



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:13 AM GMT

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
<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

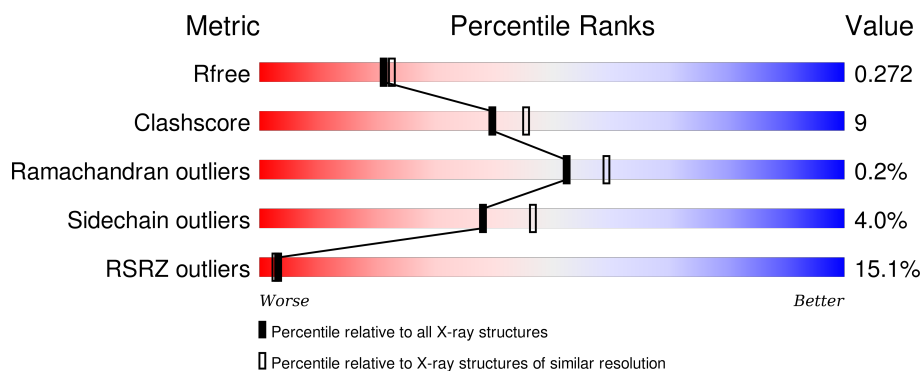
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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>79%</div> <div>17%</div> <div>..</div> </div>
1	L	214	<div> <div>35%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
2	B	227	<div> <div>5%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	H	227	<div> <div>30%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
3	X	244	<div> <div>4%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	244	

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
5	CA	Y	2001	-	-	-	X

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:

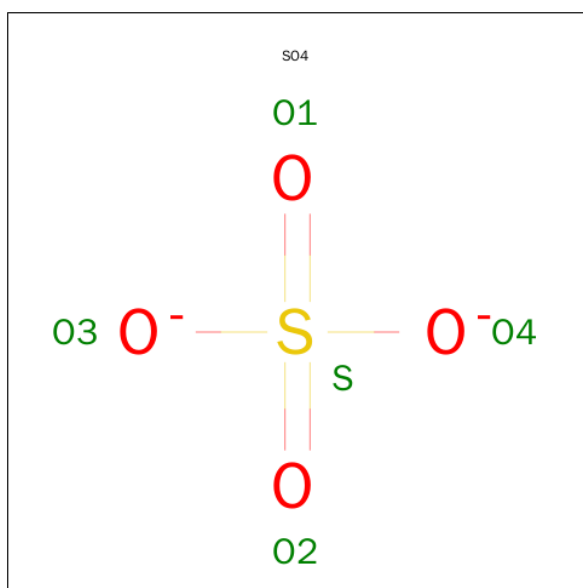
Chain	Residue	Modelled	Actual	Comment	Reference
X	1730	ALA	-	EXPRESSION TAG	UNP P46531
X	1731	ASN	-	EXPRESSION TAG	UNP P46531
X	1732	SER	-	EXPRESSION TAG	UNP P46531
X	1733	HIS	-	EXPRESSION TAG	UNP P46531
X	1734	HIS	-	EXPRESSION TAG	UNP P46531
X	1735	HIS	-	EXPRESSION TAG	UNP P46531
X	1736	HIS	-	EXPRESSION 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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

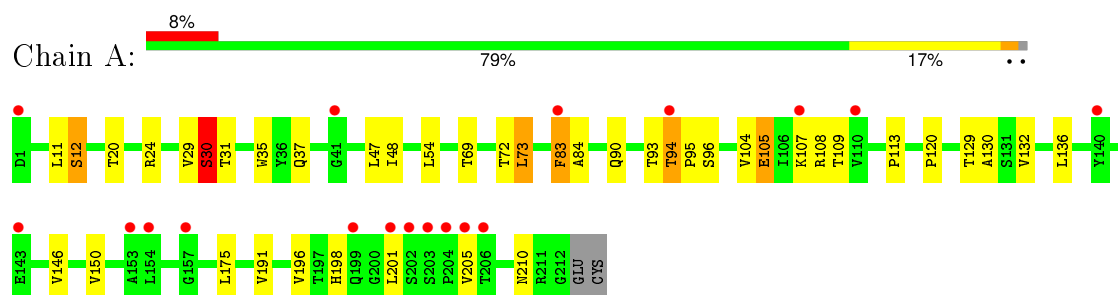
- Molecule 7 is water.

