



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 PM GMT

PDB ID : 4M4D
Title : Crystal structure of lipopolysaccharide binding protein
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Deposited on : 2013-08-07
Resolution : 2.91 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

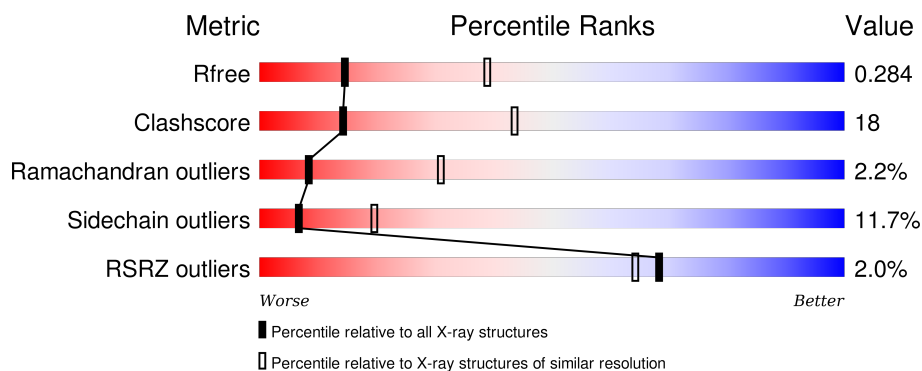
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	467	<div> <div> <div>2%</div> <div>53%</div> <div>38%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	467	<div> <div>2%</div> <div>57%</div> <div>33%</div> <div>5%</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
2	NAG	A	501	-	-	X	-
2	NAG	A	502	-	-	X	-
2	NAG	A	504	-	-	X	-
3	PC1	A	506	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7212 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 Lipopolysaccharide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3502	2252	591	644	15			
1	B	442	Total	C	N	O	S	0	0	0
			3452	2222	580	635	15			

There are 20 discrepancies between the modelled and reference sequences:

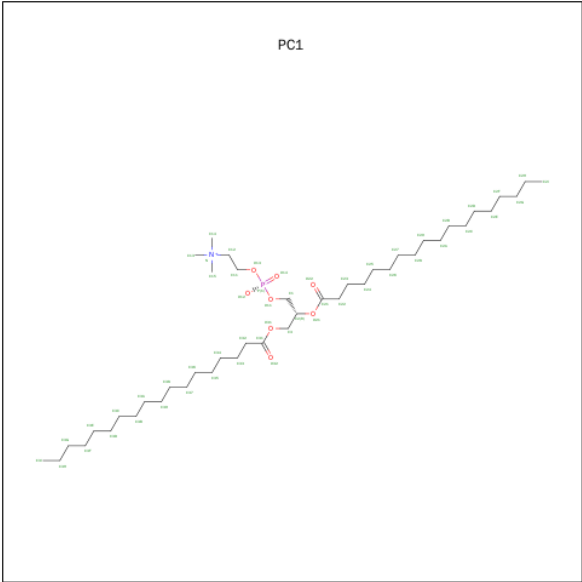
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	EXPRESSION TAG	UNP Q61805
A	23	ASP	-	EXPRESSION TAG	UNP Q61805
A	24	LEU	-	EXPRESSION TAG	UNP Q61805
A	482	SER	-	EXPRESSION TAG	UNP Q61805
A	483	GLY	-	EXPRESSION TAG	UNP Q61805
A	484	ARG	-	EXPRESSION TAG	UNP Q61805
A	485	LEU	-	EXPRESSION TAG	UNP Q61805
A	486	VAL	-	EXPRESSION TAG	UNP Q61805
A	487	PRO	-	EXPRESSION TAG	UNP Q61805
A	488	ARG	-	EXPRESSION TAG	UNP Q61805
B	22	ALA	-	EXPRESSION TAG	UNP Q61805
B	23	ASP	-	EXPRESSION TAG	UNP Q61805
B	24	LEU	-	EXPRESSION TAG	UNP Q61805
B	482	SER	-	EXPRESSION TAG	UNP Q61805
B	483	GLY	-	EXPRESSION TAG	UNP Q61805
B	484	ARG	-	EXPRESSION TAG	UNP Q61805
B	485	LEU	-	EXPRESSION TAG	UNP Q61805
B	486	VAL	-	EXPRESSION TAG	UNP Q61805
B	487	PRO	-	EXPRESSION TAG	UNP Q61805
B	488	ARG	-	EXPRESSION TAG	UNP Q61805

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).

