



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:30 PM GMT

PDB ID : 4LSX
Title : Plant steroid receptor ectodomain bound to brassinolide and SERK1 co-receptor ectodomain
Authors : Santiago, J.; Henzler, C.; Hothorn, M.
Deposited on : 2013-07-23
Resolution : 3.30 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

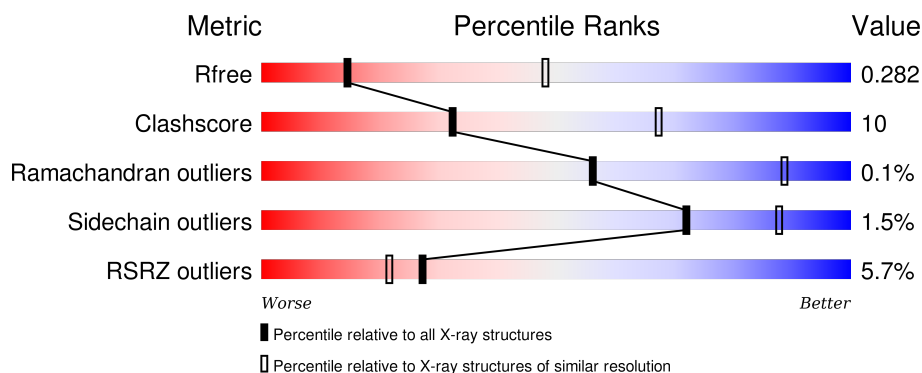
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	774	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	774	<div> <div>3%</div> <div>69%</div> <div>22%</div> <div>• 8%</div> </div>
2	C	203	<div> <div>10%</div> <div>66%</div> <div>25%</div> <div>9%</div> </div>
2	D	203	<div> <div>16%</div> <div>67%</div> <div>23%</div> <div>9%</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
3	BLD	B	801	-	-	-	X
6	NAG	A	807	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13920 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 Protein BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5454	3421	914	1088	31			
1	B	710	Total	C	N	O	S	0	0	0
			5217	3283	868	1037	29			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP O22476
A	25	SER	-	EXPRESSION TAG	UNP O22476
A	26	SER	-	EXPRESSION TAG	UNP O22476
A	27	MET	-	EXPRESSION TAG	UNP O22476
A	28	GLY	-	EXPRESSION TAG	UNP O22476
A	643	GLU	GLY	ENGINEERED MUTATION	UNP O22476
A	789	LEU	-	EXPRESSION TAG	UNP O22476
A	790	GLU	-	EXPRESSION TAG	UNP O22476
A	791	ASN	-	EXPRESSION TAG	UNP O22476
A	792	LEU	-	EXPRESSION TAG	UNP O22476
A	793	TYR	-	EXPRESSION TAG	UNP O22476
A	794	PHE	-	EXPRESSION TAG	UNP O22476
A	795	GLN	-	EXPRESSION TAG	UNP O22476
A	796	GLY	-	EXPRESSION TAG	UNP O22476
A	797	ALA	-	EXPRESSION TAG	UNP O22476
B	24	GLY	-	EXPRESSION TAG	UNP O22476
B	25	SER	-	EXPRESSION TAG	UNP O22476
B	26	SER	-	EXPRESSION TAG	UNP O22476
B	27	MET	-	EXPRESSION TAG	UNP O22476
B	28	GLY	-	EXPRESSION TAG	UNP O22476
B	643	GLU	GLY	ENGINEERED MUTATION	UNP O22476
B	789	LEU	-	EXPRESSION TAG	UNP O22476
B	790	GLU	-	EXPRESSION TAG	UNP O22476
B	791	ASN	-	EXPRESSION TAG	UNP O22476
B	792	LEU	-	EXPRESSION TAG	UNP O22476

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	793	TYR	-	EXPRESSION TAG	UNP O22476
B	794	PHE	-	EXPRESSION TAG	UNP O22476
B	795	GLN	-	EXPRESSION TAG	UNP O22476
B	796	GLY	-	EXPRESSION TAG	UNP O22476
B	797	ALA	-	EXPRESSION TAG	UNP O22476

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	185	Total	C	N	O	S	0	0	0
			1397	881	238	273	5			
2	D	185	Total	C	N	O	S	0	0	0
			1380	871	234	271	4			

There are 26 discrepancies between the modelled and reference sequences:

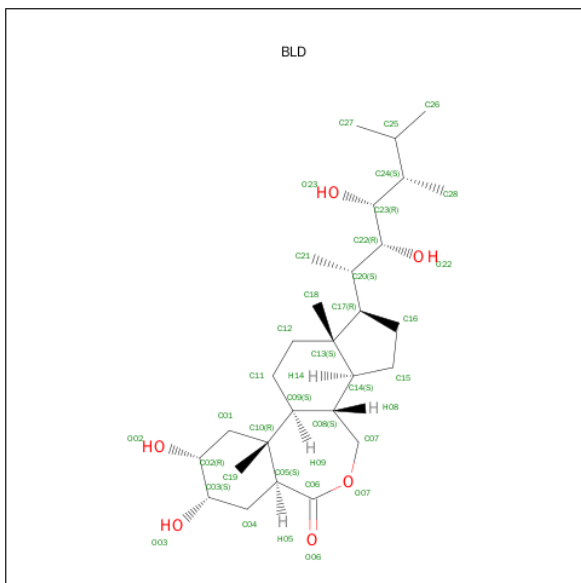
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	EXPRESSION TAG	UNP Q94AG2
C	21	SER	-	EXPRESSION TAG	UNP Q94AG2
C	22	SER	-	EXPRESSION TAG	UNP Q94AG2
C	23	MET	-	EXPRESSION TAG	UNP Q94AG2
C	214	LEU	-	EXPRESSION TAG	UNP Q94AG2
C	215	GLU	-	EXPRESSION TAG	UNP Q94AG2
C	216	ASN	-	EXPRESSION TAG	UNP Q94AG2
C	217	LEU	-	EXPRESSION TAG	UNP Q94AG2
C	218	TYR	-	EXPRESSION TAG	UNP Q94AG2
C	219	PHE	-	EXPRESSION TAG	UNP Q94AG2
C	220	GLN	-	EXPRESSION TAG	UNP Q94AG2
C	221	GLY	-	EXPRESSION TAG	UNP Q94AG2
C	222	ALA	-	EXPRESSION TAG	UNP Q94AG2
D	20	GLY	-	EXPRESSION TAG	UNP Q94AG2
D	21	SER	-	EXPRESSION TAG	UNP Q94AG2
D	22	SER	-	EXPRESSION TAG	UNP Q94AG2
D	23	MET	-	EXPRESSION TAG	UNP Q94AG2
D	214	LEU	-	EXPRESSION TAG	UNP Q94AG2
D	215	GLU	-	EXPRESSION TAG	UNP Q94AG2
D	216	ASN	-	EXPRESSION TAG	UNP Q94AG2
D	217	LEU	-	EXPRESSION TAG	UNP Q94AG2
D	218	TYR	-	EXPRESSION TAG	UNP Q94AG2
D	219	PHE	-	EXPRESSION TAG	UNP Q94AG2
D	220	GLN	-	EXPRESSION TAG	UNP Q94AG2
D	221	GLY	-	EXPRESSION TAG	UNP Q94AG2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	222	ALA	-	EXPRESSION TAG	UNP Q94AG2

- Molecule 3 is BRASSINOLIDE (three-letter code: BLD) (formula: $C_{28}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	28	6		
3	B	1	Total	C	O	0	0
			34	28	6		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		
5	B	4	Total	C	N	O	0	0
			50	28	2	20		
5	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	5	Total	C	N	O	0	0
			61	34	2	25		