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

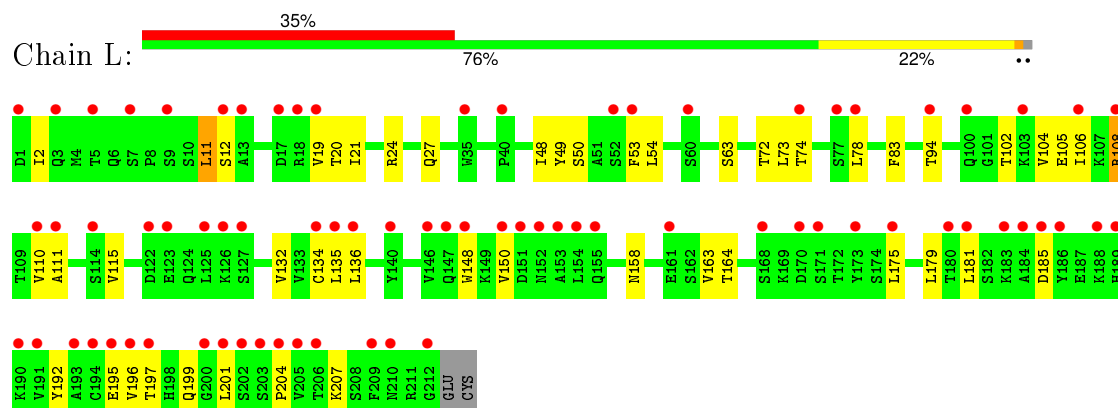
3 Residue-property plots [i](#)

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.

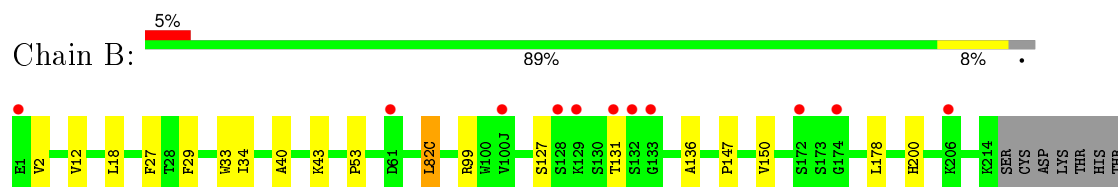
- Molecule 1: anti-NRR1 fab fragment light chain



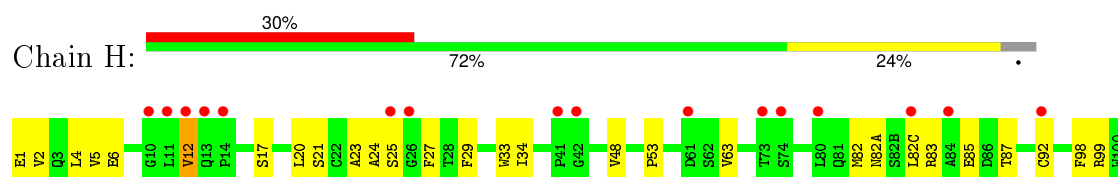
- Molecule 1: anti-NRR1 fab fragment light chain

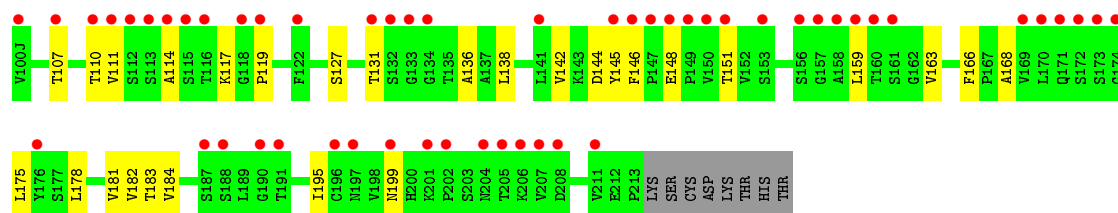


- Molecule 2: anti-NRR1 fab fragment heavy chain

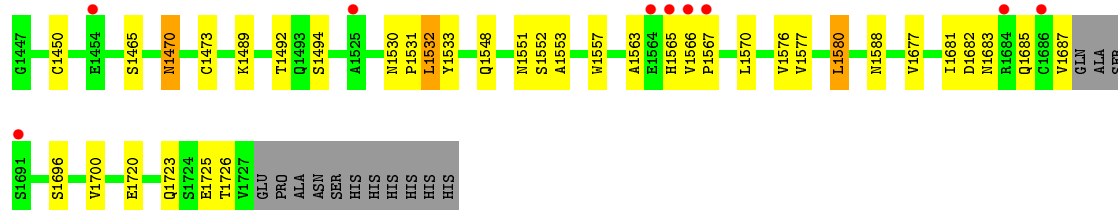
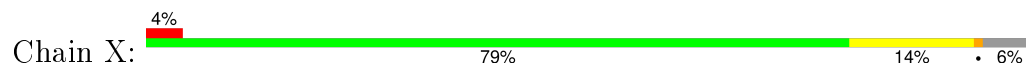