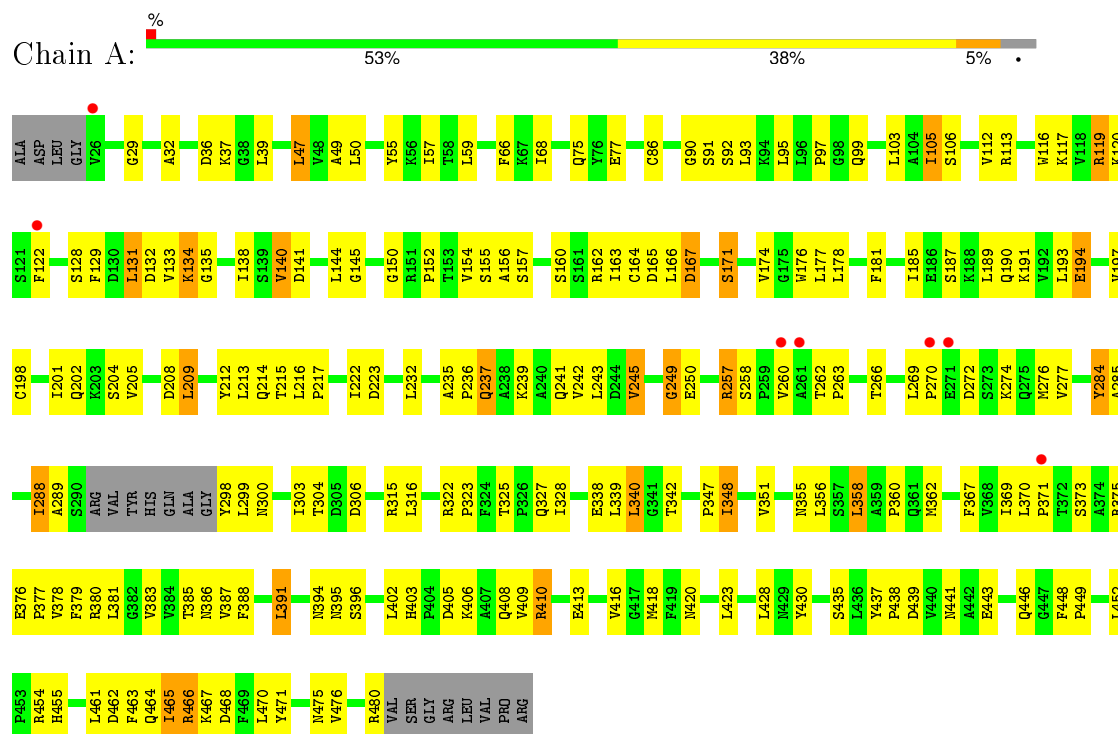


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

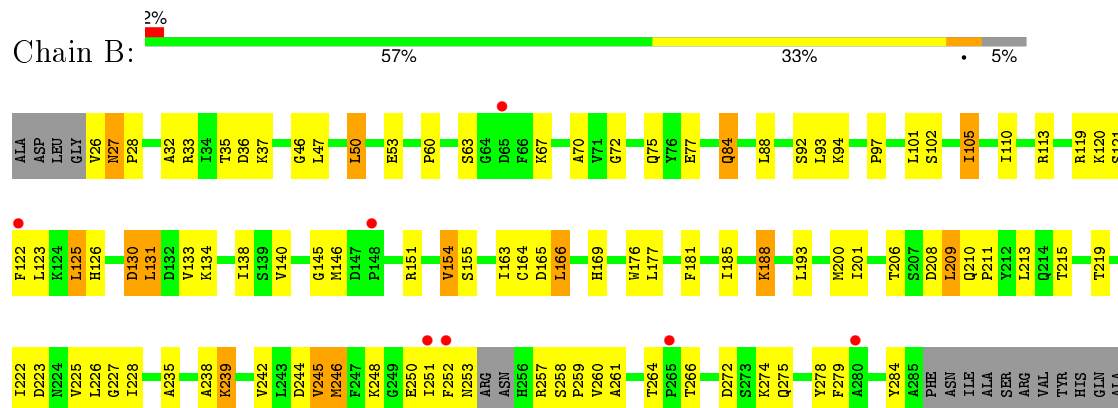
3 Residue-property plots

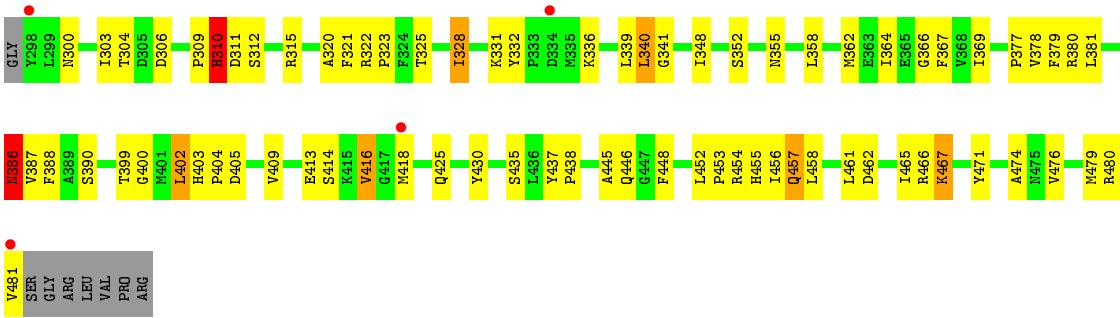
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 1: Lipopolysaccharide-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.28Å 59.91Å 119.93Å 90.00° 102.63° 90.00°	Depositor
Resolution (Å)	19.89 – 2.91 19.89 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.1 (19.89-2.91) 86.6 (19.89-2.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 2.93Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.230 , 0.277 0.230 , 0.284	Depositor DCC
R_{free} test set	1087 reflections (5.55%)	DCC
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21732 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7212	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: PC1, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/3577 (0.0%)	0.81	3/4851 (0.1%)
1	B	0.57	1/3525 (0.0%)	0.78	2/4780 (0.0%)
All	All	0.59	2/7102 (0.0%)	0.80	5/9631 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	TYR	CE2-CZ	5.18	1.45	1.38
1	B	284	TYR	CE2-CZ	5.17	1.45	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	LEU	CA-CB-CG	6.93	131.23	115.30
1	B	418	MET	CG-SD-CE	-6.91	89.14	100.20
1	A	358	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	418	MET	CG-SD-CE	-5.65	91.16	100.20
1	B	50	LEU	CB-CG-CD2	-5.20	102.16	111.00

There are no chirality outliers.

