:412:LYS:NZ	2.39	0.56
1:A:561:LEU:O	1:A:564:ASN:ND2	2.35	0.56
1:D:489:ILE:HG13	1:D:489:ILE:O	2.05	0.55
1:A:653:ILE:HG12	1:A:676:LYS:HB3	1.89	0.55
1:D:201:SER:HA	1:D:225:TYR:HB2	1.88	0.55
1:A:539:ARG:HG2	1:A:563:ARG:HD2	1.89	0.55
1:A:266:CYS:HB3	5:A:908:HOH:O	2.05	0.55
1:D:532:LEU:HD13	1:D:535:ILE:HD11	1.89	0.54
1:D:124:LYS:O	1:D:148:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:HG2	1:A:163:LEU:N	2.23	0.54
1:D:432:GLY:HA3	1:D:454:ASN:C	2.28	0.54
1:D:30:ASN:O	1:D:34:LEU:HG	2.07	0.54
1:D:149:LEU:HB3	1:D:170:ILE:HD11	1.89	0.53
1:A:72:ASP:OD2	5:A:904:HOH:O	2.19	0.53
1:D:737:ILE:HD12	1:D:738:PRO:HD2	1.91	0.53
1:D:270:LEU:HA	1:D:293:LEU:HA	1.90	0.53
1:A:651:ASP:O	1:A:653:ILE:HG13	2.07	0.53
1:D:266:CYS:HB3	1:D:290:CYS:HA	1.90	0.53
1:D:659:SER:O	1:D:661:ASN:ND2	2.42	0.52
1:D:432:GLY:HA3	1:D:454:ASN:O	2.10	0.52
1:A:148:ARG:HG2	1:A:148:ARG:NH1	2.14	0.52
1:A:406:GLU:N	1:A:406:GLU:OE2	2.41	0.52
1:D:489:ILE:HD13	1:D:491:ARG:CZ	2.39	0.52
1:D:381:ILE:HD11	1:D:406:GLU:OE1	2.09	0.52
1:D:605:THR:HG23	1:D:606:THR:OG1	2.10	0.51
1:D:36:LEU:HD11	1:D:77:VAL:HG11	1.92	0.51
1:D:678:THR:HG23	1:D:701:LEU:HD12	1.92	0.51
1:D:126:ALA:O	1:D:149:LEU:HD12	2.10	0.51
1:A:45:ARG:NH1	1:A:86:ARG:HH21	2.03	0.51
1:D:246:THR:HA	1:D:269:LEU:HA	1.92	0.51
1:A:691:LEU:HD22	1:A:694:LEU:HD22	1.93	0.51
1:A:713:PRO:HA	1:A:736:CYS:H	1.75	0.51
1:A:439:GLU:OE1	1:A:462:ARG:NH2	2.44	0.51
1:A:29:LEU:HG	1:A:62:THR:HG22	1.93	0.51
1:A:719:GLU:O	1:A:723:LEU:N	2.40	0.51
1:D:427:ILE:HB	1:D:452:PRO:HG3	1.92	0.51
1:D:258:PRO:HA	1:D:280:GLU:O	2.12	0.50
1:A:137:ASP:CG	1:A:138:LYS:H	2.14	0.50
1:D:651:ASP:O	1:D:653:ILE:HG13	2.12	0.50
1:D:360:GLY:HA3	1:D:382:GLU:HB2	1.94	0.50
1:A:72:ASP:HB2	1:A:76:ASN:H	1.77	0.49
1:D:202:MET:HB3	1:D:207:PHE:CE2	2.46	0.49
1:A:334:GLU:N	1:A:334:GLU:OE1	2.40	0.49
1:D:106:LEU:O	1:D:109:ASN:ND2	2.36	0.48
1:D:315:LYS:CG	1:D:316:ASN:H	2.25	0.48
1:A:435:SER:HB3	1:A:458:GLY:CA	2.43	0.48
1:A:543:THR:HG22	1:A:565:LEU:HB2	1.95	0.48
1:D:415:ILE:HG23	1:D:439:GLU:HB2	1.95	0.48
1:D:675:ILE:O	1:D:699:SER:OG	2.21	0.48
1:D:626:LYS:HD2	1:D:650:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:ALA:HA	1:D:448:THR:O	2.14	0.47
1:A:515:SER:OG	1:A:539:ARG:NH2	2.47	0.47
