



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:29 PM BST

PDB ID : 3L95
Title : Crystal structure of the human Notch1 Negative Regulatory Region (NRR)
bound to the fab fragment of an antagonist antibody
Authors : Hymowitz, S.G.; de Leon, G.P.
Deposited on : 2010-01-04
Resolution : 2.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

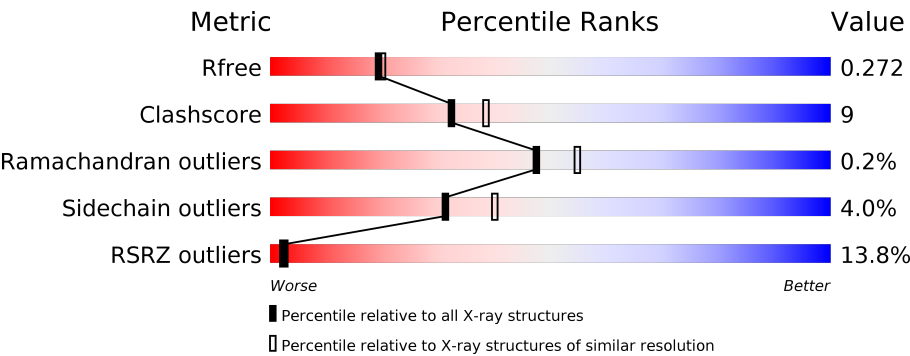
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>79%</div><div>17%</div><div>..</div></div>
1	L	214	<div><div>32%</div><div><div></div><div></div><div></div><div></div></div><div>76%</div><div>22%</div><div>..</div></div>
2	B	227	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>89%</div><div>8%</div><div>.</div></div>
2	H	227	<div><div>27%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div>24%</div><div>.</div></div>
3	X	244	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>79%</div><div>14%</div><div>• 6%</div></div>
3	Y	244	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>74%</div><div>14%</div><div>• 12%</div></div>

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Mol	Chain	Length	Quality of chain
4	C	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10113 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 anti-NRR1 fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1625	1020	269	331	5			
1	L	212	Total	C	N	O	S	0	0	0
			1625	1020	269	331	5			

- Molecule 2 is a protein called anti-NRR1 fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1648	1040	283	319	6			
2	H	219	Total	C	N	O	S	0	0	0
			1643	1037	282	318	6			

- Molecule 3 is a protein called Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	230	Total	C	N	O	S	0	0	0
			1776	1094	309	351	22			
3	Y	215	Total	C	N	O	S	0	1	0
			1676	1037	293	326	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1730	ALA	-	expression tag	UNP P46531
X	1731	ASN	-	expression tag	UNP P46531
X	1732	SER	-	expression tag	UNP P46531
X	1733	HIS	-	expression tag	UNP P46531
X	1734	HIS	-	expression tag	UNP P46531
X	1735	HIS	-	expression tag	UNP P46531
X	1736	HIS	-	expression tag	UNP P46531
X	1737	HIS	-	expression tag	UNP P46531

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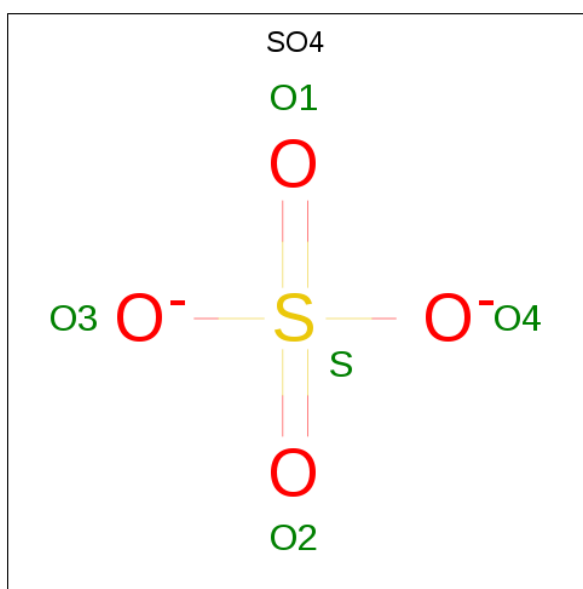
Chain	Residue	Modelled	Actual	Comment	Reference
X	1738	HIS	-	expression tag	UNP P46531
Y	1730	ALA	-	expression tag	UNP P46531
Y	1731	ASN	-	expression tag	UNP P46531
Y	1732	SER	-	expression tag	UNP P46531
Y	1733	HIS	-	expression tag	UNP P46531
Y	1734	HIS	-	expression tag	UNP P46531
Y	1735	HIS	-	expression tag	UNP P46531
Y	1736	HIS	-	expression tag	UNP P46531
Y	1737	HIS	-	expression tag	UNP P46531
Y	1738	HIS	-	expression tag	UNP P46531

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	3	Total Ca 3 3	0	0
6	Y	3	Total Ca 3 3	0	0