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	3502	0	3557	138	1
1	B	3452	0	3508	104	1
2	A	75	0	75	23	0
2	B	75	0	74	5	0
3	A	54	0	88	15	0
3	B	54	0	88	12	0
All	All	7212	0	7390	264	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 18.

All (264) 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:340:LEU:HD13	2:A:502:NAG:H62	1.36	1.08
3:B:501:PC1:H381	3:B:501:PC1:H3C1	1.45	0.96
3:A:506:PC1:H381	3:A:506:PC1:H3C1	1.53	0.90
2:A:501:NAG:H62	2:A:502:NAG:H5	1.56	0.87
1:A:112:VAL:HB	1:A:131:LEU:HD13	1.58	0.85
3:B:501:PC1:H381	3:B:501:PC1:C3C	2.06	0.83
1:A:216:LEU:CD1	3:A:506:PC1:H3I1	2.09	0.82
1:B:133:VAL:HG11	1:B:163:ILE:HG23	1.62	0.82
1:B:481:VAL:HG11	3:B:501:PC1:H152	1.62	0.81
3:A:506:PC1:C3C	3:A:506:PC1:H381	2.11	0.81
1:A:216:LEU:HD12	3:A:506:PC1:H3I1	1.61	0.81
1:A:213:LEU:HD13	3:A:506:PC1:H2I3	1.63	0.79
1:A:380:ARG:HH12	2:A:502:NAG:H3	1.46	0.79
1:A:269:LEU:HG	1:A:270:PRO:HD2	1.65	0.78
1:A:338:GLU:HB2	1:A:367:PHE:HB2	1.66	0.78
1:B:311:ASP:OD1	1:B:430:TYR:OH	2.00	0.77
1:A:378:VAL:HG13	1:A:416:VAL:HG21	1.63	0.77
1:B:387:VAL:HG23	1:B:404:PRO:HA	1.67	0.77
1:A:181:PHE:HA	1:A:185:ILE:HD12	1.67	0.76
1:A:134:LYS:HD3	1:A:135:GLY:H	1.50	0.76
1:A:380:ARG:HB3	1:A:413:GLU:HG2	1.65	0.75
1:B:26:VAL:HG23	1:B:27:ASN:H	1.52	0.75
1:A:386:ASN:O	1:A:405:ASP:HB3	1.88	0.72
1:A:269:LEU:HD11	1:A:466:ARG:HE	1.55	0.71
1:B:300:ASN:HD21	2:B:502:NAG:H62	1.55	0.70
1:B:131:LEU:HD21	1:B:166:LEU:HD13	1.75	0.68
1:A:388:PHE:HB2	1:A:403:HIS:HB2	1.76	0.67
1:A:166:LEU:HD12	1:A:190:GLN:HE21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:ND2	2:B:502:NAG:H62	2.09	0.67
1:B:84:GLN:HB3	1:B:113:ARG:HE	1.60	0.67
1:A:300:ASN:ND2	2:A:501:NAG:H2	2.08	0.67
1:A:300:ASN:HD21	2:A:501:NAG:H2	1.60	0.67
1:A:355:ASN:ND2	2:A:503:NAG:O1	2.29	0.66
3:A:506:PC1:H11	3:A:506:PC1:H112	1.78	0.65
1:B:252:PHE:HA	1:B:257:ARG:HG3	1.77	0.65
1:A:284:TYR:HD1	1:A:288:ILE:HG13	1.61	0.65
1:A:476:VAL:HG21	3:A:506:PC1:H3B2	1.79	0.65
1:B:133:VAL:HG22	1:B:166:LEU:HD22	1.78	0.65
1:A:356:LEU:HD11	1:A:463:PHE:CE2	2.31	0.65
1:A:383:VAL:HG22	1:A:409:VAL:HG13	1.79	0.65
1:A:284:TYR:HB2	1:A:288:ILE:HB	1.79	0.65
1:A:140:VAL:HG11	1:A:201:ILE:HG21	1.79	0.64
3:B:501:PC1:H112	3:B:501:PC1:H11	1.79	0.64
1:A:222:ILE:HG23	1:A:223:ASP:H	1.62	0.64
1:B:32:ALA:HB3	1:B:245:VAL:HG13	1.80	0.64
1:B:386:ASN:O	1:B:405:ASP:HB3	1.98	0.63
1:A:216:LEU:HD12	3:A:506:PC1:C3I	2.29	0.63
1:B:105:ILE:HD12	1:B:138:ILE:HD12	1.81	0.63
1:B:105:ILE:HG23	1:B:138:ILE:HB	1.81	0.62
1:A:300:ASN:HD21	2:A:501:NAG:C1	2.13	0.62
1:B:213:LEU:HD13	3:B:501:PC1:H2I3	1.81	0.62
1:B:27:ASN:ND2	1:B:266:THR:OG1	2.32	0.62
1:A:128:SER:H	1:A:171:SER:HB3	1.65	0.61
1:A:237:GLN:HB3	1:A:239:LYS:HE2	1.81	0.61
2:A:504:NAG:H62	2:A:505:NAG:H1	1.82	0.61
1:A:32:ALA:HB3	1:A:245:VAL:HG13	1.83	0.61
1:A:262:THR:N	1:A:263:PRO:HD3	2.16	0.61
1:B:378:VAL:HG12	1:B:416:VAL:HG21	1.83	0.60
1:B:404:PRO:HB3	1:B:437:TYR:CD1	2.36	0.60
1:A:405:ASP:CG	1:A:406:LYS:H	2.04	0.60
1:B:35:THR:HG22	1:B:37:LYS:H	1.67	0.60