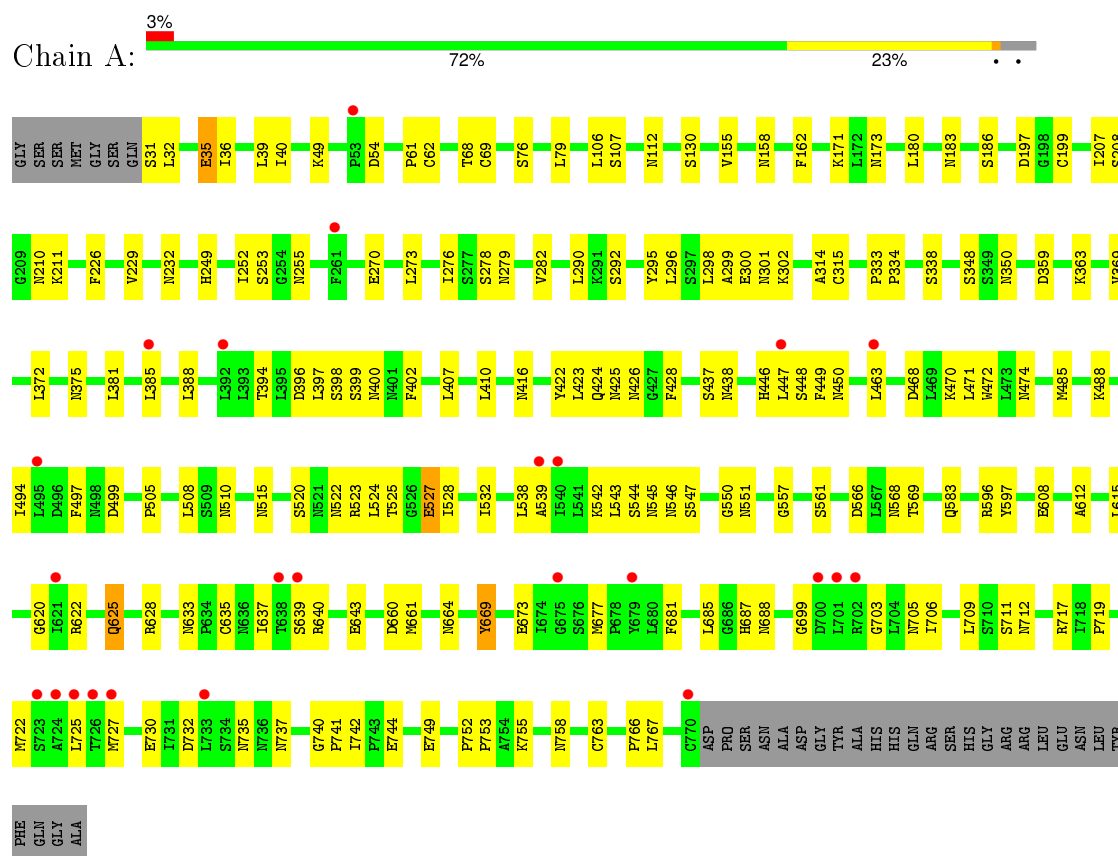
- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	3	Total	C	N	O	0	0
			39	22	2	15		

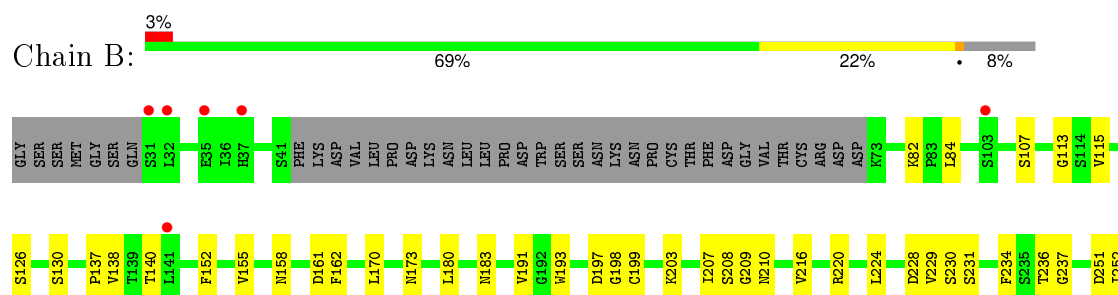
3 Residue-property plots

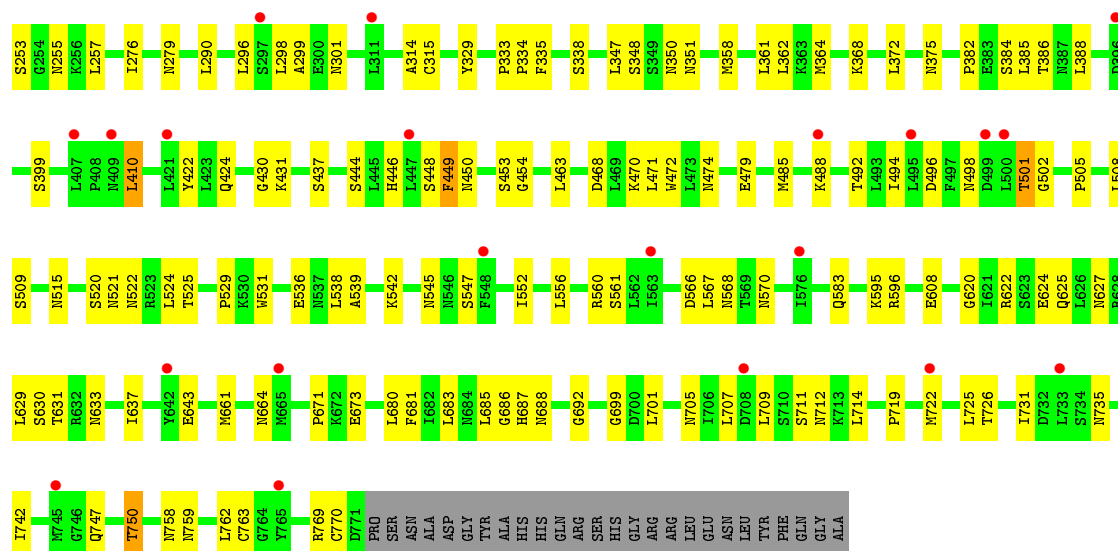
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