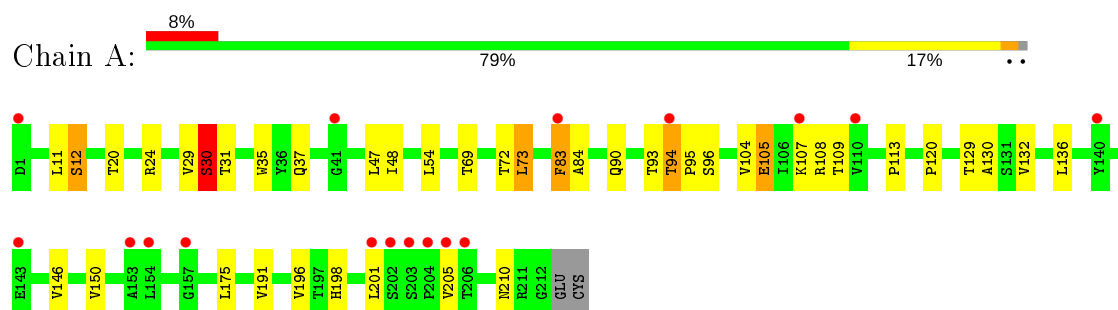
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	11	Total O 11 11	0	0
7	B	14	Total O 14 14	0	0
7	X	37	Total O 37 37	0	0
7	L	4	Total O 4 4	0	0
7	H	3	Total O 3 3	0	0
7	Y	12	Total O 12 12	0	0

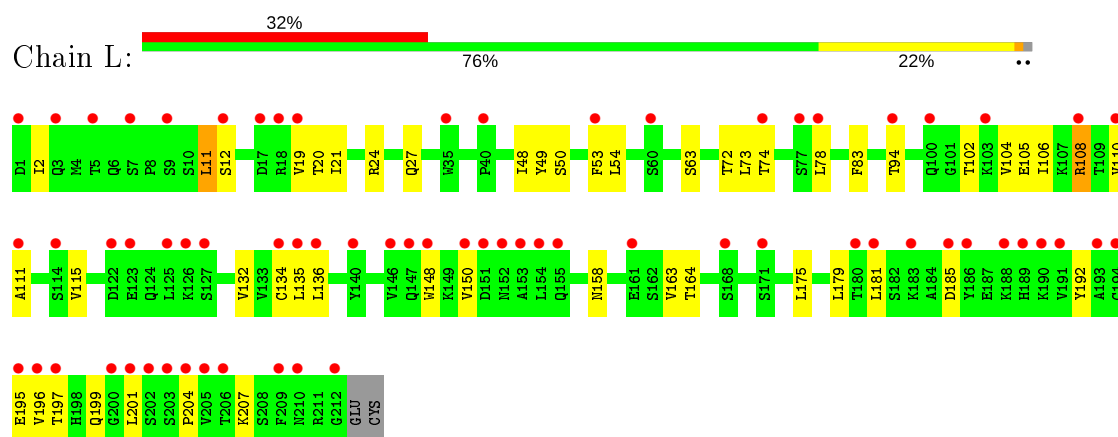
3 Residue-property plots [i](#)

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

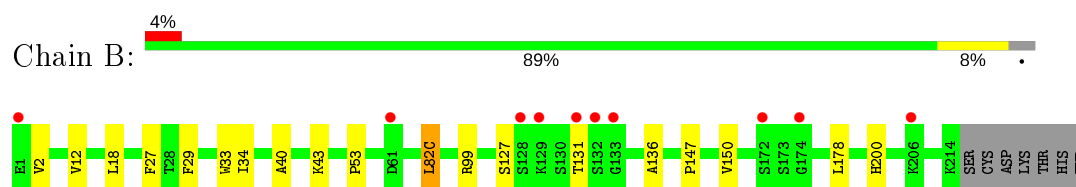
- Molecule 1: anti-NRR1 fab fragment light chain



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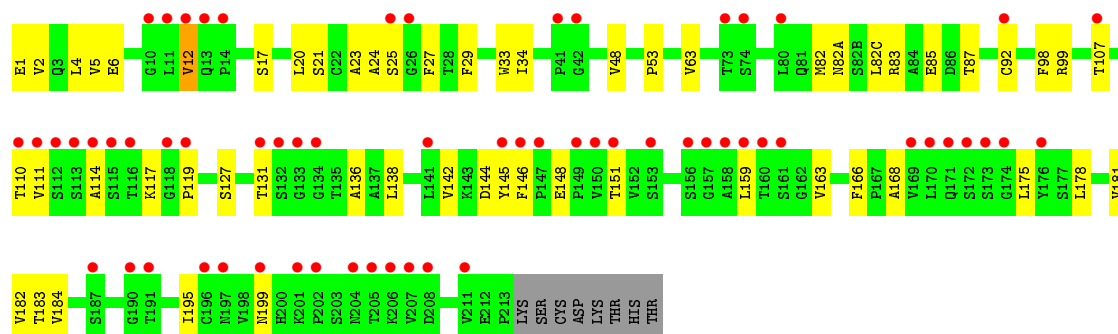