1:A:356:LEU:HD11	1:A:463:PHE:HE2	1.67	0.60
1:B:452:LEU:HD23	3:B:501:PC1:H3F2	1.84	0.59
1:B:300:ASN:HD21	2:B:502:NAG:C6	2.15	0.59
1:B:379:PHE:HA	1:B:414:SER:HA	1.85	0.59
2:A:501:NAG:H62	2:A:502:NAG:C5	2.29	0.59
1:A:50:LEU:HD21	1:A:201:ILE:HG12	1.84	0.59
1:A:162:ARG:NH1	1:A:164:CYS:SG	2.76	0.59
1:B:258:SER:O	1:B:260:VAL:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD11	1:B:201:ILE:HG12	1.86	0.58
1:B:63:SER:OG	1:B:77:GLU:HG3	2.04	0.58
1:A:300:ASN:HD21	2:A:501:NAG:C2	2.17	0.57
2:A:501:NAG:H5	2:A:502:NAG:C8	2.34	0.57
1:A:269:LEU:HD13	1:A:471:TYR:CG	2.39	0.57
1:A:338:GLU:HG3	1:A:375:ARG:HG2	1.85	0.57
1:A:351:VAL:HB	1:A:355:ASN:HD22	1.70	0.57
1:B:145:GLY:HA2	1:B:235:ALA:HB1	1.87	0.57
1:A:187:SER:O	1:A:191:LYS:HG2	2.05	0.56
1:B:435:SER:C	1:B:438:PRO:HD2	2.26	0.56
1:B:452:LEU:HD11	1:B:458:LEU:HD21	1.87	0.56
1:A:36:ASP:OD2	1:A:37:LYS:N	2.38	0.56
1:A:131:LEU:HD21	1:A:189:LEU:HD13	1.88	0.55
1:B:33:ARG:HD2	1:B:471:TYR:OH	2.06	0.55
1:B:336:LYS:HB2	1:B:369:ILE:HD12	1.88	0.55
2:A:501:NAG:H5	2:A:502:NAG:H83	1.89	0.55
1:B:244:ASP:HB3	1:B:246:MET:HE3	1.88	0.55
3:A:506:PC1:O13	3:A:506:PC1:H153	2.07	0.55
1:B:250:GLU:O	1:B:251:ILE:HG23	2.07	0.54
1:B:133:VAL:HG13	1:B:164:CYS:O	2.08	0.54
3:B:501:PC1:H153	3:B:501:PC1:O13	2.07	0.54
1:A:394:ASN:OD1	2:A:504:NAG:H82	2.07	0.54
1:B:340:LEU:HD12	1:B:367:PHE:HE1	1.73	0.54
1:B:380:ARG:HB3	1:B:413:GLU:HG2	1.88	0.54
1:B:341:GLY:HA2	1:B:364:ILE:HA	1.89	0.54
1:A:262:THR:H	1:A:263:PRO:HD3	1.72	0.54
1:A:216:LEU:HD11	3:A:506:PC1:H3I1	1.88	0.54
1:B:303:ILE:HB	1:B:339:LEU:HB2	1.88	0.54
1:B:455:HIS:NE2	3:B:501:PC1:H133	2.23	0.54
1:A:152:PRO:HD2	1:A:214:GLN:HG2	1.89	0.54
1:A:95:LEU:O	1:A:97:PRO:HD3	2.07	0.54
1:B:239:LYS:HA	1:B:239:LYS:HE2	1.90	0.54
1:A:284:TYR:HE1	1:A:470:LEU:HD13	1.73	0.53
1:A:394:ASN:OD1	2:A:504:NAG:H3	2.08	0.53
2:A:504:NAG:H62	2:A:505:NAG:C1	2.38	0.53
1:A:284:TYR:H	1:A:288:ILE:HG13	1.73	0.53
1:A:394:ASN:OD1	2:A:504:NAG:C3	2.57	0.53
3:B:501:PC1:H3C1	3:B:501:PC1:C38	2.24	0.52
1:A:348:ILE:H	1:A:348:ILE:HD12	1.74	0.52
1:B:331:LYS:HG2	1:B:332:TYR:CE1	2.45	0.52
1:A:465:ILE:O	1:A:466:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:PRO:HD2	1:B:456:ILE:HD12	1.91	0.52
1:B:181:PHE:HA	1:B:185:ILE:HD12	1.91	0.52
1:A:105:ILE:HG12	1:A:106:SER:N	2.25	0.52
1:B:251:ILE:HD11	1:B:260:VAL:HG11	1.91	0.52
1:A:216:LEU:CD1	3:A:506:PC1:C3I	2.84	0.51
1:A:284:TYR:OH	1:A:470:LEU:HD22	2.12	0.50
1:A:355:ASN:CG	2:A:503:NAG:O1	2.50	0.50
1:B:348:ILE:HG13	1:B:358:LEU:HG	1.93	0.50
1:A:463:PHE:HE1	1:A:470:LEU:HB3	1.76	0.50
1:B:35:THR:HG22	1:B:36:ASP:N	2.26	0.50
2:A:501:NAG:C6	2:A:502:NAG:H5	2.36	0.50
1:A:66:PHE:CD1	1:A:68:ILE:HG12	2.47	0.49
1:B:53:GLU:HB3	1:B:200:MET:HE2	1.93	0.49
1:B:458:LEU:HD23	1:B:476:VAL:HG12	1.94	0.49
1:A:410:ARG:HB2	1:A:410:ARG:HH11	1.77	0.49
1:A:55:TYR:CE1	1:A:86:CYS:HB3	2.47	0.49
1:B:215:THR:HB	1:B:454:ARG:HG2	1.93	0.49
1:B:154:VAL:HG11	1:B:209:LEU:HD13	1.95	0.49
1:A:29:GLY:HA3	1:A:249:GLY:O	2.13	0.49