1:D:256:GLN:HA	1:D:278:GLU:O	2.13	0.47
1:D:150:GLU:O	1:D:173:LEU:HD12	2.14	0.47
1:D:331:ILE:HG21	1:D:346:LEU:HD13	1.96	0.47
1:A:263:SER:O	1:A:265:ASN:O	2.32	0.47
1:D:170:ILE:HG12	1:D:173:LEU:HB2	1.97	0.47
1:D:196:GLU:O	1:D:198:VAL:HG23	2.15	0.47
1:D:349:ASN:HB3	1:D:351:LEU:HD13	1.97	0.47
1:A:722:LEU:O	1:A:722:LEU:HD22	2.15	0.46
1:A:256:GLN:HA	1:A:278:GLU:O	2.15	0.46
1:D:715:PRO:HD2	1:D:718:LEU:HD12	1.95	0.46
1:A:443:ILE:HA	1:A:467:GLY:O	2.16	0.46
1:A:722:LEU:HD23	1:A:729:PHE:CD2	2.50	0.46
1:D:308:PRO:HG2	1:D:311:LEU:HG	1.96	0.46
1:A:144:ASP:HB2	1:A:166:SER:HB2	1.98	0.46
1:A:300:SER:HA	1:A:324:GLU:O	2.16	0.46
1:A:737:ILE:HD12	1:A:738:PRO:HD2	1.98	0.46
1:D:170:ILE:HG21	1:D:173:LEU:HD22	1.98	0.46
1:D:653:ILE:O	1:D:678:THR:HB	2.14	0.46
1:A:594:VAL:HB	1:A:619:PRO:HG3	1.98	0.45
1:D:232:VAL:HG12	1:D:254:SER:HB2	1.97	0.45
1:D:315:LYS:HG2	1:D:316:ASN:H	1.80	0.45
1:D:533:SER:HA	1:D:556:LEU:HA	1.98	0.45
1:D:519:GLU:HG2	1:D:541:ARG:HB3	1.97	0.45
1:D:29:LEU:HD21	1:D:31:SER:HB3	1.99	0.45
1:D:461:LEU:O	1:D:484:THR:HG23	2.17	0.45
1:D:236:PRO:HG2	1:D:239:LEU:HD22	1.99	0.45
1:D:245:LEU:HD21	1:D:248:LEU:HD22	1.99	0.45
1:D:126:ALA:HB2	1:D:148:ARG:HE	1.82	0.45
1:A:428:PRO:HA	1:A:429:PRO:HD3	1.83	0.44
1:A:719:GLU:O	1:A:723:LEU:HG	2.17	0.44
1:A:384:TRP:HE3	1:A:410:MET:CE	2.30	0.44
1:D:489:ILE:HD12	1:D:491:ARG:HG2	1.98	0.44
1:D:443:ILE:HD11	1:D:489:ILE:CG1	2.48	0.44
1:D:263:SER:O	1:D:266:CYS:HB2	2.18	0.44
1:D:29:LEU:HB2	1:D:76:ASN:OD1	2.16	0.44
1:D:266:CYS:O	1:D:267:LYS:HB2	2.17	0.44
1:A:508:LEU:HD21	1:A:511:LEU:HD12	1.98	0.44
1:A:587:PHE:CE2	1:A:611:GLU:HG3	2.53	0.44
1:D:55:LYS:HA	1:D:55:LYS:HD3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:VAL:HA	1:A:254:SER:O	2.17	0.44
1:A:627:LYS:HD3	1:A:627:LYS:HA	1.85	0.44
1:D:322:LEU:HD23	1:D:322:LEU:HA	1.69	0.44
1:A:532:LEU:HD13	1:A:535:ILE:HD11	1.99	0.44
1:A:642:ILE:O	1:A:668:PRO:HG3	2.18	0.44
1:D:260:ARG:HG3	1:D:260:ARG:H	1.59	0.43
1:D:294:ASP:O	1:D:318:THR:N	2.47	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.81	0.43
1:D:202:MET:HB3	1:D:207:PHE:HE2	1.84	0.43
1:A:162:GLU:HG2	1:A:163:LEU:H	1.82	0.43
1:D:670:LYS:HD2	1:D:670:LYS:HA	1.83	0.43
1:A:39:LEU:HA	1:A:42:HIS:HD2	1.84	0.43