- Molecule 2: anti-NRR1 fab fragment heavy chain

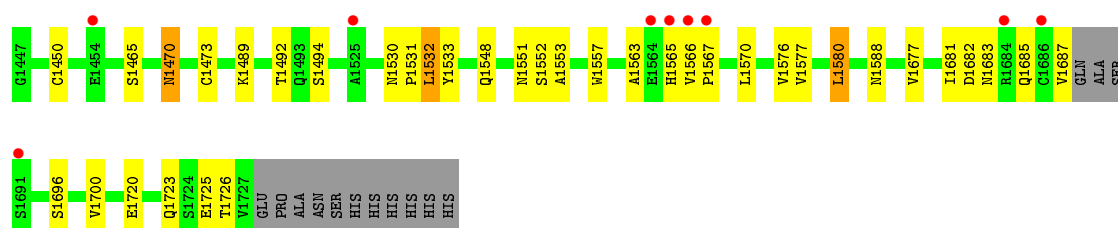
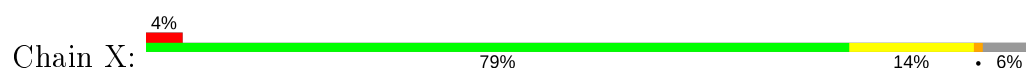


- Molecule 2: anti-NRR1 fab fragment heavy chain

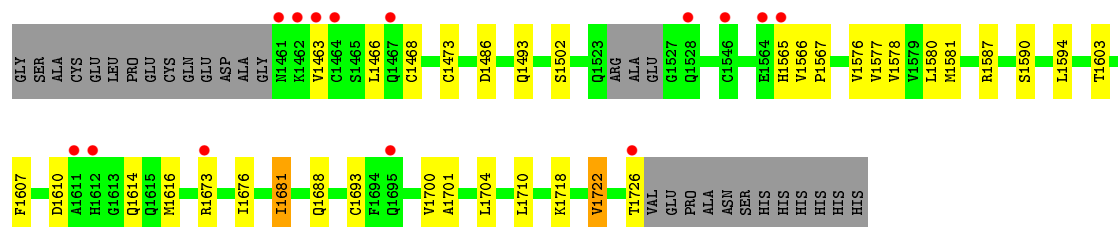




• Molecule 3: Neurogenic locus notch homolog protein 1



• Molecule 3: Neurogenic locus notch homolog protein 1



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.25Å 163.93Å 179.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.19 29.45 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.19) 97.8 (29.45-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.271 0.227 , 0.272	Depositor DCC
R_{free} test set	6979 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10113	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.44	0/1661	0.59	0/2257
1	L	0.34	0/1661	0.50	0/2257
2	B	0.45	0/1691	0.58	0/2307
2	H	0.37	0/1686	0.52	0/2300
3	X	0.51	0/1816	0.64	0/2461
3	Y	0.41	0/1719	0.55	0/2330
All	All	0.42	0/10234	0.56	0/13912