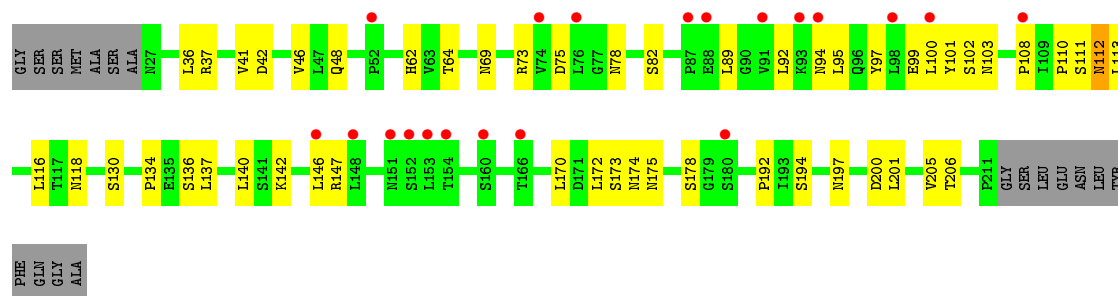


• Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1

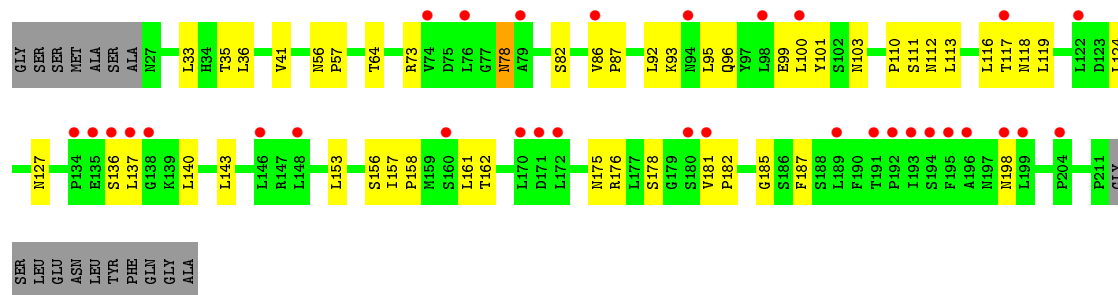




• Molecule 2: Somatic embryogenesis receptor kinase 1



• Molecule 2: Somatic embryogenesis receptor kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	69.90Å 69.90Å 873.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.53 – 3.30 48.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.53-3.30) 96.4 (48.53-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1334)	Depositor
R, R_{free}	0.246 , 0.285 0.243 , 0.282	Depositor DCC
R_{free} test set	1982 reflections (6.07%)	DCC
Wilson B-factor (Å ²)	85.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.7	EDS
Estimated twinning fraction	0.457 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 35233 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13920	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/5553	0.45	0/7543
1	B	0.22	0/5311	0.44	0/7218
2	C	0.25	0/1427	0.47	0/1959
2	D	0.24	0/1410	0.47	0/1940
All	All	0.23	0/13701	0.45	0/18660

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5454	0	5251	113	0
1	B	5217	0	5032	109	0
2	C	1397	0	1366	31	0
2	D	1380	0	1332	30	0
3	A	34	0	47	5	0
3	B	34	0	47	5	0
4	A	28	0	26	3	0
4	B	14	0	13	1	0
4	C	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	26	0	0
5	A	50	0	43	1	0
5	B	100	0	86	4	0
6	A	28	0	25	2	0
6	B	28	0	25	0	0
7	A	61	0	52	1	0
8	B	39	0	34	0	0
All	All	13920	0	13431	286	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 10.