1:A:719:GLU:HA	1:A:722:LEU:HB3	2.00	0.43
1:A:460:LYS:HE2	1:A:460:LYS:HB3	1.67	0.43
1:D:307:ILE:HD12	1:D:331:ILE:HG22	2.00	0.43
1:D:410:MET:O	1:D:434:ASN:ND2	2.41	0.43
1:A:348:ASP:OD2	2:J:18:ARG:NH2	2.50	0.43
1:D:593:SER:HA	1:D:615:SER:O	2.19	0.43
1:A:448:THR:HG22	1:A:470:LEU:HB2	2.01	0.42
1:D:120:GLY:O	1:D:145:SER:HB2	2.19	0.42
1:D:270:LEU:N	1:D:270:LEU:HD23	2.34	0.42
1:D:50:VAL:HA	1:D:54:TRP:CD1	2.55	0.42
1:A:384:TRP:CD1	1:A:404:PRO:HG2	2.54	0.42
1:A:478:SER:O	1:A:481:HIS:CD2	2.72	0.42
1:D:521:PRO:HA	1:D:543:THR:O	2.20	0.42
1:D:174:GLN:O	1:D:198:VAL:N	2.43	0.42
1:D:315:LYS:O	1:D:316:ASN:HB2	2.20	0.42
1:D:443:ILE:HA	1:D:467:GLY:O	2.19	0.42
1:A:426:ALA:HA	1:A:448:THR:O	2.20	0.42
1:A:85:SER:HB2	1:A:87:VAL:HG23	2.01	0.42
1:D:107:SER:HB3	1:D:129:ASP:CG	2.40	0.42
1:D:29:LEU:HG	1:D:31:SER:N	2.34	0.42
1:D:522:ILE:O	1:D:547:PRO:HG3	2.20	0.42
1:D:104:LEU:HD23	1:D:128:LEU:HD13	2.02	0.42
1:A:722:LEU:HD23	1:A:729:PHE:CE2	2.55	0.41
1:D:78:ALA:O	1:D:101:LEU:HD12	2.20	0.41
1:A:647:GLY:HA3	1:A:670:LYS:HB3	2.02	0.41
1:A:678:THR:HG22	1:A:679:ARG:CG	2.49	0.41
1:A:732:ASN:HA	1:A:733:PRO:HD2	1.84	0.41
1:A:418:LEU:HB3	1:A:423:PHE:CE2	2.56	0.41
1:A:680:LEU:O	1:A:703:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:MET:O	1:A:410:MET:HG3	2.19	0.41
1:D:42:HIS:CD2	1:D:92:GLY:HA3	2.55	0.41
1:D:173:LEU:O	1:D:196:GLU:HB3	2.20	0.41
1:D:519:GLU:CD	1:D:520:GLY:H	2.24	0.41
1:D:618:ILE:HD11	1:D:663:LEU:HD21	2.02	0.41
1:A:224:LEU:HD23	1:A:248:LEU:HD13	2.03	0.41
1:A:514:ASN:HA	1:A:538:SER:O	2.21	0.41
1:A:690:SER:O	1:A:691:LEU:HB2	2.21	0.41
1:D:428:PRO:HA	1:D:429:PRO:HD3	1.85	0.41
1:A:44:ASP:N	1:A:88:SER:O	2.53	0.41
1:D:390:THR:HA	1:D:412:LYS:O	2.21	0.41
1:D:550:LEU:HD13	1:D:559:MET:CE	2.51	0.41
1:D:348:ASP:OD2	2:P:18:ARG:NH2	2.54	0.41
1:A:724:SER:C	1:A:726:PRO:HD3	2.40	0.40
1:D:142:THR:C	1:D:144:ASP:H	2.24	0.40
1:A:596:SER:HA	1:A:621:PHE:CD2	2.57	0.40
1:D:33:GLY:O	1:D:37:LEU:HD22	2.20	0.40
1:D:455:LEU:HD23	1:D:455:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	708/710 (100%)	690 (98%)	18 (2%)	0	100	100
1	D	708/710 (100%)	685 (97%)	23 (3%)	0	100	100
2	J	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	P	14/17 (82%)	14 (100%)	0	0	100	100