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	1625	0	1578	30	0
1	L	1625	0	1578	50	0
2	B	1648	0	1606	11	0
2	H	1643	0	1604	40	0
3	X	1776	0	1605	23	0
3	Y	1676	0	1522	26	0
4	C	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
6	X	3	0	0	0	0
6	Y	3	0	0	0	0
7	A	11	0	0	0	0
7	B	14	0	0	0	0
7	H	3	0	0	1	0
7	L	4	0	0	1	0
7	X	37	0	0	1	0
7	Y	12	0	0	0	0
All	All	10113	0	9518	171	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 (171) 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:L:148:TRP:CD2	1:L:179:LEU:HD11	1.91	1.03
1:L:148:TRP:CE2	1:L:179:LEU:HD11	2.00	0.96
3:Y:1576:VAL:CG1	3:Y:1676:ILE:HD11	1.99	0.93
3:Y:1681:ILE:HD12	3:Y:1700:VAL:HG21	1.54	0.88
1:A:90:GLN:NE2	1:A:93:THR:H	1.72	0.87
1:L:21:ILE:HD12	1:L:102:THR:HG21	1.58	0.86
2:H:151:THR:HG22	2:H:199:ASN:HB3	1.61	0.82
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.60	0.81
1:L:135:LEU:CD2	2:H:181:VAL:HG11	2.11	0.81
1:A:136:LEU:HD11	1:A:196:VAL:HG21	1.63	0.80
3:X:1588:ASN:ND2	7:X:19:HOH:O	2.16	0.78
3:Y:1681:ILE:HD11	3:Y:1700:VAL:HG11	1.65	0.77
1:A:20:THR:HG23	1:A:72:THR:CG2	2.17	0.75
2:B:12:VAL:HG21	2:B:82(C):LEU:HD23	1.67	0.74
2:H:33:TRP:CZ2	2:H:99:ARG:HD3	2.24	0.72
3:Y:1576:VAL:HG12	3:Y:1676:ILE:HD11	1.72	0.71
2:H:159:LEU:CD2	2:H:182:VAL:HG21	2.20	0.71
1:L:135:LEU:HD22	2:H:181:VAL:HG11	1.73	0.71
1:L:20:THR:HG23	1:L:72:THR:HG23	1.73	0.69
2:H:33:TRP:CE2	2:H:99:ARG:HD3	2.28	0.69
3:Y:1576:VAL:HG13	3:Y:1676:ILE:HD11	1.73	0.69
2:H:131:THR:HG22	2:H:136:ALA:HB2	1.74	0.68
3:X:1489:LYS:HD2	4:C:1:NAG:H82	1.75	0.67
2:B:40:ALA:HB3	2:B:43:LYS:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD13	1:A:205:VAL:HG23	1.78	0.65
1:L:135:LEU:HD21	2:H:181:VAL:HG11	1.79	0.65
1:L:150:VAL:HG23	1:L:150:VAL:O	1.98	0.64
1:A:90:GLN:HE22	1:A:93:THR:H	1.44	0.64
1:A:30:SER:OG	1:A:31:THR:N	2.32	0.63
1:A:20:THR:HG23	1:A:72:THR:HG23	1.81	0.62
3:X:1726:THR:HG22	3:X:1726:THR:O	2.00	0.61
1:L:148:TRP:CE3	1:L:179:LEU:HD11	2.35	0.61
3:X:1570:LEU:HD23	3:X:1682:ASP:HA	1.81	0.61
3:X:1548:GLN:NE2	3:X:1551:ASN:HD22	1.99	0.60
1:L:158:ASN:HD22	1:L:181:LEU:HD21	1.66	0.60
2:B:2:VAL:HG13	2:B:27:PHE:CD2	2.36	0.60
1:A:11:LEU:HD12	1:A:11:LEU:C	2.20	0.60
1:L:148:TRP:CE2	1:L:179:LEU:CD1	2.81	0.60
1:L:164:THR:HG23	2:H:166:PHE:CE1	2.37	0.60
1:A:29:VAL:HG11	1:A:90:GLN:HG3	1.84	0.59
1:A:11:LEU:HD11	1:A:104:VAL:HG13	1.84	0.59
3:X:1548:GLN:HE22	3:X:1551:ASN:HD22	1.51	0.59
1:L:78:LEU:HD21	1:L:106:ILE:CD1	2.33	0.59
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.37	0.58
1:A:146:VAL:HG22	1:A:196:VAL:HG22	1.85	0.58
1:L:163:VAL:HG22	1:L:175:LEU:HD12	1.85	0.58
2:H:131:THR:HG22	2:H:136:ALA:CB	2.33	0.57
2:H:99:ARG:NH2	3:Y:1710:LEU:HD13	2.19	0.57
2:B:131:THR:HG22	2:B:136:ALA:HB2	1.85	0.57
1:A:48:ILE:CD1	1:A:54:LEU:HD12	2.35	0.57
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.88	0.56
1:A:136:LEU:HD11	1:A:196:VAL:CG2	2.33	0.56
1:A:94:THR:HG23	1:A:95:PRO:HD3	1.87	0.56