1:B:208:ASP:HB3	3:B:501:PC1:O22	2.12	0.49
1:A:222:ILE:HG23	1:A:223:ASP:N	2.27	0.49
1:A:370:LEU:H	1:A:370:LEU:HD23	1.78	0.48
1:A:303:ILE:HG22	1:A:316:LEU:HD11	1.95	0.48
1:A:338:GLU:HG2	1:A:369:ILE:HD11	1.95	0.48
1:B:300:ASN:HD21	2:B:502:NAG:C5	2.26	0.48
1:A:150:GLY:O	1:A:232:LEU:HD23	2.14	0.48
1:B:121:SER:C	1:B:123:LEU:H	2.17	0.48
1:A:141:ASP:O	1:A:156:ALA:HA	2.14	0.48
1:B:47:LEU:HD12	1:B:88:LEU:HB3	1.94	0.48
1:A:383:VAL:HA	1:A:408:GLN:O	2.13	0.48
1:A:439:ASP:O	1:A:443:GLU:HG3	2.13	0.47
2:A:504:NAG:H83	2:A:504:NAG:O3	2.14	0.47
1:A:129:PHE:HE2	1:A:131:LEU:HD11	1.78	0.47
1:B:84:GLN:CB	1:B:113:ARG:HE	2.24	0.47
1:A:91:SER:HA	1:A:105:ILE:HA	1.95	0.47
1:A:455:HIS:NE2	3:A:506:PC1:H133	2.30	0.47
1:B:27:ASN:HA	1:B:28:PRO:HD2	1.81	0.47
1:B:110:ILE:HD11	1:B:163:ILE:HD11	1.97	0.47
1:A:133:VAL:HG11	1:A:163:ILE:HG23	1.97	0.47
1:A:289:ALA:HB1	1:A:299:LEU:HD21	1.96	0.46
1:A:59:LEU:HD11	1:A:193:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:506:PC1:C38	3:A:506:PC1:H3C1	2.29	0.46
1:A:464:GLN:OE1	1:A:466:ARG:NH2	2.48	0.46
1:A:269:LEU:HD22	1:A:471:TYR:CE2	2.51	0.46
1:A:378:VAL:HG13	1:A:416:VAL:CG2	2.39	0.46
1:B:120:LYS:HD3	1:B:121:SER:HB2	1.98	0.46
1:A:75:GLN:OE1	1:A:119:ARG:HD2	2.15	0.46
1:A:394:ASN:OD1	2:A:504:NAG:C8	2.63	0.46
1:A:448:PHE:CD1	1:A:449:PRO:HD2	2.51	0.46
1:A:435:SER:O	1:A:438:PRO:HD2	2.16	0.46
2:A:501:NAG:O6	2:A:502:NAG:N2	2.50	0.46
1:B:388:PHE:HB2	1:B:403:HIS:HB2	1.96	0.46
1:A:303:ILE:HB	1:A:339:LEU:HB2	1.98	0.45
1:B:222:ILE:HG13	1:B:227:GLY:HA2	1.97	0.45
1:A:131:LEU:HA	1:A:167:ASP:O	2.17	0.45
1:A:388:PHE:O	1:A:403:HIS:N	2.49	0.45
1:B:367:PHE:CD2	1:B:377:PRO:HA	2.52	0.45
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.74	0.45
1:B:310:HIS:HB3	1:B:311:ASP:H	1.62	0.45
1:A:190:GLN:O	1:A:194:GLU:HG2	2.15	0.45
1:B:465:ILE:HG12	1:B:465:ILE:H	1.62	0.45
1:B:97:PRO:HA	1:B:238:ALA:O	2.16	0.45
1:A:405:ASP:CG	1:A:406:LYS:N	2.70	0.45
1:A:322:ARG:HB3	1:A:323:PRO:HD3	1.98	0.45
1:B:215:THR:CB	1:B:454:ARG:HG2	2.46	0.45
1:B:226:LEU:HD23	1:B:253:ASN:HB2	1.98	0.45
1:B:279:PHE:HZ	1:B:452:LEU:HD21	1.80	0.45
1:A:154:VAL:CG2	1:A:213:LEU:HD12	2.47	0.45
1:B:26:VAL:HG23	1:B:27:ASN:N	2.27	0.45
1:B:480:ARG:HD3	1:B:480:ARG:HA	1.63	0.45
1:A:232:LEU:HD11	1:A:245:VAL:HG23	2.00	0.44
1:B:390:SER:O	1:B:400:GLY:HA2	2.17	0.44
1:B:322:ARG:HB3	1:B:323:PRO:HD3	1.97	0.44
1:A:103:LEU:HB3	1:A:140:VAL:HG22	1.99	0.44
1:A:376:GLU:HA	1:A:377:PRO:HD3	1.72	0.44
1:B:461:LEU:HD12	1:B:462:ASP:N	2.32	0.44
1:A:216:LEU:HD23	1:A:217:PRO:HD2	1.98	0.44
1:A:129:PHE:CE2	1:A:131:LEU:HD11	2.51	0.44
1:A:463:PHE:CZ	1:A:470:LEU:HD23	2.52	0.44
1:B:35:THR:HG22	1:B:36:ASP:OD2	2.18	0.44
1:A:77:GLU:O	1:A:116:TRP:HA	2.17	0.44
1:B:275:GLN:HB3	1:B:474:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD22	3:A:506:PC1:H271	1.98	0.44
1:B:457:GLN:HG3	1:B:479:MET:SD	2.57	0.44
1:B:125:LEU:HD23	1:B:126:HIS:H	1.83	0.44
1:B:93:LEU:HD22	1:B:101:LEU:HB3	2.00	0.44
1:A:217:PRO:HD3	1:A:452:LEU:O	2.18	0.44
1:A:77:GLU:OE1	1:A:117:LYS:HE2	2.17	0.44