- Molecule 2: anti-NRR1 fab fragment heavy chain

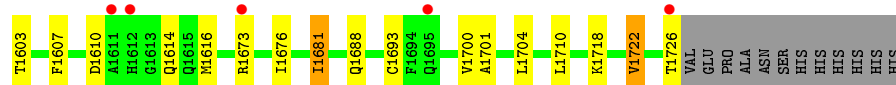
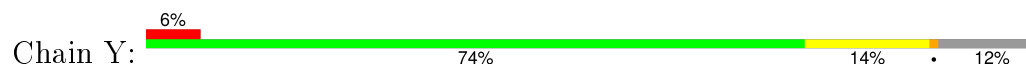




• Molecule 3: Neurogenic locus notch homolog protein 1



• Molecule 3: Neurogenic locus notch homolog protein 1



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 (11.09%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 69909 reflections	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, 0.375 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: 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	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	X	3	0	0	0	0
5	Y	3	0	0	0	0
6	X	28	0	25	3	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
3:Y:1576:VAL:HG13	3:Y:1676:ILE:HD11	1.73	0.69
2:H:33:TRP:CE2	2:H:99:ARG:HD3	2.28	0.69
2:H:131:THR:HG22	2:H:136:ALA:HB2	1.74	0.68
3:X:1489:LYS:HD2	6:X:2004: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:94:THR:HG23	1:A:95:PRO:HD3	1.87	0.56
1:A:136:LEU:HD11	1:A:196:VAL:CG2	2.33	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
3:X:1530:ASN:OD1	3:X:1532:LEU:HD22	2.09	0.52
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.90	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
3:Y:1566:VAL:HG13	3:Y:1567:PRO:HD2	1.93	0.51
3:X:1683:ASN:O	3:X:1687:VAL:HG22	2.11	0.51
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.45	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
2:B:33:TRP:CE2	2:B:99:ARG:HD2	2.47	0.48
1:A:150:VAL:O	1:A:150:VAL:HG13	2.12	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:150:VAL:CG2	1:L:150:VAL:O	2.63	0.45
1:L:115:VAL:HG13	1:L:207:LYS:HG3	1.98	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
3:X:1557:TRP:CB	3:X:1685:GLN:HE22	2.31	0.43
1:L:110:VAL:O	1:L:110:VAL:HG23	2.19	0.43
3:Y:1587:ARG:O	3:Y:1590:SER:HB2	2.19	0.43
1:L:148:TRP:CZ2	1:L:179:LEU:HD11	2.51	0.42
3:X:1489:LYS:CD	6:X:2004:NAG:H82	2.46	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
1:L:48:ILE:HD13	1:L:54:LEU:HA	2.00	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
3:X:1532:LEU:HD23	3:X:1533:TYR:CE1	2.54	0.42
3:X:1696:SER:HB3	6:X:2005:NAG:H83	2.01	0.42
1:A:129:THR:HG22	1:A:130:ALA:N	2.34	0.42
3:Y:1578:VAL:CG2	3:Y:1676:ILE:HD13	2.50	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
1:L:136:LEU:N	1:L:136:LEU:HD12	2.34	0.42
2:H:151:THR:CG2	2:H:199:ASN:HB3	2.42	0.42
1:A:35:TRP:CE3	1:A:73:LEU:HD12	2.54	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
3:Y:1578:VAL:HG22	3:Y:1676:ILE:HD13	2.03	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
1:A:83:PHE:O	1:A:84:ALA:HB2	2.21	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
3:Y:1681:ILE:HD12	3:Y:1700:VAL:CG2	2.37	0.41
1:L:181:LEU:HD22	1:L:185:ASP:OD2	2.20	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
2:H:17:SER:HB3	2:H:82(A):ASN:HD22	1.85	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%)	34 35

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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%)	39	42
3	Y	212/244 (87%)	206 (97%)	5 (2%)	1 (0%)	34	35
All	All	1293/1370 (94%)	1245 (96%)	45 (4%)	3 (0%)	52	59

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%)	27	31
1	L	186/188 (99%)	179 (96%)	7 (4%)	40	49
2	B	182/190 (96%)	179 (98%)	3 (2%)	70	82
2	H	182/190 (96%)	174 (96%)	8 (4%)	35	42
3	X	196/208 (94%)	188 (96%)	8 (4%)	37	45
3	Y	186/208 (89%)	177 (95%)	9 (5%)	31	37
All	All	1118/1172 (95%)	1073 (96%)	45 (4%)	38	47