2:H:195:ILE:O	2:H:195:ILE:HD12	2.05	0.55
1:L:148:TRP:CG	1:L:179:LEU:HD21	2.42	0.55
2:H:83:ARG:O	2:H:111:VAL:HG21	2.07	0.55
2:B:29:PHE:CE1	2:B:34:ILE:HD11	2.43	0.54
1:A:191:VAL:HG22	1:A:210:ASN:ND2	2.22	0.54
3:X:1576:VAL:HG21	3:X:1725:GLU:HG3	1.91	0.53
2:H:127:SER:O	2:H:131:THR:HG23	2.08	0.52
3:X:1450:CYS:SG	3:X:1470:ASN:OD1	2.66	0.52
2:H:195:ILE:C	2:H:195:ILE:HD12	2.29	0.52
2:H:163:VAL:HG22	2:H:182:VAL:HB	1.91	0.52
3:Y:1701:ALA:HB1	3:Y:1722:VAL:HG13	1.90	0.52
1:A:90:GLN:HE21	1:A:93:THR:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:PRO:O	2:B:200:HIS:HE1	1.91	0.52
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.90	0.52
3:X:1530:ASN:OD1	3:X:1532:LEU:HD22	2.09	0.52
1:A:136:LEU:HD22	1:A:175:LEU:HD22	1.91	0.52
1:L:195:GLU:OE2	1:L:197:THR:HG23	2.09	0.52
2:H:48:VAL:HG13	2:H:63:VAL:HG21	1.91	0.52
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.92	0.51
1:L:148:TRP:CB	1:L:179:LEU:HD21	2.40	0.51
1:L:53:PHE:CE1	3:Y:1463:VAL:HG13	2.45	0.51
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.45	0.51
3:X:1683:ASN:O	3:X:1687:VAL:HG22	2.11	0.51
3:Y:1566:VAL:HG13	3:Y:1567:PRO:HD2	1.93	0.51
2:H:148:GLU:OE2	2:H:168:ALA:HB3	2.11	0.51
2:H:2:VAL:HG13	2:H:27:PHE:CE2	2.46	0.51
2:H:12:VAL:O	2:H:111:VAL:HG12	2.11	0.50
1:L:104:VAL:HG12	1:L:104:VAL:O	2.11	0.50
2:H:87:THR:OG1	2:H:111:VAL:HG22	2.11	0.50
2:H:146:PHE:HB2	2:H:175:LEU:HD23	1.92	0.50
1:A:93:THR:HG22	1:A:95:PRO:HD2	1.94	0.50
2:H:119:PRO:HB2	2:H:142:VAL:HG13	1.94	0.50
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.47	0.49
3:Y:1681:ILE:CD1	3:Y:1700:VAL:HG11	2.38	0.49
3:X:1557:TRP:HB3	3:X:1685:GLN:HE22	1.76	0.49
2:H:4:LEU:HD23	2:H:92:CYS:SG	2.52	0.49
2:H:117:LYS:HZ1	2:H:144:ASP:HB3	1.77	0.49
2:H:5:VAL:HB	2:H:23:ALA:HB3	1.94	0.49
2:B:178:LEU:HD12	2:B:178:LEU:C	2.33	0.49
2:H:20:LEU:HD22	2:H:107:THR:HG21	1.95	0.48
1:A:150:VAL:O	1:A:150:VAL:HG13	2.12	0.48
2:B:33:TRP:CE2	2:B:99:ARG:HD2	2.47	0.48
1:L:48:ILE:HD11	1:L:54:LEU:HD12	1.96	0.48
3:X:1552:SER:HA	3:X:1557:TRP:CZ3	2.47	0.48
1:L:108:ARG:NH1	1:L:111:ALA:HB2	2.29	0.48
1:L:63:SER:O	1:L:73:LEU:HD12	2.14	0.48
2:H:138:LEU:HD21	2:H:184:VAL:HG21	1.95	0.47
3:Y:1610:ASP:OD2	3:Y:1614:GLN:N	2.46	0.47
1:A:191:VAL:HG22	1:A:210:ASN:HD21	1.80	0.47
1:L:53:PHE:HE1	3:Y:1463:VAL:HG13	1.80	0.47
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.49	0.47
1:L:150:VAL:HG12	1:L:192:TYR:CD1	2.49	0.47
1:A:11:LEU:O	1:A:105:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ILE:CD1	1:L:54:LEU:HD12	2.45	0.46
3:X:1681:ILE:HG13	3:X:1700:VAL:HG21	1.98	0.46
2:B:34:ILE:HD12	2:B:53:PRO:HG3	1.98	0.46
1:L:197:THR:HG22	1:L:204:PRO:HG3	1.98	0.46
1:L:2:ILE:HD11	1:L:27:GLN:HE21	1.81	0.46
2:H:114:ALA:HB1	7:H:224:HOH:O	2.16	0.45
1:L:115:VAL:HG13	1:L:207:LYS:HG3	1.98	0.45
1:L:150:VAL:CG2	1:L:150:VAL:O	2.63	0.45
1:L:136:LEU:HD21	1:L:196:VAL:HG13	1.99	0.45
2:B:40:ALA:HB3	2:B:43:LYS:CD	2.46	0.45