1:B:325:THR:HB	1:B:328:ILE:HD11	2.00	0.44
1:A:266:THR:HG21	1:B:67:LYS:NZ	2.33	0.44
1:A:276:MET:HG3	1:A:475:ASN:OD1	2.18	0.44
1:B:366:GLY:HA3	1:B:379:PHE:CZ	2.53	0.44
1:B:278:TYR:HB3	1:B:471:TYR:CZ	2.52	0.44
1:A:328:ILE:HA	1:A:416:VAL:HG11	2.00	0.43
1:A:133:VAL:CG1	1:A:163:ILE:HG23	2.48	0.43
1:A:420:ASN:OD1	1:A:423:LEU:HB2	2.18	0.43
1:A:328:ILE:HD11	1:A:378:VAL:HG11	2.00	0.43
1:B:188:LYS:HE3	1:B:188:LYS:HB2	1.68	0.43
1:B:467:LYS:HA	1:B:467:LYS:HD3	1.76	0.43
1:B:134:LYS:HB3	1:B:134:LYS:HE3	1.89	0.43
1:B:435:SER:O	1:B:438:PRO:HD2	2.19	0.43
1:B:75:GLN:HB2	1:B:119:ARG:HB2	2.00	0.43
1:B:223:ASP:C	1:B:225:VAL:H	2.22	0.43
1:A:144:LEU:HB3	1:A:236:PRO:HG2	1.99	0.43
1:A:258:SER:O	1:A:260:VAL:N	2.49	0.43
1:B:367:PHE:HA	1:B:378:VAL:HG23	2.01	0.43
1:B:210:GLN:HB3	1:B:211:PRO:HD3	2.01	0.43
1:B:399:THR:HG23	1:B:445:ALA:HA	2.00	0.43
1:A:47:LEU:HD22	1:A:47:LEU:HA	1.85	0.42
1:B:309:PRO:HG2	1:B:312:SER:HB3	2.01	0.42
1:B:92:SER:HB2	1:B:94:LYS:HE3	2.01	0.42
1:B:130:ASP:HB3	1:B:169:HIS:ND1	2.33	0.42
1:A:435:SER:C	1:A:438:PRO:HD2	2.40	0.42
1:B:355:ASN:HA	1:B:390:SER:HA	2.01	0.42
1:A:402:LEU:HB2	1:A:441:ASN:OD1	2.20	0.42
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.83	0.42
1:A:215:THR:HB	1:A:454:ARG:HG2	2.00	0.42
1:A:381:LEU:HA	1:A:381:LEU:HD23	1.81	0.42
1:B:93:LEU:HD13	1:B:101:LEU:HD13	2.02	0.42
1:A:371:PRO:C	1:A:373:SER:H	2.21	0.42
2:A:501:NAG:C6	2:A:502:NAG:O4	2.67	0.42
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.79	0.42
1:B:244:ASP:HB3	1:B:246:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLY:HA2	1:A:235:ALA:HB1	2.01	0.42
1:A:347:PRO:O	1:A:358:LEU:HA	2.19	0.42
1:B:300:ASN:CG	2:B:502:NAG:H62	2.41	0.41
1:A:204:SER:O	1:A:208:ASP:HB2	2.19	0.41
1:B:193:LEU:HD12	1:B:193:LEU:HA	1.74	0.41
1:B:110:ILE:HD11	1:B:163:ILE:CD1	2.50	0.41
1:A:395:ASN:O	1:A:396:SER:OG	2.26	0.41
1:A:138:ILE:HG21	1:A:201:ILE:CD1	2.50	0.41
1:A:402:LEU:HA	1:A:402:LEU:HD23	1.84	0.41
1:A:250:GLU:OE2	1:A:257:ARG:NH2	2.53	0.41
1:B:46:GLY:O	1:B:50:LEU:HB2	2.21	0.41
1:A:49:ALA:HB2	1:A:480:ARG:HH22	1.84	0.41
1:A:360:PRO:HD2	1:A:385:THR:HG1	1.86	0.41
3:B:501:PC1:H111	3:B:501:PC1:H142	1.87	0.41
1:A:437:TYR:O	1:A:441:ASN:HB2	2.21	0.41
1:B:399:THR:HG22	1:B:400:GLY:N	2.36	0.41
1:A:327:GLN:HB2	1:A:416:VAL:O	2.20	0.41
1:A:144:LEU:HD23	1:A:154:VAL:HG13	2.01	0.41
1:A:212:TYR:CE2	3:A:506:PC1:H342	2.55	0.41
1:A:378:VAL:HG12	1:A:379:PHE:CD2	2.56	0.41
1:A:133:VAL:HG22	1:A:166:LEU:HD21	2.03	0.41
1:A:205:VAL:HA	1:A:209:LEU:HB2	2.02	0.41
1:B:219:THR:HA	1:B:228:ILE:O	2.21	0.41
1:A:304:THR:HG22	1:A:338:GLU:OE1	2.22	0.41
1:B:387:VAL:HG21	1:B:402:LEU:HG	2.02	0.41
1:A:461:LEU:HD12	1:A:462:ASP:N	2.35	0.41
3:B:501:PC1:H342	3:B:501:PC1:H372	1.89	0.40
1:A:57:ILE:HD11	1:A:197:VAL:HA	2.04	0.40
1:A:269:LEU:HD13	1:A:471:TYR:CD2	2.56	0.40
2:A:501:NAG:C5	2:A:502:NAG:H83	2.50	0.40
1:B:228:ILE:HD11	1:B:448:PHE:CZ	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:A:430:TYR:OH	1:B:320:ALA:O[1_654]	2.16	0.04