All (286) 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:551:ASN:HD21	4:A:814:NAG:H82	1.39	0.86
1:A:290:LEU:HB3	1:A:314:ALA:HB2	1.71	0.73
2:C:64:THR:HB	2:C:73:ARG:HB2	1.72	0.72
2:D:140:LEU:HD12	2:D:143:LEU:HD22	1.72	0.71
1:B:198:GLY:HA2	1:B:220:ARG:HH12	1.56	0.71
2:C:94:ASN:HA	2:C:118:ASN:HD22	1.56	0.70
1:A:155:VAL:O	1:A:158:ASN:ND2	2.25	0.69
1:B:449:PHE:HE1	1:B:625:GLN:HB3	1.58	0.68
1:B:191:VAL:HG11	1:B:216:VAL:HG13	1.74	0.68
1:B:661:MET:O	1:B:664:ASN:ND2	2.26	0.67
1:A:685:LEU:O	1:A:688:ASN:ND2	2.27	0.67
1:B:347:LEU:O	1:B:350:ASN:ND2	2.28	0.67
1:B:290:LEU:HB3	1:B:314:ALA:HB2	1.77	0.67
7:A:811:BMA:H62	7:A:813:MAN:H2	1.77	0.67
1:A:633:ASN:ND2	1:A:635:CYS:SG	2.67	0.67
2:D:162:THR:HB	2:D:185:GLY:HA3	1.77	0.65
1:A:397:LEU:O	1:A:400:ASN:ND2	2.29	0.65
1:B:437:SER:HA	1:B:463:LEU:HD21	1.78	0.65
1:A:423:LEU:O	1:A:426:ASN:ND2	2.30	0.65
1:A:229:VAL:O	1:A:232:ASN:ND2	2.29	0.65
1:A:471:LEU:O	1:A:474:ASN:ND2	2.28	0.65
1:A:520:SER:O	1:A:522:ASN:ND2	2.30	0.64
1:A:687:HIS:HA	1:A:711:SER:HB2	1.79	0.64
1:A:753:PRO:HG3	1:A:766:PRO:HB2	1.78	0.64
1:A:468:ASP:HB3	1:A:470:LYS:HE3	1.79	0.63
1:B:685:LEU:O	1:B:688:ASN:ND2	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LEU:O	1:A:712:ASN:ND2	2.31	0.63
2:C:172:LEU:O	2:C:175:ASN:ND2	2.31	0.63
1:A:276:ILE:O	1:A:279:ASN:ND2	2.31	0.62
1:B:180:LEU:O	1:B:183:ASN:ND2	2.33	0.62
1:B:155:VAL:O	1:B:158:ASN:ND2	2.28	0.62
1:B:520:SER:O	1:B:522:ASN:ND2	2.31	0.62
1:A:35:GLU:O	1:A:39:LEU:HG	1.99	0.62
1:B:515:ASN:HA	1:B:538:LEU:HA	1.81	0.62
2:D:100:LEU:O	2:D:103:ASN:ND2	2.32	0.61
1:A:207:ILE:HG22	1:A:229:VAL:HA	1.81	0.61
1:A:661:MET:O	1:A:664:ASN:ND2	2.34	0.61
2:D:110:PRO:HB2	2:D:113:LEU:HG	1.82	0.61
1:A:472:TRP:HB3	1:A:494:ILE:HG22	1.83	0.60
1:A:551:ASN:ND2	4:A:814:NAG:H82	2.15	0.60
1:B:431:LYS:HG3	1:B:454:GLY:HA3	1.82	0.60
1:B:567:LEU:O	1:B:570:ASN:ND2	2.34	0.60
1:A:180:LEU:O	1:A:183:ASN:ND2	2.33	0.60
1:B:747:GLN:HG2	2:D:101:TYR:OH	2.01	0.60
1:B:471:LEU:O	1:B:474:ASN:ND2	2.35	0.60
2:D:157:ILE:HD12	2:D:181:VAL:HG22	1.84	0.60
1:B:207:ILE:O	1:B:210:ASN:ND2	2.34	0.60
1:A:545:ASN:HA	1:A:569:THR:HB	1.83	0.60
1:A:448:SER:O	1:A:450:ASN:ND2	2.34	0.60
1:A:543:LEU:O	1:A:546:ASN:ND2	2.34	0.60
1:A:299:ALA:O	1:A:301:ASN:ND2	2.35	0.59
2:C:73:ARG:HG2	2:C:97:TYR:HB2	1.84	0.59
2:C:36:LEU:HD22	2:C:89:LEU:HD21	1.83	0.59
3:A:801:BLD:O02	2:C:62:HIS:ND1	2.35	0.59
2:C:100:LEU:O	2:C:103:ASN:ND2	2.36	0.59
1:A:437:SER:HA	1:A:463:LEU:HD21	1.83	0.59
2:D:92:LEU:HD12	2:D:95:LEU:HD22	1.83	0.59
1:A:719:PRO:HG2	1:A:722:MET:HG3	1.85	0.58
1:A:735:ASN:OD1	1:A:758:ASN:ND2	2.35	0.58
1:B:424:GLN:HE21	1:B:620:GLY:HA3	1.69	0.58
1:A:399:SER:O	1:A:622:ARG:NH2	2.37	0.58
2:C:92:LEU:HD12	2:C:95:LEU:HD22	1.86	0.57
2:D:87:PRO:O	2:D:112:ASN:ND2	2.35	0.57
1:B:372:LEU:O	1:B:375:ASN:ND2	2.34	0.57
2:C:174:ASN:OD1	2:C:197:ASN:ND2	2.28	0.57
5:A:804:NAG:H83	5:A:804:NAG:H3	1.86	0.56
1:A:732:ASP:HA	1:A:755:LYS:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:PRO:HB2	2:C:113:LEU:HG	1.87	0.56
1:B:735:ASN:OD1	1:B:758:ASN:ND2	2.37	0.56
1:A:527:GLU:OE1	1:A:528:ILE:N	2.34	0.56
1:B:399:SER:O	1:B:622:ARG:NH2	2.39	0.56
5:B:804:NAG:H83	5:B:804:NAG:H3	1.86	0.55
1:A:252:ILE:O	1:A:255:ASN:ND2	2.36	0.55
1:B:315:CYS:SG	1:B:338:SER:OG	2.64	0.55
1:A:706:ILE:HG12	1:A:730:GLU:HB3	1.88	0.55
3:A:801:BLD:O02	2:C:62:HIS:N	2.38	0.55
2:D:99:GLU:HB3	2:D:101:TYR:CE2	2.42	0.55
1:A:253:SER:HB2	6:A:807:NAG:H62	1.89	0.55
1:B:472:TRP:HB3	1:B:494:ILE:HG22	1.89	0.55
2:D:153:LEU:HB2	2:D:175:ASN:HD21	1.71	0.55
1:B:750:THR:HG23	2:D:73:ARG:HH12	1.72	0.55
1:A:424:GLN:HE21	1:A:620:GLY:HA3	1.71	0.54
2:D:95:LEU:HD23	2:D:116:LEU:HD13	1.90	0.54
2:D:64:THR:HB	2:D:73:ARG:HB2	1.88	0.54
1:A:525:THR:HG22	1:A:547:SER:HB2	1.89	0.54
1:A:68:THR:HB	1:A:76:SER:HB3	1.90	0.54
1:B:208:SER:O	1:B:210:ASN:ND2	2.41	0.54
1:A:717:ARG:HG2	1:A:740:GLY:HA3	1.90	0.54
1:A:542:LYS:NZ	1:A:566:ASP:OD1	2.41	0.54
1:B:536:GLU:O	1:B:561:SER:OG	2.20	0.54
1:A:515:ASN:HA	1:A:538:LEU:HA	1.90	0.54
1:A:596:ARG:NH2	1:A:643:GLU:OE2	2.39	0.53
1:A:640:ARG:NH2	2:C:69:ASN:OD1	2.40	0.53
1:A:597:TYR:HB2	1:A:615:LEU:HD11	1.90	0.52
1:B:203:LYS:HA	1:B:224:LEU:HA	1.91	0.52
1:B:207:ILE:HD11	1:B:229:VAL:HG12	1.91	0.52
1:B:560:ARG:NH1	1:B:583:GLN:OE1	2.41	0.52
1:A:375:ASN:O	1:A:622:ARG:NH2	2.43	0.52