All	All	1445/1454 (99%)	1403 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	628/628 (100%)	589 (94%)	39 (6%)	23	43
1	D	628/628 (100%)	572 (91%)	56 (9%)	12	22
2	J	14/14 (100%)	13 (93%)	1 (7%)	18	35
2	P	13/14 (93%)	12 (92%)	1 (8%)	16	30
All	All	1283/1284 (100%)	1186 (92%)	97 (8%)	16	31

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	72	ASP
1	A	88	SER
1	A	114	THR
1	A	123	THR
1	A	143	LEU
1	A	148	ARG
1	A	175	VAL
1	A	196	GLU
1	A	200	LEU
1	A	250	VAL
1	A	260	ARG
1	A	266	CYS
1	A	309	SER
1	A	311	LEU
1	A	359	LEU
1	A	460	LYS
1	A	464	LEU
1	A	481	HIS
1	A	483	LYS
1	A	488	PHE
1	A	503	SER
1	A	504	GLN
1	A	555	ASN

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Mol	Chain	Res	Type
1	A	590	LEU
1	A	625	LEU
1	A	644	SER
1	A	663	LEU
1	A	675	ILE
1	A	691	LEU
1	A	695	LYS
1	A	716	ASP
1	A	718	LEU
1	A	719	GLU
1	A	722	LEU
1	A	725	GLU
1	A	735	LEU
1	A	736	CYS
1	A	737	ILE
1	D	37	LEU
1	D	50	VAL
1	D	55	LYS
1	D	97	GLU
1	D	99	LYS
1	D	114	THR
1	D	123	THR
1	D	146	LEU
1	D	159	LEU
1	D	175	VAL
1	D	179	ASP
1	D	182	ASN
1	D	189	GLN
1	D	196	GLU
1	D	197	LEU
1	D	215	ILE
1	D	239	LEU
1	D	250	VAL
1	D	255	LEU
1	D	260	ARG
1	D	266	CYS
1	D	270	LEU
1	D	314	LEU
1	D	326	ARG
1	D	337	ASN
1	D	350	GLN
1	D	351	LEU

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Mol	Chain	Res	Type
1	D	366	GLU
1	D	381	ILE
1	D	382	GLU
1	D	393	LEU
1	D	399	LEU
1	D	403	LEU
1	D	460	LYS
1	D	464	LEU
1	D	481	HIS
1	D	487	ARG
1	D	488	PHE
1	D	489	ILE
1	D	494	ASN
1	D	508	LEU
1	D	534	SER
1	D	556	LEU
1	D	611	GLU
1	D	625	LEU
1	D	627	LYS
1	D	646	ILE
1	D	663	LEU
1	D	675	ILE
1	D	705	VAL
1	D	716	ASP
1	D	719	GLU
1	D	725	GLU
1	D	735	LEU
1	D	736	CYS
1	D	737	ILE
2	J	18	ARG
2	P	14	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	717	ASN
1	D	396	GLN
1	D	494	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 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$
3	NAG	A	801	1	14,14,15	0.49	0	15,19,21	1.78	7 (46%)
3	NAG	A	802	1	14,14,15	0.50	0	15,19,21	1.61	3 (20%)
3	NAG	A	803	1,3	14,14,15	0.61	0	15,19,21	1.30	1 (6%)
3	NAG	A	804	3	14,14,15	0.56	0	15,19,21	1.40	2 (13%)
3	NAG	A	805	1	14,14,15	0.61	0	15,19,21	1.11	0
3	NAG	A	806	1	14,14,15	0.51	0	15,19,21	1.18	1 (6%)