1:L:136:LEU:HD21	1:L:196:VAL:CG1	2.47	0.45
3:Y:1580:LEU:HD11	3:Y:1673:ARG:NE	2.32	0.45
1:A:20:THR:CG2	1:A:72:THR:HG23	2.45	0.45
2:H:34:ILE:HD12	2:H:53:PRO:HG3	1.99	0.45
1:L:132:VAL:HB	1:L:179:LEU:HD13	1.98	0.44
3:Y:1704:LEU:HD12	3:Y:1722:VAL:HG21	1.99	0.44
3:Y:1577:VAL:HG22	3:Y:1722:VAL:HG23	1.98	0.44
3:X:1553:ALA:HB2	3:X:1557:TRP:CZ2	2.53	0.44
1:L:11:LEU:HD12	1:L:12:SER:N	2.33	0.43
1:L:110:VAL:O	1:L:110:VAL:HG23	2.19	0.43
3:X:1557:TRP:CB	3:X:1685:GLN:HE22	2.31	0.43
3:Y:1587:ARG:O	3:Y:1590:SER:HB2	2.19	0.43
3:X:1489:LYS:CD	4:C:1:NAG:H82	2.46	0.42
1:L:148:TRP:CZ2	1:L:179:LEU:HD11	2.51	0.42
1:L:48:ILE:HD13	1:L:54:LEU:HA	2.00	0.42
1:L:78:LEU:HD21	1:L:106:ILE:HD13	2.00	0.42
3:X:1532:LEU:HD23	3:X:1533:TYR:CD1	2.54	0.42
3:Y:1594:LEU:HD11	3:Y:1607:PHE:CD2	2.54	0.42
3:Y:1603:THR:HG21	3:Y:1681:ILE:HG23	2.01	0.42
3:Y:1580:LEU:HD23	3:Y:1718:LYS:HE2	2.01	0.42
2:H:29:PHE:CE1	2:H:34:ILE:HD11	2.54	0.42
2:H:98:PHE:HB2	3:Y:1466:LEU:HD11	1.99	0.42
1:A:129:THR:HG22	1:A:130:ALA:N	2.34	0.42
3:X:1696:SER:HB3	4:C:2:NAG:H83	2.01	0.42
3:X:1532:LEU:HD23	3:X:1533:TYR:CE1	2.54	0.42
1:L:108:ARG:HH12	1:L:111:ALA:HB2	1.85	0.42
3:Y:1468:CYS:O	3:Y:1473:CYS:HB2	2.20	0.42
3:Y:1578:VAL:CG2	3:Y:1676:ILE:HD13	2.50	0.42
1:L:136:LEU:N	1:L:136:LEU:HD12	2.34	0.42
1:A:35:TRP:CE3	1:A:73:LEU:HD12	2.54	0.42
2:H:151:THR:CG2	2:H:199:ASN:HB3	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:1580:LEU:CD2	3:X:1720:GLU:HB3	2.50	0.42
1:L:20:THR:OG1	1:L:74:THR:HG22	2.20	0.41
3:X:1566:VAL:HG13	3:X:1567:PRO:HD2	2.01	0.41
1:L:148:TRP:HB3	1:L:179:LEU:HD21	2.01	0.41
1:L:24:ARG:HD2	7:L:215:HOH:O	2.19	0.41
1:L:20:THR:HG23	1:L:72:THR:CG2	2.45	0.41
2:H:145:TYR:OH	2:H:178:LEU:HD23	2.20	0.41
1:A:83:PHE:O	1:A:84:ALA:HB2	2.21	0.41
2:B:127:SER:O	2:B:131:THR:HG23	2.21	0.41
1:L:110:VAL:HG11	1:L:199:GLN:NE2	2.36	0.41
3:Y:1578:VAL:HG22	3:Y:1676:ILE:HD13	2.03	0.41
1:L:72:THR:HG22	1:L:74:THR:HG23	2.01	0.41
1:A:11:LEU:HD12	1:A:12:SER:N	2.36	0.41
1:L:181:LEU:HD22	1:L:185:ASP:OD2	2.20	0.41
3:Y:1681:ILE:HD12	3:Y:1700:VAL:CG2	2.37	0.41
2:H:17:SER:HB3	2:H:82(A):ASN:HD22	1.85	0.41
2:H:82:MET:HE3	2:H:82(C):LEU:HD21	2.03	0.41
1:L:49:TYR:CG	3:Y:1466:LEU:HD22	2.56	0.41
3:Y:1616:MET:HB3	3:Y:1616:MET:HE2	1.75	0.41
1:L:11:LEU:C	1:L:11:LEU:HD12	2.42	0.40
1:A:24:ARG:HA	1:A:69:THR:O	2.22	0.40
3:X:1492:THR:HG22	3:X:1494:SER:H	1.85	0.40
3:X:1577:VAL:HB	3:X:1677:VAL:HG22	2.02	0.40
1:L:11:LEU:HD21	1:L:19:VAL:HG11	2.04	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	210/214 (98%)	202 (96%)	7 (3%)	1 (0%)	29 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	B	218/227 (96%)	215 (99%)	3 (1%)	0	100	100
2	H	217/227 (96%)	206 (95%)	11 (5%)	0	100	100
3	X	226/244 (93%)	219 (97%)	6 (3%)	1 (0%)	34	37
3	Y	212/244 (87%)	206 (97%)	5 (2%)	1 (0%)	29	31
All	All	1293/1370 (94%)	1245 (96%)	45 (4%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	X	1563	ALA
1	A	30	SER
3	Y	1486	ASP