1:B:686:GLY:O	1:B:688:ASN:ND2	2.41	0.52
1:A:568:ASN:OD1	1:A:569:THR:N	2.42	0.52
1:B:680:LEU:HD21	1:B:683:LEU:HB2	1.91	0.52
1:B:596:ARG:NH2	1:B:643:GLU:OE2	2.42	0.52
1:B:448:SER:O	1:B:450:ASN:ND2	2.43	0.52
1:A:717:ARG:HE	1:A:741:PRO:HD2	1.75	0.52
1:B:681:PHE:CD2	3:B:801:BLD:H112	2.45	0.52
1:B:252:ILE:O	1:B:255:ASN:ND2	2.43	0.51
1:A:270:GLU:OE1	1:A:292:SER:OG	2.23	0.51
1:A:485:MET:O	1:A:488:LYS:NZ	2.32	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ASP:OD2	1:B:568:ASN:ND2	2.40	0.51
1:B:479:GLU:HG2	1:B:502:GLY:HA3	1.92	0.51
1:A:669:TYR:HD1	1:A:669:TYR:H	1.57	0.51
1:A:207:ILE:O	1:A:210:ASN:ND2	2.44	0.50
1:B:276:ILE:O	1:B:279:ASN:ND2	2.43	0.50
1:A:542:LYS:HG3	1:A:566:ASP:HB3	1.92	0.50
2:D:93:LYS:O	2:D:118:ASN:ND2	2.44	0.50
1:A:171:LYS:HA	1:A:197:ASP:HB2	1.93	0.50
1:B:348:SER:O	1:B:350:ASN:ND2	2.44	0.50
1:B:631:THR:O	5:B:811:NAG:O4	2.30	0.50
1:B:362:LEU:HD11	1:B:384:SER:HB2	1.92	0.50
2:D:41:VAL:HB	2:D:82:SER:HB3	1.93	0.50
1:B:505:PRO:HG2	1:B:508:LEU:HG	1.93	0.50
1:B:299:ALA:O	1:B:301:ASN:ND2	2.45	0.50
1:B:422:TYR:HE1	1:B:444:SER:HG	1.59	0.50
1:A:744:GLU:OE1	1:A:744:GLU:N	2.40	0.50
1:B:333:PRO:HB2	1:B:335:PHE:CD2	2.47	0.50
1:A:295:TYR:CZ	6:A:807:NAG:H82	2.47	0.50
1:B:138:VAL:N	1:B:161:ASP:O	2.45	0.49
1:A:226:PHE:HA	1:A:249:HIS:HB3	1.94	0.49
1:B:173:ASN:ND2	1:B:197:ASP:OD1	2.45	0.49
2:C:192:PRO:HG3	2:C:205:VAL:O	2.11	0.49
1:A:416:ASN:ND2	1:A:438:ASN:O	2.45	0.49
1:B:629:LEU:O	1:B:633:ASN:N	2.45	0.49
1:B:742:ILE:N	1:B:763:CYS:O	2.42	0.49
1:A:699:GLY:HA2	1:A:725:LEU:HD21	1.94	0.49
1:A:208:SER:O	1:A:210:ASN:ND2	2.45	0.49
1:A:488:LYS:HZ2	1:A:510:ASN:HB3	1.78	0.49
1:A:425:ASN:H	1:A:449:PHE:HB3	1.78	0.49
1:A:639:SER:HB3	1:A:640:ARG:HB2	1.94	0.49
1:A:673:GLU:N	1:A:673:GLU:OE1	2.46	0.49
2:C:41:VAL:HB	2:C:82:SER:HB2	1.94	0.49
1:A:557:GLY:O	1:A:583:GLN:HB2	2.13	0.49
1:A:278:SER:H	1:A:300:GLU:HB2	1.78	0.49
2:C:118:ASN:HA	2:C:142:LYS:HD2	1.94	0.48
1:B:329:TYR:HB3	1:B:351:ASN:HB3	1.94	0.48
1:A:385:LEU:HD12	1:A:388:LEU:HD12	1.94	0.48
1:B:358:MET:HG3	1:B:382:PRO:HB2	1.95	0.48
1:A:539:ALA:HA	1:A:561:SER:O	2.13	0.48
1:B:296:LEU:HD11	1:B:298:LEU:HD13	1.95	0.48
1:B:542:LYS:NZ	1:B:566:ASP:OD1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:THR:HG22	1:B:502:GLY:H	1.78	0.48
2:C:146:LEU:O	2:C:170:LEU:HA	2.14	0.48
2:C:178:SER:HA	2:C:200:ASP:O	2.13	0.48
1:B:709:LEU:O	1:B:712:ASN:ND2	2.45	0.48
1:B:335:PHE:O	1:B:338:SER:OG	2.22	0.48
1:A:348:SER:O	1:A:350:ASN:ND2	2.47	0.48
1:A:173:ASN:ND2	1:A:197:ASP:OD1	2.47	0.47
1:A:742:ILE:N	1:A:763:CYS:O	2.45	0.47
2:C:78:ASN:HD22	2:C:102:SER:HB3	1.79	0.47
2:C:99:GLU:HB3	2:C:101:TYR:CE2	2.50	0.47
1:A:372:LEU:O	1:A:375:ASN:ND2	2.41	0.47
1:A:315:CYS:SG	1:A:338:SER:OG	2.71	0.47
1:A:527:GLU:HG2	1:A:550:GLY:HA3	1.97	0.47
1:B:209:GLY:H	1:B:231:SER:HB2	1.80	0.47
1:A:449:PHE:HE1	1:A:625:GLN:HB3	1.80	0.47
2:C:112:ASN:HD22	2:C:112:ASN:H	1.61	0.47
1:B:385:LEU:HD12	1:B:388:LEU:HD12	1.95	0.47
1:A:608:GLU:OE1	1:A:608:GLU:N	2.48	0.47
1:B:692:GLY:H	1:B:714:LEU:HA	1.80	0.46
1:B:525:THR:HG22	1:B:547:SER:HB2	1.96	0.46
1:A:36:ILE:O	1:A:40:ILE:HG12	2.15	0.46
1:B:386:THR:HG22	1:B:410:LEU:HA	1.97	0.46
1:B:687:HIS:HA	1:B:711:SER:HB2	1.96	0.46
1:A:664:ASN:N	1:A:688:ASN:OD1	2.46	0.46
1:A:752:PRO:HA	1:A:753:PRO:HD3	1.85	0.46
2:C:173:SER:N	2:C:194:SER:O	2.48	0.46
1:A:62:CYS:HB3	1:A:69:CYS:HB3	1.91	0.46
1:A:447:LEU:O	1:A:450:ASN:ND2	2.41	0.46
1:A:186:SER:HA	1:A:211:LYS:O	2.14	0.46
1:B:449:PHE:CE1	1:B:625:GLN:HB3	2.45	0.46
1:B:468:ASP:HB3	1:B:470:LYS:HE3	1.98	0.46
2:C:62:HIS:HB3	2:C:75:ASP:O	2.15	0.46
2:D:35:THR:HG22	2:D:86:VAL:HG11	1.98	0.46
1:B:759:ASN:HB3	1:B:762:LEU:HB2	1.99	0.45
1:B:333:PRO:HA	1:B:334:PRO:HD3	1.81	0.45
1:B:681:PHE:HD2	3:B:801:BLD:H112	1.81	0.45
2:C:42:ASP:OD2	2:C:46:VAL:N	2.50	0.45
1:B:236:THR:OG1	1:B:237:GLY:N	2.47	0.45
2:C:134:PRO:HB2	2:C:137:LEU:HG	1.98	0.45
1:A:722:MET:O	1:A:725:LEU:HG	2.17	0.45
2:D:182:PRO:HG2	2:D:187:PHE:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:THR:OG1	2:D:118:ASN:ND2	2.50	0.45
1:A:333:PRO:HA	1:A:334:PRO:HD3	1.75	0.45
2:D:124:LEU:O	2:D:127:ASN:ND2	2.50	0.45
1:A:249:HIS:NE2	1:A:273:LEU:HD22	2.32	0.45
1:A:402:PHE:HB3	1:A:428:PHE:CE1	2.52	0.45
1:B:529:PRO:HB3	1:B:531:TRP:CE2	2.53	0.44
1:B:552:ILE:HG23	1:B:556:LEU:HD12	1.99	0.44