4	SO4	A	807	-	4,4,4	0.15	0	6,6,6	0.15	0
3	NAG	D	801	1,3	14,14,15	1.02	1 (7%)	15,19,21	1.79	2 (13%)
3	NAG	D	802	3	14,14,15	0.53	0	15,19,21	0.91	0
3	NAG	D	803	1	14,14,15	0.87	0	15,19,21	1.69	3 (20%)
3	NAG	D	804	1,3	14,14,15	0.48	0	15,19,21	1.25	1 (6%)
3	NAG	D	805	3	14,14,15	0.54	0	15,19,21	1.10	1 (6%)
3	NAG	D	806	1	14,14,15	0.65	0	15,19,21	1.29	3 (20%)
3	NAG	D	807	1	14,14,15	0.72	0	15,19,21	1.52	3 (20%)

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	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	804	3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	1	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
4	SO4	A	807	-	-	0/0/0/0	0/0/0/0
3	NAG	D	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	802	3	-	0/6/23/26	0/1/1/1
3	NAG	D	803	1	-	0/6/23/26	0/1/1/1
3	NAG	D	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	805	3	-	0/6/23/26	0/1/1/1
3	NAG	D	806	1	-	0/6/23/26	0/1/1/1
3	NAG	D	807	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	NAG	O7-C7	-2.06	1.18	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	NAG	O5-C5-C4	-4.32	102.98	110.13
3	A	803	NAG	C2-N2-C7	-4.09	117.79	123.11
3	D	801	NAG	O3-C3-C2	-3.45	101.99	109.37
3	A	801	NAG	C2-N2-C7	-3.42	118.65	123.11
3	A	804	NAG	C3-C4-C5	-3.36	104.23	110.23
3	A	802	NAG	C6-C5-C4	-2.69	106.23	112.99
3	A	801	NAG	C4-C3-C2	-2.31	107.75	111.34
3	A	801	NAG	C3-C4-C5	-2.29	106.14	110.23
3	D	803	NAG	C3-C4-C5	-2.28	106.16	110.23
3	A	806	NAG	C2-N2-C7	-2.19	120.25	123.11
3	D	806	NAG	C6-C5-C4	-2.17	107.55	112.99
3	D	807	NAG	O6-C6-C5	-2.08	104.36	111.30
3	A	801	NAG	C6-C5-C4	-2.03	107.90	112.99
3	D	807	NAG	C4-C3-C2	-2.03	108.19	111.34
3	D	806	NAG	O7-C7-C8	-2.02	118.35	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	NAG	C1-O5-C5	2.04	115.15	112.14
3	D	806	NAG	O5-C5-C6	2.28	112.22	107.34
3	A	801	NAG	O4-C4-C3	2.34	115.64	110.36
3	D	805	NAG	C1-O5-C5	2.39	115.65	112.14
3	A	804	NAG	C1-O5-C5	2.44	115.73	112.14
3	A	802	NAG	O5-C5-C4	2.52	114.31	110.13
3	A	801	NAG	O5-C5-C6	2.82	113.37	107.34
3	D	803	NAG	C1-O5-C5	2.96	116.49	112.14
3	D	804	NAG	C1-O5-C5	3.20	116.84	112.14
3	D	807	NAG	C1-O5-C5	3.64	117.49	112.14
3	A	802	NAG	C1-O5-C5	4.25	118.39	112.14