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	444/467 (95%)	403 (91%)	35 (8%)	6 (1%)	14	44
1	B	436/467 (93%)	390 (89%)	33 (8%)	13 (3%)	5	22
All	All	880/934 (94%)	793 (90%)	68 (8%)	19 (2%)	8	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	467	LYS
1	B	70	ALA
1	B	310	HIS
1	B	386	ASN
1	A	90	GLY
1	A	165	ASP
1	A	249	GLY
1	B	259	PRO
1	B	467	LYS
1	B	239	LYS
1	B	261	ALA
1	B	264	THR
1	B	27	ASN
1	B	248	LYS
1	A	285	ALA
1	B	60	PRO
1	B	72	GLY
1	B	416	VAL

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	392/406 (97%)	342 (87%)	50 (13%)	5	16
1	B	387/406 (95%)	346 (89%)	41 (11%)	8	25
All	All	779/812 (96%)	688 (88%)	91 (12%)	7	19

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	92	SER
1	A	93	LEU
1	A	99	GLN
1	A	105	ILE
1	A	113	ARG
1	A	119	ARG
1	A	120	LYS
1	A	122	PHE
1	A	131	LEU
1	A	132	ASP
1	A	134	LYS
1	A	140	VAL
1	A	155	SER
1	A	157	SER
1	A	160	SER
1	A	167	ASP
1	A	171	SER
1	A	174	VAL
1	A	176	TRP
1	A	178	LEU
1	A	194	GLU
1	A	198	CYS
1	A	202	GLN
1	A	209	LEU
1	A	237	GLN
1	A	241	GLN
1	A	242	VAL
1	A	243	LEU
1	A	245	VAL
1	A	272	ASP
1	A	274	LYS
1	A	277	VAL

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Mol	Chain	Res	Type
1	A	288	ILE
1	A	298	TYR
1	A	306	ASP
1	A	315	ARG
1	A	325	THR
1	A	340	LEU
1	A	342	THR
1	A	348	ILE
1	A	362	MET
1	A	387	VAL
1	A	391	LEU
1	A	410	ARG
1	A	428	LEU
1	A	446	GLN
1	A	465	ILE
1	A	466	ARG
1	A	468	ASP
1	B	84	GLN
1	B	102	SER
1	B	105	ILE
1	B	122	PHE
1	B	125	LEU
1	B	130	ASP
1	B	131	LEU
1	B	140	VAL
1	B	146	MET
1	B	151	ARG
1	B	154	VAL
1	B	155	SER
1	B	165	ASP
1	B	166	LEU
1	B	176	TRP
1	B	177	LEU
1	B	188	LYS
1	B	206	THR
1	B	209	LEU
1	B	242	VAL
1	B	245	VAL
1	B	246	MET
1	B	272	ASP
1	B	274	LYS
1	B	304	THR