2:D:56:ASN:HB2	2:D:57:PRO:HD2	1.99	0.44
2:D:111:SER:O	2:D:136:SER:OG	2.25	0.44
3:A:801:BLD:H328	3:A:801:BLD:H22	1.70	0.44
1:B:539:ALA:HA	1:B:561:SER:O	2.18	0.44
1:A:499:ASP:OD1	1:A:523:ARG:NH2	2.50	0.44
2:D:137:LEU:O	2:D:140:LEU:HG	2.18	0.44
1:B:705:ASN:ND2	3:B:801:BLD:H101	2.32	0.44
2:D:175:ASN:O	2:D:198:ASN:HA	2.16	0.44
1:A:107:SER:HA	1:A:130:SER:O	2.18	0.44
1:A:36:ILE:HB	1:A:61:PRO:HG3	2.00	0.44
2:C:116:LEU:O	2:C:140:LEU:HD22	2.18	0.44
1:B:673:GLU:OE1	1:B:673:GLU:N	2.49	0.44
1:B:430:GLY:O	1:B:453:SER:N	2.49	0.44
1:A:396:ASP:OD1	1:A:398:SER:OG	2.23	0.44
1:B:126:SER:HA	1:B:152:PHE:HB3	2.00	0.43
2:C:137:LEU:O	2:C:140:LEU:HG	2.17	0.43
1:B:255:ASN:O	1:B:279:ASN:HA	2.18	0.43
1:A:505:PRO:HG2	1:A:508:LEU:HG	2.00	0.43
2:D:116:LEU:O	2:D:140:LEU:HD22	2.19	0.43
1:B:113:GLY:HA2	4:B:802:NAG:H82	1.99	0.43
3:A:801:BLD:H23	3:A:801:BLD:H121	1.79	0.43
1:B:726:THR:OG1	2:D:78:ASN:HB2	2.18	0.43
1:B:276:ILE:HD11	1:B:298:LEU:HG	2.01	0.43
2:D:96:GLN:HA	2:D:119:LEU:HA	1.99	0.43
1:A:753:PRO:HB3	1:A:767:LEU:HD23	2.00	0.43
2:C:111:SER:O	2:C:136:SER:OG	2.27	0.43
1:B:498:ASN:H	1:B:522:ASN:ND2	2.16	0.43
2:D:175:ASN:OD1	2:D:176:ARG:N	2.42	0.43
1:B:361:LEU:HD23	1:B:364:MET:HE3	2.01	0.43
1:A:681:PHE:O	1:A:705:ASN:N	2.43	0.43
1:A:749:GLU:CD	2:C:147:ARG:HH12	2.22	0.43
1:B:624:GLU:O	1:B:627:ASN:ND2	2.52	0.42
1:B:130:SER:HB2	5:B:803:NAG:H62	2.02	0.42
1:A:705:ASN:HA	1:A:727:MET:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG13	1:A:394:THR:HB	2.01	0.42
1:A:449:PHE:CE1	1:A:625:GLN:HB3	2.54	0.42
1:B:630:SER:HB2	5:B:813:MAN:H62	2.00	0.42
1:B:699:GLY:HA2	1:B:725:LEU:HD21	2.02	0.42
1:A:296:LEU:HD11	1:A:298:LEU:HD13	2.00	0.42
1:B:251:ASP:OD1	1:B:253:SER:OG	2.23	0.42
1:A:612:ALA:N	1:A:660:ASP:OD2	2.30	0.42
2:C:108:PRO:HA	2:C:130:SER:O	2.20	0.42
1:B:498:ASN:H	1:B:522:ASN:HD21	1.67	0.42
2:D:156:SER:HA	2:D:178:SER:O	2.20	0.42
1:B:707:LEU:O	1:B:731:ILE:HA	2.20	0.42
3:B:801:BLD:H23	3:B:801:BLD:H121	1.69	0.42
1:A:677:MET:HE3	1:A:677:MET:HB2	1.94	0.42
1:B:170:LEU:N	1:B:193:TRP:O	2.50	0.42
1:B:769:ARG:HG2	1:B:770:CYS:N	2.35	0.42
1:A:422:TYR:HD1	1:A:446:HIS:HB2	1.85	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.82	0.41
1:B:521:ASN:HA	1:B:545:ASN:HB3	2.01	0.41
1:A:449:PHE:CE1	1:A:628:ARG:HD2	2.55	0.41
1:B:229:VAL:HG23	1:B:252:ILE:HA	2.02	0.41
1:A:381:LEU:HB2	1:A:407:LEU:HD21	2.02	0.41
1:A:359:ASP:O	1:A:363:LYS:HG2	2.21	0.41
1:A:544:SER:O	1:A:546:ASN:ND2	2.53	0.41
1:B:485:MET:O	1:B:488:LYS:NZ	2.43	0.41
1:B:719:PRO:HG2	1:B:722:MET:HG3	2.02	0.41
1:B:234:PHE:HB3	1:B:257:LEU:HD21	2.03	0.41
1:A:688:ASN:HB2	1:A:712:ASN:OD1	2.21	0.41
1:B:496:ASP:HA	1:B:520:SER:H	1.86	0.41
1:B:333:PRO:HB2	1:B:335:PHE:CE2	2.55	0.41
1:B:671:PRO:HB2	1:B:673:GLU:OE1	2.21	0.41
1:B:137:PRO:HG2	1:B:140:THR:HG23	2.03	0.41
1:B:492:THR:HG21	1:B:595:LYS:HE3	2.03	0.41
1:B:228:ASP:OD1	1:B:230:SER:OG	2.23	0.41
1:A:375:ASN:O	1:A:400:ASN:HA	2.21	0.41
1:B:470:LYS:HG2	1:B:494:ILE:HG12	2.03	0.41
3:B:801:BLD:H115	3:B:801:BLD:H207	1.93	0.41
1:A:681:PHE:HA	1:A:703:GLY:O	2.21	0.41
1:B:115:VAL:HB	1:B:140:THR:HB	2.03	0.41
1:A:31:SER:OG	1:A:32:LEU:N	2.54	0.41
2:D:158:PRO:HB2	2:D:161:LEU:HG	2.03	0.41
1:A:737:ASN:O	1:A:737:ASN:ND2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:HG12	1:A:302:LYS:HB2	2.02	0.41
3:A:801:BLD:H115	3:A:801:BLD:H207	1.89	0.40
2:C:201:LEU:HB3	2:C:206:THR:HG21	2.02	0.40
1:A:497:PHE:N	1:A:520:SER:O	2.44	0.40
1:B:542:LYS:HG3	1:B:566:ASP:HB3	2.03	0.40
1:B:701:LEU:O	1:B:725:LEU:HD22	2.21	0.40
1:B:368:LYS:HA	1:B:368:LYS:HD3	1.81	0.40
2:D:33:LEU:O	2:D:36:LEU:HB3	2.21	0.40
1:B:82:LYS:O	1:B:84:LEU:N	2.51	0.40
1:A:112:ASN:HD22	4:A:802:NAG:C7	2.33	0.40
2:C:37:ARG:NH2	2:C:48:GLN:HA	2.36	0.40
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.89	0.40
1:B:509:SER:HB3	1:B:531:TRP:CD2	2.56	0.40
1:B:608:GLU:OE1	1:B:608:GLU:N	2.55	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	738/774 (95%)	710 (96%)	27 (4%)	1 (0%)	56	89
1	B	706/774 (91%)	680 (96%)	25 (4%)	1 (0%)	56	89
2	C	183/203 (90%)	176 (96%)	7 (4%)	0	100	100
2	D	183/203 (90%)	177 (97%)	6 (3%)	0	100	100
All	All	1810/1954 (93%)	1743 (96%)	65 (4%)	2 (0%)	56	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	637	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	637	ILE