3	D	801	NAG	C1-O5-C5	4.70	119.06	112.14

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	710/710 (100%)	0.82	60 (8%) 13 10	10, 27, 65, 106	0
1	D	710/710 (100%)	0.99	117 (16%) 2 1	17, 45, 63, 74	0
2	J	17/17 (100%)	0.57	0 100 100	15, 23, 44, 46	0
2	P	16/17 (94%)	1.39	4 (25%) 1 0	28, 38, 63, 80	0
All	All	1453/1454 (99%)	0.90	181 (12%) 5 4	10, 36, 63, 106	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	LEU	11.0
1	D	160	THR	6.9
1	D	170	ILE	6.8
1	D	169	ARG	5.7
1	A	729	PHE	5.6
1	A	737	ILE	5.6
2	P	11	LYS	5.4
1	D	207	PHE	5.2
1	D	221	LEU	5.1
1	D	204	ALA	5.1
1	A	29	LEU	4.9
1	A	714	ILE	4.6
1	A	723	LEU	4.6
1	A	694	LEU	4.4
1	A	686	ASN	4.4
1	A	687	LEU	4.3
1	A	667	ILE	4.3
1	D	735	LEU	4.3
1	D	435	SER	4.3
1	D	245	LEU	4.3
1	D	217	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	161	GLY	4.2
1	D	197	LEU	4.2
1	D	156	ILE	4.2
1	D	222	GLN	4.1
1	D	29	LEU	4.0
1	A	710	PHE	4.0
1	D	128	LEU	4.0
1	D	314	LEU	4.0
1	A	663	LEU	4.0
1	D	242	LEU	3.9
1	D	206	GLN	3.9
1	A	702	HIS	3.9
1	D	208	SER	3.9
1	D	268	ASN	3.8
1	A	697	LEU	3.8
1	D	185	GLY	3.7
1	D	167	LEU	3.7
1	A	682	ILE	3.7
1	D	244	ASN	3.7
1	D	293	LEU	3.7
1	A	725	GLU	3.7
1	D	101	LEU	3.7
1	D	714	ILE	3.6
1	D	335	LEU	3.6
1	D	343	LEU	3.6
1	D	232	VAL	3.6
2	P	10	GLY	3.6
1	D	125	LEU	3.6
1	D	103	ILE	3.6
1	A	664	THR	3.5
1	A	662	GLY	3.5
1	D	168	PHE	3.5
1	A	736	CYS	3.4
1	D	298	ILE	3.4
1	D	173	LEU	3.3
1	D	78	ALA	3.3
1	D	434	ASN	3.3
1	D	287	LEU	3.3
1	D	205	ASN	3.3
1	D	151	VAL	3.3
1	D	184	THR	3.3
1	D	479	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	723	LEU	3.2
1	A	705	VAL	3.2
2	P	9	ARG	3.2
1	D	701	LEU	3.2
1	A	703	VAL	3.2
1	D	159	LEU	3.2
1	A	738	PRO	3.1
1	D	230	LYS	3.1
1	D	433	VAL	3.1
1	D	59	SER	3.1
1	D	341	LEU	3.1
1	D	358	ALA	3.1
1	D	218	SER	3.1
1	D	183	LEU	3.1
1	D	346	LEU	3.1
1	A	728	SER	3.1
1	A	691	LEU	3.1
1	D	436	SER	3.0
1	D	481	HIS	3.0
1	D	148	ARG	3.0
1	A	696	GLY	3.0
1	A	688	THR	3.0
1	D	307	ILE	3.0
1	D	177	TYR	3.0
1	D	198	VAL	2.9
2	P	8	GLN	2.9
1	D	193	ASP	2.9
1	D	729	PHE	2.9
1	A	385	LYS	2.8
1	D	541	ARG	2.8
1	D	359	LEU	2.8
1	D	422	SER	2.7
1	D	349	ASN	2.7
1	A	505	ASP	2.7
1	A	652	LEU	2.7
1	D	319	ILE	2.7
1	A	732	ASN	2.7
1	D	143	LEU	2.7
1	D	84	ARG	2.6
1	D	350	GLN	2.6
1	A	733	PRO	2.6