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Mol	Chain	Res	Type
1	B	306	ASP
1	B	310	HIS
1	B	315	ARG
1	B	321	PHE
1	B	328	ILE
1	B	340	LEU
1	B	352	SER
1	B	362	MET
1	B	381	LEU
1	B	386	ASN
1	B	402	LEU
1	B	409	VAL
1	B	425	GLN
1	B	446	GLN
1	B	457	GLN
1	B	466	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	190	GLN
1	A	300	ASN
1	A	355	ASN
1	A	422	ASN
1	B	27	ASN
1	B	253	ASN
1	B	350	ASN
1	B	395	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 ⓘ

12 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	$\# Z > 2$
2	NAG	A	501	-	15,15,15	0.41	0	17,21,21	0.63	0
2	NAG	A	502	-	15,15,15	0.42	0	17,21,21	0.62	0
2	NAG	A	503	-	15,15,15	0.53	0	17,21,21	0.67	0
2	NAG	A	504	-	15,15,15	0.45	0	17,21,21	0.80	0
2	NAG	A	505	-	15,15,15	0.51	0	17,21,21	0.56	0
3	PC1	A	506	-	53,53,53	0.59	0	57,61,61	1.03	4 (7%)
3	PC1	B	501	-	53,53,53	0.59	0	57,61,61	1.06	3 (5%)
2	NAG	B	502	-	15,15,15	0.51	0	17,21,21	0.55	0
2	NAG	B	503	-	15,15,15	0.50	0	17,21,21	0.60	0
2	NAG	B	504	-	15,15,15	0.51	0	17,21,21	0.57	0
2	NAG	B	505	-	15,15,15	0.51	0	17,21,21	0.54	0
2	NAG	B	506	-	15,15,15	0.63	0	17,21,21	0.62	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
2	NAG	A	501	-	-	0/6/26/26	0/1/1/1
2	NAG	A	502	-	-	0/6/26/26	0/1/1/1
2	NAG	A	503	-	-	0/6/26/26	0/1/1/1
2	NAG	A	504	-	-	1/6/26/26	0/1/1/1
2	NAG	A	505	-	-	0/6/26/26	0/1/1/1
3	PC1	A	506	-	-	0/57/57/57	0/0/0/0
3	PC1	B	501	-	-	0/57/57/57	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	502	-	-	0/6/26/26	0/1/1/1
2	NAG	B	503	-	-	0/6/26/26	0/1/1/1
2	NAG	B	504	-	-	0/6/26/26	0/1/1/1
2	NAG	B	505	-	-	0/6/26/26	0/1/1/1
2	NAG	B	506	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	PC1	C2-O21-C21	-3.46	109.59	117.89
3	A	506	PC1	C2-O21-C21	-3.38	109.79	117.89
3	A	506	PC1	C3-O31-C31	-2.11	110.96	116.85
3	A	506	PC1	O31-C31-C32	2.13	118.38	111.90
3	B	501	PC1	O31-C31-C32	2.38	119.16	111.90
3	A	506	PC1	O21-C21-C22	3.83	119.86	111.53
3	B	501	PC1	O21-C21-C22	3.86	119.92	111.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	504	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	12	0
2	A	502	NAG	10	0
2	A	503	NAG	2	0
2	A	504	NAG	7	0
2	A	505	NAG	2	0
3	A	506	PC1	15	0
3	B	501	PC1	12	0
2	B	502	NAG	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	448/467 (95%)	-0.10	7 (1%) 74 72	40, 67, 101, 132	0
1	B	442/467 (94%)	-0.07	11 (2%) 61 55	44, 69, 104, 141	0
All	All	890/934 (95%)	-0.08	18 (2%) 68 64	40, 68, 102, 141	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	ALA	4.9
1	A	260	VAL	4.1
1	A	26	VAL	3.7
1	A	270	PRO	3.4
1	B	122	PHE	3.0
1	B	418	MET	3.0
1	B	481	VAL	2.6
1	A	371	PRO	2.6
1	B	65	ASP	2.5
1	A	122	PHE	2.3
1	B	148	PRO	2.3
1	B	265	PRO	2.3
1	B	334	ASP	2.3
1	B	252	PHE	2.2
1	B	280	ALA	2.2
1	B	298	TYR	2.2
1	B	251	ILE	2.1
1	A	271	GLU	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](#)

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	PC1	A	506	54/54	0.76	0.35	3.95	69,76,116,117	0
3	PC1	B	501	54/54	0.83	0.30	1.68	66,77,115,115	0
2	NAG	B	505	15/15	0.76	0.20	1.55	115,120,121,122	0
2	NAG	A	503	15/15	0.84	0.17	-0.30	80,84,89,90	0
2	NAG	A	501	15/15	0.74	0.30	-	119,121,122,123	0
2	NAG	B	506	15/15	0.67	0.35	-	137,138,138,138	0
2	NAG	A	504	15/15	0.77	0.27	-	120,122,123,124	0
2	NAG	A	505	15/15	0.52	0.55	-	173,176,177,177	0
2	NAG	B	504	15/15	0.90	0.17	-	80,81,84,84	0
2	NAG	B	503	15/15	0.81	0.23	-	100,101,102,103	0
2	NAG	B	502	15/15	0.69	0.39	-	116,117,118,119	0
2	NAG	A	502	15/15	0.77	0.31	-	110,114,117,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.