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	611/680 (90%)	600 (98%)	11 (2%)	66	85
1	B	580/680 (85%)	571 (98%)	9 (2%)	70	87
2	C	165/182 (91%)	164 (99%)	1 (1%)	90	95
2	D	161/182 (88%)	160 (99%)	1 (1%)	90	95
All	All	1517/1724 (88%)	1495 (98%)	22 (2%)	72	88

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	49	LYS
1	A	54	ASP
1	A	162	PHE
1	A	199	CYS
1	A	410	LEU
1	A	524	LEU
1	A	527	GLU
1	A	532	ILE
1	A	625	GLN
1	A	669	TYR
1	B	107	SER
1	B	162	PHE
1	B	199	CYS
1	B	410	LEU
1	B	446	HIS
1	B	449	PHE
1	B	501	THR
1	B	524	LEU
1	B	750	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	112	ASN
2	D	78	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	551	ASN
1	B	705	ASN
2	C	78	ASN
2	C	112	ASN
2	D	94	ASN
2	D	118	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 ⓘ

24 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	$\# Z > 2$
5	NAG	A	803	1,5	14,14,15	0.25	0	15,19,21	0.39	0
5	NAG	A	804	5	14,14,15	0.46	0	15,19,21	1.30	1 (6%)
5	BMA	A	805	5	11,11,12	0.69	0	14,15,17	1.01	1 (7%)
5	MAN	A	806	5	11,11,12	0.71	0	14,15,17	0.98	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	807	1,6	14,14,15	0.34	0	15,19,21	0.42	0
6	NAG	A	808	6	14,14,15	0.39	0	15,19,21	0.65	1 (6%)
7	NAG	A	809	1,7	14,14,15	0.29	0	15,19,21	0.32	0
7	NAG	A	810	7	14,14,15	0.21	0	15,19,21	0.23	0
7	BMA	A	811	7	11,11,12	0.97	1 (9%)	14,15,17	0.91	0
7	MAN	A	812	7	11,11,12	0.71	0	14,15,17	1.00	2 (14%)
7	MAN	A	813	7	11,11,12	0.76	0	14,15,17	1.76	4 (28%)
5	NAG	B	803	1,5	14,14,15	0.31	0	15,19,21	0.33	0
5	NAG	B	804	5	14,14,15	0.47	0	15,19,21	1.30	1 (6%)
5	BMA	B	805	5	11,11,12	0.62	0	14,15,17	0.97	1 (7%)
5	MAN	B	806	5	11,11,12	0.75	0	14,15,17	1.02	2 (14%)
8	NAG	B	807	1,8	14,14,15	0.62	1 (7%)	15,19,21	0.49	0
8	NAG	B	808	8	14,14,15	0.64	1 (7%)	15,19,21	0.54	0
8	BMA	B	809	8	11,11,12	0.62	0	14,15,17	1.07	2 (14%)
5	NAG	B	810	1,5	14,14,15	0.22	0	15,19,21	0.40	0
5	NAG	B	811	5	14,14,15	0.49	0	15,19,21	0.37	0
5	BMA	B	812	5	11,11,12	1.34	3 (27%)	14,15,17	1.55	3 (21%)
5	MAN	B	813	5	11,11,12	0.79	1 (9%)	14,15,17	1.08	2 (14%)
6	NAG	B	814	1,6	14,14,15	0.40	0	15,19,21	0.28	0
6	NAG	B	815	6	14,14,15	0.23	0	15,19,21	0.29	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
5	NAG	A	803	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	804	5	-	0/6/23/26	0/1/1/1
5	BMA	A	805	5	-	0/2/19/22	0/1/1/1
5	MAN	A	806	5	-	0/2/19/22	0/1/1/1
6	NAG	A	807	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	808	6	-	0/6/23/26	0/1/1/1
7	NAG	A	809	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	810	7	-	0/6/23/26	0/1/1/1
7	BMA	A	811	7	-	0/2/19/22	0/1/1/1
7	MAN	A	812	7	-	0/2/19/22	0/1/1/1
7	MAN	A	813	7	-	0/2/19/22	0/1/1/1
5	NAG	B	803	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	804	5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	B	805	5	-	0/2/19/22	0/1/1/1
5	MAN	B	806	5	-	0/2/19/22	0/1/1/1
8	NAG	B	807	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	808	8	-	0/6/23/26	0/1/1/1
8	BMA	B	809	8	-	0/2/19/22	0/1/1/1
5	NAG	B	810	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	811	5	-	0/6/23/26	0/1/1/1
5	BMA	B	812	5	-	0/2/19/22	0/1/1/1
5	MAN	B	813	5	-	0/2/19/22	0/1/1/1
6	NAG	B	814	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	815	6	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	812	BMA	O5-C1	-2.92	1.38	1.43
8	B	808	NAG	O5-C1	-2.24	1.40	1.43
8	B	807	NAG	O5-C1	-2.20	1.40	1.43
5	B	813	MAN	O5-C1	-2.17	1.40	1.43
7	A	811	BMA	C2-C3	2.01	1.55	1.52
5	B	812	BMA	C4-C3	2.14	1.58	1.52
5	B	812	BMA	C2-C3	2.28	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	809	BMA	O2-C2-C3	-2.42	105.25	110.12
8	B	809	BMA	C1-C2-C3	-2.36	106.75	109.54
5	B	806	MAN	O2-C2-C3	-2.30	105.48	110.12
7	A	813	MAN	O2-C2-C3	-2.30	105.49	110.12
5	B	813	MAN	O2-C2-C3	-2.26	105.57	110.12
7	A	812	MAN	O2-C2-C3	-2.16	105.78	110.12
5	A	806	MAN	O2-C2-C3	-2.15	105.79	110.12
5	A	805	BMA	C1-C2-C3	2.00	111.91	109.54
5	A	806	MAN	C1-O5-C5	2.10	114.91	112.25
5	B	805	BMA	C1-C2-C3	2.11	112.04	109.54
7	A	812	MAN	C1-O5-C5	2.16	115.00	112.25
5	B	806	MAN	C1-O5-C5	2.17	115.00	112.25
5	B	812	BMA	C1-C2-C3	2.18	112.12	109.54
5	B	813	MAN	C1-O5-C5	2.30	115.17	112.25
6	A	808	NAG	C1-O5-C5	2.49	115.41	112.25
7	A	813	MAN	O5-C1-C2	2.74	115.30	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	812	BMA	C3-C4-C5	2.92	115.28	110.20
7	A	813	MAN	C1-C2-C3	3.03	113.12	109.54
5	B	812	BMA	C2-C3-C4	3.91	117.69	111.04
7	A	813	MAN	C1-O5-C5	4.17	117.54	112.25
5	B	804	NAG	C2-N2-C7	4.73	129.12	123.04
5	A	804	NAG	C2-N2-C7	4.74	129.13	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	NAG	1	0
6	A	807	NAG	2	0
7	A	811	BMA	1	0
7	A	813	MAN	1	0
5	B	803	NAG	1	0
5	B	804	NAG	1	0
5	B	811	NAG	1	0
5	B	813	MAN	1	0

5.6 Ligand geometry ⓘ

9 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	BLD	A	801	-	36,37,37	3.10	13 (36%)	45,59,59	1.91	12 (26%)
4	NAG	A	802	1	14,14,15	0.35	0	15,19,21	0.48	0
4	NAG	A	814	1	14,14,15	0.57	0	15,19,21	1.21	1 (6%)
3	BLD	B	801	-	36,37,37	3.08	12 (33%)	45,59,59	1.79	10 (22%)
4	NAG	B	802	1	14,14,15	0.23	0	15,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1000	2	14,14,15	1.07	1 (7%)	15,19,21	0.58	0
4	NAG	C	1001	2	14,14,15	0.19	0	15,19,21	0.37	0
4	NAG	D	1001	2	14,14,15	0.36	0	15,19,21	0.31	0
4	NAG	D	1002	2	14,14,15	1.75	1 (7%)	15,19,21	1.44	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BLD	A	801	-	-	0/20/85/85	0/4/4/4
4	NAG	A	802	1	-	0/6/23/26	0/1/1/1
4	NAG	A	814	1	-	0/6/23/26	0/1/1/1
3	BLD	B	801	-	-	0/20/85/85	0/4/4/4
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1000	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1002	2	-	0/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	BLD	O07-C07	-11.30	1.30	1.45
3	B	801	BLD	O07-C07	-11.13	1.30	1.45
3	B	801	BLD	C15-C14	-4.70	1.43	1.54
3	A	801	BLD	C15-C14	-4.67	1.43	1.54
3	A	801	BLD	C20-C17	-3.23	1.49	1.54
3	B	801	BLD	O22-C22	-3.16	1.35	1.43
3	A	801	BLD	O22-C22	-3.11	1.35	1.43
3	B	801	BLD	C20-C17	-3.06	1.49	1.54
3	A	801	BLD	C28-C24	-2.71	1.47	1.53
3	B	801	BLD	C28-C24	-2.69	1.47	1.53
3	B	801	BLD	C13-C14	-2.22	1.50	1.55
3	A	801	BLD	C13-C14	-2.13	1.50	1.55
3	A	801	BLD	C07-C08	-2.06	1.50	1.52
3	A	801	BLD	O07-C06	-2.03	1.32	1.34
3	B	801	BLD	O07-C06	-2.02	1.32	1.34
3	A	801	BLD	C08-C14	2.13	1.57	1.53
3	B	801	BLD	C08-C14	2.30	1.58	1.53
3	A	801	BLD	C15-C16	2.50	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	BLD	C15-C16	2.56	1.61	1.54
3	A	801	BLD	C19-C10	3.20	1.60	1.54
3	B	801	BLD	C19-C10	3.21	1.60	1.54
4	C	1000	NAG	O5-C1	3.43	1.49	1.43
3	B	801	BLD	C11-C09	4.52	1.61	1.53
3	A	801	BLD	C11-C09	4.66	1.62	1.53
4	D	1002	NAG	C1-C2	6.16	1.61	1.52
3	A	801	BLD	O06-C06	9.81	1.46	1.21
3	B	801	BLD	O06-C06	9.90	1.46	1.21