1	A	721	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	286	ALA	2.6
1	A	680	LEU	2.6
1	A	718	LEU	2.6
1	D	180	TYR	2.6
1	D	61	ALA	2.5
1	A	700	LEU	2.5
1	A	727	SER	2.5
1	D	280	GLU	2.5
1	D	276	TYR	2.5
1	A	531	ASN	2.5
1	A	75	LYS	2.5
1	D	138	LYS	2.5
1	A	674	LEU	2.4
1	D	363	ARG	2.4
1	D	565	LEU	2.4
1	D	703	VAL	2.4
1	D	155	TYR	2.4
1	A	709	GLN	2.4
1	A	713	PRO	2.4
1	A	669	ALA	2.4
1	A	698	THR	2.4
1	D	215	ILE	2.4
1	A	433	VAL	2.4
1	D	355	ILE	2.4
1	D	710	PHE	2.3
1	A	108	THR	2.3
1	D	62	THR	2.3
1	D	82	PHE	2.3
1	A	555	ASN	2.3
1	D	269	LEU	2.3
1	D	683	SER	2.3
1	A	722	LEU	2.3
1	D	162	GLU	2.3
1	A	111	PHE	2.3
1	D	178	LEU	2.3
1	D	328	SER	2.2
1	D	447	LEU	2.2
1	D	738	PRO	2.2
1	A	481	HIS	2.2
1	A	711	THR	2.2
1	D	139	ILE	2.2
1	A	526	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	476	PRO	2.2
1	D	373	ASN	2.2
1	A	590	LEU	2.2
1	D	691	LEU	2.2
1	D	203	TYR	2.2
1	D	315	LYS	2.2
1	D	477	ALA	2.2
1	A	576	ASN	2.2
1	D	451	ILE	2.2
1	D	209	GLY	2.2
1	A	646	ILE	2.1
1	D	186	PRO	2.1
1	A	457	HIS	2.1
1	D	385	LYS	2.1
1	D	146	LEU	2.1
1	A	44	ASP	2.1
1	D	383	ILE	2.1
1	D	67	PHE	2.1
1	A	690	SER	2.1
1	D	149	LEU	2.1
1	D	118	THR	2.1
1	D	702	HIS	2.1
1	A	67	PHE	2.1
1	A	642	ILE	2.0
1	D	682	ILE	2.0
1	D	154	LEU	2.0
1	D	270	LEU	2.0
1	D	414	LYS	2.0
1	D	396	GLN	2.0
1	D	431	LEU	2.0
1	A	196	GLU	2.0
1	D	115	ILE	2.0
1	D	419	PHE	2.0
1	D	313	MET	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 carbohydrates 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. 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	NAG	D	807	14/15	0.86	0.23	0.17	36,41,50,50	0
3	NAG	A	805	14/15	0.98	0.19	0.04	15,19,23,25	0
3	NAG	A	802	14/15	0.92	0.19	-0.19	20,26,33,33	0
3	NAG	D	806	14/15	0.94	0.18	-0.25	19,25,29,29	0
3	NAG	D	804	14/15	0.94	0.19	-0.28	36,38,49,51	0
3	NAG	D	805	14/15	0.85	0.18	-0.42	36,46,48,51	0
3	NAG	A	803	14/15	0.93	0.20	-0.76	13,19,32,38	0
4	SO4	A	807	5/5	0.93	0.14	-1.96	35,39,45,63	0
3	NAG	D	801	14/15	0.95	0.23	-	33,38,43,54	0
3	NAG	A	806	14/15	0.95	0.14	-	18,29,34,35	0
3	NAG	A	801	14/15	0.85	0.19	-	28,34,43,46	0
3	NAG	D	802	14/15	0.86	0.41	-	30,45,53,55	0
3	NAG	A	804	14/15	0.85	0.19	-	29,40,53,56	0
3	NAG	D	803	14/15	0.92	0.14	-	31,40,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.