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	186/188 (99%)	176 (95%)	10 (5%)	22	26
1	L	186/188 (99%)	179 (96%)	7 (4%)	33	42
2	B	182/190 (96%)	179 (98%)	3 (2%)	62	76
2	H	182/190 (96%)	174 (96%)	8 (4%)	28	35
3	X	196/208 (94%)	188 (96%)	8 (4%)	30	39
3	Y	186/208 (89%)	177 (95%)	9 (5%)	25	32
All	All	1118/1172 (95%)	1073 (96%)	45 (4%)	31	40

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	30	SER
1	A	73	LEU

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Mol	Chain	Res	Type
1	A	83	PHE
1	A	94	THR
1	A	96	SER
1	A	105	GLU
1	A	107	LYS
1	A	108	ARG
1	A	109	THR
2	B	18	LEU
2	B	82(C)	LEU
2	B	150	VAL
3	X	1465	SER
3	X	1470	ASN
3	X	1473	CYS
3	X	1531	PRO
3	X	1532	LEU
3	X	1565	HIS
3	X	1580	LEU
3	X	1723	GLN
1	L	11	LEU
1	L	50	SER
1	L	83	PHE
1	L	94	THR
1	L	105	GLU
1	L	108	ARG
1	L	201	LEU
2	H	1	GLU
2	H	6	GLU
2	H	12	VAL
2	H	21	SER
2	H	25	SER
2	H	85	GLU
2	H	110	THR
2	H	183	THR
3	Y	1493	GLN
3	Y	1502	SER
3	Y	1565	HIS
3	Y	1581	MET
3	Y	1681	ILE
3	Y	1688	GLN
3	Y	1693	CYS
3	Y	1722	VAL
3	Y	1726	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	90	GLN
1	A	155	GLN
1	A	199	GLN
1	A	210	ASN
2	B	13	GLN
2	B	35	HIS
2	B	39	GLN
2	B	55	ASN
2	B	82(A)	ASN
2	B	164	HIS
2	B	171	GLN
2	B	200	HIS
3	X	1470	ASN
3	X	1483	ASN
3	X	1548	GLN
3	X	1585	GLN
3	X	1615	GLN
3	X	1685	GLN
1	L	27	GLN
1	L	38	GLN
1	L	79	GLN
1	L	124	GLN
1	L	199	GLN
2	H	39	GLN
2	H	81	GLN
2	H	82(A)	ASN
3	Y	1471	HIS
3	Y	1505	HIS
3	Y	1523	GLN
3	Y	1551	ASN
3	Y	1683	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

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	C	1	3,4	14,14,15	0.59	0	17,19,21	2.32	3 (17%)
4	NAG	C	2	4	14,14,15	0.54	0	17,19,21	1.31	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
4	C	1	NAG	C1-O5-C5	7.71	122.64	112.19
4	C	1	NAG	O5-C1-C2	3.35	116.58	111.29
4	C	1	NAG	O4-C4-C5	2.90	116.51	109.30
4	C	2	NAG	C1-O5-C5	2.80	115.98	112.19
4	C	2	NAG	C3-C4-C5	2.67	115.01	110.24
4	C	2	NAG	O5-C1-C2	-2.31	107.64	111.29
4	C	2	NAG	C6-C5-C4	-2.20	107.85	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O7-C7-N2-C2
4	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	NAG	1	0
4	C	1	NAG	2	0