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	BLD	C15-C14-C08	-5.48	110.37	119.03
3	B	801	BLD	C15-C14-C08	-5.24	110.74	119.03
3	A	801	BLD	O07-C06-O06	-4.72	108.67	116.53
3	B	801	BLD	O07-C06-O06	-4.49	109.07	116.53
3	A	801	BLD	C17-C20-C22	-3.42	105.47	111.24
3	B	801	BLD	C11-C09-C08	-3.15	107.17	111.74
3	A	801	BLD	C11-C09-C08	-3.08	107.27	111.74
3	A	801	BLD	C16-C17-C20	-2.64	108.97	112.59
3	A	801	BLD	C16-C15-C14	-2.54	100.02	105.12
3	A	801	BLD	C14-C08-C09	-2.40	105.90	109.06
3	B	801	BLD	C17-C20-C22	-2.34	107.29	111.24
3	B	801	BLD	C16-C17-C20	-2.32	109.42	112.59
3	B	801	BLD	C16-C15-C14	-2.29	100.51	105.12
3	A	801	BLD	C24-C23-C22	-2.11	109.93	114.87
3	B	801	BLD	C14-C08-C09	-2.09	106.31	109.06
3	A	801	BLD	C28-C24-C25	-2.06	108.76	112.45
3	B	801	BLD	C21-C20-C22	-2.01	107.09	111.24
3	B	801	BLD	C12-C13-C17	2.24	120.54	116.56
3	A	801	BLD	C12-C13-C14	2.32	111.08	107.31
3	A	801	BLD	C12-C13-C17	2.44	120.89	116.56
4	A	814	NAG	C1-O5-C5	3.72	116.97	112.25
4	D	1002	NAG	C2-N2-C7	4.03	128.21	123.04
3	A	801	BLD	C01-C10-C05	4.91	114.83	107.16
3	B	801	BLD	C01-C10-C05	5.16	115.22	107.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	BLD	5	0
4	A	802	NAG	1	0
4	A	814	NAG	2	0
3	B	801	BLD	5	0
4	B	802	NAG	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	740/774 (95%)	0.06	24 (3%)	51	44	47, 114, 169, 224	0
1	B	710/774 (91%)	0.07	27 (3%)	44	37	57, 115, 166, 222	0
2	C	185/203 (91%)	0.44	20 (10%)	8	6	88, 145, 192, 210	0
2	D	185/203 (91%)	0.77	32 (17%)	2	2	105, 146, 225, 259	0
All	All	1820/1954 (93%)	0.18	103 (5%)	27	22	47, 121, 183, 259	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	726	THR	8.3
2	D	192	PRO	6.8
2	D	138	GLY	6.6
2	D	137	LEU	6.6
2	D	98	LEU	6.5
2	D	196	ALA	6.2
1	A	723	SER	6.0
2	D	146	LEU	5.9
2	D	195	PHE	5.5
1	B	31	SER	4.9
1	B	500	LEU	4.8
1	A	725	LEU	4.8
2	C	87	PRO	4.5
2	D	74	VAL	4.4
2	D	135	GLU	4.4
2	D	79	ALA	4.3
2	D	189	LEU	4.3
2	D	76	LEU	4.3
1	A	702	ARG	4.2
1	A	724	ALA	4.2
2	C	98	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	76	LEU	4.2
1	A	675	GLY	4.1
1	A	733	LEU	4.1
2	C	74	VAL	4.0
2	D	172	LEU	4.0
2	C	180	SER	3.9
2	D	100	LEU	3.8
2	D	148	LEU	3.8
2	D	94	ASN	3.7
2	D	198	ASN	3.7
2	D	194	SER	3.7
1	A	539	ALA	3.6
1	A	463	LEU	3.5
1	A	53	PRO	3.5
2	D	122	LEU	3.5
2	D	199	LEU	3.4
2	D	134	PRO	3.4
2	C	153	LEU	3.3
1	A	701	LEU	3.3
2	D	136	SER	3.3
2	D	171	ASP	3.2
2	C	146	LEU	3.2
1	B	103	SER	3.1
2	C	108	PRO	2.9
1	A	621	ILE	2.9
2	C	160	SER	2.9
1	B	733	LEU	2.9
2	C	152	SER	2.9
2	C	148	LEU	2.9
1	B	765	TYR	2.9
2	D	204	PRO	2.8
2	C	91	VAL	2.8
1	A	638	THR	2.7
1	A	679	TYR	2.7
1	B	35	GLU	2.7
2	C	154	THR	2.7
2	D	117	THR	2.7
2	D	191	THR	2.7
1	B	447	LEU	2.7
1	B	311	LEU	2.6
2	D	160	SER	2.6
1	A	540	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	181	VAL	2.6
2	C	100	LEU	2.6
1	B	642	TYR	2.6
1	B	409	ASN	2.6
2	C	94	ASN	2.6
2	D	180	SER	2.6
1	A	392	LEU	2.5
1	B	708	ASP	2.5
2	C	88	GLU	2.5
1	B	722	MET	2.5
2	C	93	LYS	2.4
1	A	639	SER	2.4
1	A	727	MET	2.4
1	A	495	LEU	2.4
1	B	396	ASP	2.3
1	B	297	SER	2.3
2	C	52	PRO	2.3
1	B	488	LYS	2.3
1	A	261	PHE	2.3
1	B	37	HIS	2.3
2	D	86	VAL	2.3
2	D	170	LEU	2.2
1	B	499	ASP	2.2
1	B	745	MET	2.2
1	A	700	ASP	2.2
1	B	141	LEU	2.2
2	C	166	THR	2.2
1	B	407	LEU	2.2
1	B	548	PHE	2.2
1	A	447	LEU	2.2
1	B	563	ILE	2.1
1	A	385	LEU	2.1
1	B	421	LEU	2.1
2	D	193	ILE	2.1
1	A	770	CYS	2.1
1	B	32	LEU	2.1
1	B	495	LEU	2.1
1	B	665	MET	2.1
1	B	576	ILE	2.0
2	C	151	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	A	807	14/15	0.92	0.26	2.21	92,102,111,111	0
7	NAG	A	809	14/15	0.90	0.24	0.34	111,121,148,149	0
5	NAG	B	803	14/15	0.92	0.21	-0.25	110,124,137,137	0
8	NAG	B	807	14/15	0.93	0.17	-0.40	72,85,96,100	0
5	NAG	B	810	14/15	0.83	0.19	-0.46	86,99,107,109	0
5	NAG	A	803	14/15	0.95	0.17	-0.68	48,61,73,95	0
5	NAG	B	811	14/15	0.93	0.16	-1.06	98,120,128,130	0
7	NAG	A	810	14/15	0.93	0.15	-1.62	88,102,106,111	0
8	NAG	B	808	14/15	0.93	0.13	-	93,114,124,132	0
6	NAG	A	808	14/15	0.88	0.17	-	107,112,122,127	0
5	BMA	A	805	11/12	0.89	0.13	-	77,110,116,116	0
5	NAG	A	804	14/15	0.94	0.12	-	108,114,118,120	0
8	BMA	B	809	11/12	0.81	0.19	-	136,138,139,143	0
6	NAG	B	815	14/15	0.93	0.26	-	72,85,107,107	0
5	BMA	B	805	11/12	0.79	0.18	-	125,136,149,156	0
5	MAN	B	813	11/12	0.95	0.13	-	84,92,96,99	0
5	MAN	A	806	11/12	0.90	0.13	-	83,104,121,128	0
7	MAN	A	812	11/12	0.87	0.17	-	128,135,139,143	0
5	MAN	B	806	11/12	0.77	0.27	-	150,157,165,169	0
7	BMA	A	811	11/12	0.91	0.13	-	101,118,146,149	0
5	NAG	B	804	14/15	0.93	0.19	-	109,116,136,136	0
6	NAG	B	814	14/15	0.85	0.20	-	93,107,121,122	0
7	MAN	A	813	11/12	0.87	0.21	-	76,87,117,130	0
5	BMA	B	812	11/12	0.85	0.16	-	98,131,145,150	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(\AA^2)	Q<0.9
3	BLD	B	801	34/34	0.90	0.42	1.50	85,127,138,149	0
3	BLD	A	801	34/34	0.94	0.22	-0.73	61,109,134,140	0
4	NAG	D	1002	14/15	0.91	0.12	-	81,98,108,109	0
4	NAG	B	802	14/15	0.86	0.17	-	96,105,113,114	0
4	NAG	A	802	14/15	0.64	0.41	-	138,158,174,175	0
4	NAG	C	1001	14/15	0.84	0.18	-	77,91,108,109	0
4	NAG	C	1000	14/15	0.90	0.19	-	96,99,105,106	0
4	NAG	A	814	14/15	0.79	0.20	-	88,94,101,103	0
4	NAG	D	1001	14/15	0.85	0.20	-	102,115,132,134	0

6.5 Other polymers

There are no such residues in this entry.