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	222	-	4,4,4	0.26	0	6,6,6	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	212/214 (99%)	0.57	17 (8%) 12 11	20, 35, 47, 57	0
1	L	212/214 (99%)	1.75	68 (32%) 0 0	20, 35, 47, 56	0
2	B	220/227 (96%)	0.34	10 (4%) 33 32	17, 30, 46, 57	0
2	H	219/227 (96%)	1.57	62 (28%) 0 0	18, 30, 45, 57	0
3	X	230/244 (94%)	0.25	9 (3%) 39 37	12, 26, 56, 80	0
3	Y	215/244 (88%)	0.39	14 (6%) 18 17	14, 28, 50, 77	0
All	All	1308/1370 (95%)	0.80	180 (13%) 2 2	12, 31, 48, 80	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	202	SER	8.8
2	H	174	GLY	7.9
1	L	205	VAL	7.4
2	H	160	THR	7.2
1	L	204	PRO	6.8
1	L	153	ALA	6.5
2	H	41	PRO	6.4
1	A	154	LEU	6.4
1	L	201	LEU	6.3
2	H	112	SER	6.3
3	Y	1726	THR	6.2
2	H	158	ALA	6.2
1	L	110	VAL	6.2
2	H	204	ASN	6.0
1	L	151	ASP	5.7
2	H	146	PHE	5.6
1	A	83	PHE	5.5
1	L	191	VAL	5.4
1	L	196	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	L	1	ASP	5.2
2	H	111	VAL	5.1
1	L	147	GLN	5.1
2	H	206	LYS	4.9
1	L	195	GLU	4.9
2	H	116	THR	4.9
2	H	176	TYR	4.8
1	L	17	ASP	4.8
1	L	203	SER	4.7
2	B	131	THR	4.6
2	H	149	PRO	4.5
1	L	9	SER	4.5
2	H	199	ASN	4.4
3	X	1525	ALA	4.4
1	L	148	TRP	4.4
3	Y	1462	LYS	4.4
1	A	206	THR	4.3
1	L	212	GLY	4.2
2	H	11	LEU	4.2
2	H	131	THR	4.2
2	H	145	TYR	4.2
1	L	200	GLY	4.2
3	X	1565	HIS	4.2
1	L	197	THR	4.1
1	L	189	HIS	4.1
1	L	206	THR	4.1
1	L	40	PRO	4.1
2	H	119	PRO	4.1
1	A	201	LEU	4.1
2	H	170	LEU	4.1
2	H	118	GLY	4.0
1	L	180	THR	4.0
3	Y	1612	HIS	3.9
2	H	42	GLY	3.9
1	L	154	LEU	3.9
2	H	10	GLY	3.9
2	H	173	SER	3.9
2	H	74	SER	3.8
2	H	12	VAL	3.7
2	H	171	GLN	3.7
2	H	208	ASP	3.7
2	H	211	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	133	GLY	3.7
3	X	1564	GLU	3.7
2	H	190	GLY	3.7
1	L	140	TYR	3.6
1	L	122	ASP	3.6
1	L	181	LEU	3.6
1	A	94	THR	3.6
1	L	185	ASP	3.5
1	L	111	ALA	3.5
2	B	132	SER	3.5
1	A	143	GLU	3.4
2	H	14	PRO	3.4
2	H	13	GLN	3.4
1	L	60	SER	3.4
2	B	206	LYS	3.4
2	H	205	THR	3.4
3	X	1684	ARG	3.3
1	A	1	ASP	3.3
2	H	187	SER	3.3
1	L	150	VAL	3.3
2	B	128	SER	3.2
1	L	155	GLN	3.2
3	Y	1695	GLN	3.2
1	A	203	SER	3.2
1	L	3	GLN	3.2
2	H	150	VAL	3.1
2	H	132	SER	3.1
1	L	188	LYS	3.1
2	H	134	GLY	3.1
1	L	210	ASN	3.1
1	L	125	LEU	3.0
2	H	26	GLY	3.0
3	Y	1564	GLU	3.0
1	A	204	PRO	3.0
2	H	113	SER	3.0
3	Y	1461	ASN	3.0
1	L	171	SER	3.0
1	A	202	SER	3.0
2	H	110	THR	3.0
2	H	156	SER	2.9
1	L	12	SER	2.9
3	X	1686	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	78	LEU	2.9
2	B	172	SER	2.9
2	H	115	SER	2.9
1	L	108	ARG	2.8
2	H	151	THR	2.8
1	A	157	GLY	2.8
1	L	146	VAL	2.8
1	A	140	TYR	2.8
1	L	5	THR	2.7
1	L	94	THR	2.7
2	H	107	THR	2.7
2	H	92	CYS	2.7
1	L	53	PHE	2.7
3	Y	1611	ALA	2.7
1	L	127	SER	2.7
1	L	168	SER	2.7
1	L	18	ARG	2.6
1	L	183	LYS	2.6
2	H	196	CYS	2.6
1	L	209	PHE	2.6
2	H	201	LYS	2.6
2	H	147	PRO	2.6
3	X	1567	PRO	2.6
1	L	126	LYS	2.5
2	B	129	LYS	2.5
1	L	136	LEU	2.5
3	Y	1464	CYS	2.5
1	L	103	LYS	2.5
3	Y	1673	ARG	2.5
1	L	194	CYS	2.5
3	Y	1463	VAL	2.5
1	A	110	VAL	2.5
2	H	161	SER	2.5
1	L	193	ALA	2.5
2	H	141	LEU	2.4
1	L	114	SER	2.4
2	H	207	VAL	2.4
1	L	100	GLN	2.4
2	B	1	GLU	2.4
2	H	73	THR	2.4
1	L	190	LYS	2.4
1	L	161	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	153	ALA	2.4
2	H	157	GLY	2.4
3	Y	1565	HIS	2.3
1	A	205	VAL	2.3
3	X	1566	VAL	2.3
1	L	77	SER	2.3
2	H	172	SER	2.3
2	B	61	ASP	2.3
1	L	74	THR	2.2
1	L	35	TRP	2.2
1	L	123	GLU	2.2
3	Y	1467	GLN	2.2
1	A	41	GLY	2.2
1	L	134	CYS	2.2
2	H	169	VAL	2.2
3	Y	1546	CYS	2.2
1	L	152	ASN	2.2
2	H	197	ASN	2.2
1	L	7	SER	2.1
2	H	25	SER	2.1
1	L	186	TYR	2.1
2	H	114	ALA	2.1
3	X	1454	GLU	2.1
2	H	153	SER	2.1
2	B	174	GLY	2.1
3	X	1691	SER	2.1
2	H	202	PRO	2.1
1	L	135	LEU	2.0
1	L	19	VAL	2.0
2	H	191	THR	2.0
3	Y	1528	GLN	2.0
1	A	107	LYS	2.0
2	H	80	LEU	2.0
2	H	159	LEU	2.0
2	B	133	GLY	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	2	14/15	0.84	0.21	53,56,61,64	0
4	NAG	C	1	14/15	0.91	0.14	31,40,50,50	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CA	Y	2001	1/1	0.86	0.43	67,67,67,67	0
6	CA	X	2001	1/1	0.97	0.18	43,43,43,43	0
6	CA	X	2003	1/1	0.99	0.03	21,21,21,21	0
6	CA	Y	2003	1/1	0.99	0.06	23,23,23,23	0
5	SO4	B	222	5/5	0.99	0.06	31,32,32,33	0
6	CA	Y	2002	1/1	0.99	0.06	21,21,21,21	0
6	CA	X	2002	1/1	1.00	0.03	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.