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 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
6	NAG	X	2004	3,6	14,14,15	0.57	0	15,19,21	2.43	2 (13%)
6	NAG	X	2005	6	14,14,15	0.51	0	15,19,21	1.25	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	2004	3,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2005	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	2005	NAG	C6-C5-C4	-2.09	107.85	113.02
6	X	2004	NAG	O4-C4-C5	2.74	116.51	109.24
6	X	2005	NAG	C3-C4-C5	2.76	115.01	110.20
6	X	2005	NAG	C1-O5-C5	2.94	115.98	112.25
6	X	2004	NAG	C1-O5-C5	8.19	122.64	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	2004	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	2005	NAG	1	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	$\# Z > 2$
4	SO4	B	222	-	4,4,4	0.52	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	222	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.64	18 (8%) 13 12	20, 35, 47, 57	0
1	L	212/214 (99%)	1.86	75 (35%) 0 0	20, 35, 47, 56	0
2	B	220/227 (96%)	0.41	11 (5%) 32 32	17, 30, 46, 57	0
2	H	219/227 (96%)	1.68	69 (31%) 1 0	18, 30, 45, 57	0
3	X	230/244 (94%)	0.31	9 (3%) 43 42	12, 26, 56, 80	0
3	Y	215/244 (88%)	0.45	15 (6%) 19 19	14, 28, 50, 77	0
All	All	1308/1370 (95%)	0.88	197 (15%) 3 3	12, 31, 48, 80	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	202	SER	9.0
2	H	174	GLY	8.3
1	L	205	VAL	8.2
2	H	160	THR	7.5
1	L	204	PRO	7.0
1	A	154	LEU	6.8
1	L	153	ALA	6.7
1	L	110	VAL	6.6
2	H	41	PRO	6.6
1	L	201	LEU	6.6
2	H	112	SER	6.6
3	Y	1726	THR	6.5
2	H	158	ALA	6.4
2	H	204	ASN	6.1
2	H	146	PHE	5.9
1	A	83	PHE	5.9
1	L	151	ASP	5.9
1	L	191	VAL	5.7
1	L	1	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	L	147	GLN	5.3
1	L	196	VAL	5.3
2	H	111	VAL	5.3
2	H	116	THR	5.1
2	H	206	LYS	5.0
1	L	195	GLU	5.0
1	L	17	ASP	4.9
2	B	131	THR	4.9
1	L	203	SER	4.8
2	H	176	TYR	4.7
1	L	148	TRP	4.7
2	H	199	ASN	4.7
1	L	9	SER	4.7
3	X	1525	ALA	4.6
2	H	149	PRO	4.6
1	L	212	GLY	4.6
2	H	11	LEU	4.6
2	H	145	TYR	4.6
3	Y	1462	LYS	4.5
1	A	206	THR	4.5
2	H	170	LEU	4.5
2	H	131	THR	4.4
1	L	197	THR	4.4
1	L	189	HIS	4.3
1	L	206	THR	4.3
2	H	118	GLY	4.3
1	L	180	THR	4.3
1	A	201	LEU	4.3
1	L	40	PRO	4.2
1	L	200	GLY	4.2
2	H	119	PRO	4.2
3	X	1565	HIS	4.2
2	H	42	GLY	4.2
2	H	12	VAL	4.1
1	L	154	LEU	4.1
2	H	10	GLY	4.1
3	Y	1612	HIS	4.0
2	H	211	VAL	4.0
2	H	133	GLY	4.0
2	H	173	SER	4.0
2	H	190	GLY	4.0
2	H	208	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	171	GLN	3.9
2	H	74	SER	3.9
3	X	1564	GLU	3.9
1	L	140	TYR	3.8
1	L	122	ASP	3.8
1	L	181	LEU	3.8
1	L	111	ALA	3.7
2	H	14	PRO	3.7
1	A	94	THR	3.7
1	L	185	ASP	3.7
1	L	60	SER	3.6
2	B	132	SER	3.6
1	A	143	GLU	3.6
2	H	13	GLN	3.6
1	L	150	VAL	3.6
2	H	205	THR	3.5
2	B	206	LYS	3.5
2	H	187	SER	3.5
1	A	1	ASP	3.5
1	A	203	SER	3.5
1	L	155	GLN	3.4
3	X	1684	ARG	3.4
2	H	150	VAL	3.4
2	B	128	SER	3.4
3	Y	1695	GLN	3.3
2	H	134	GLY	3.3
1	L	3	GLN	3.3
2	H	132	SER	3.3
2	H	113	SER	3.2
2	H	26	GLY	3.2
1	L	210	ASN	3.2
1	L	125	LEU	3.2
3	X	1686	CYS	3.2
3	Y	1461	ASN	3.2
1	L	188	LYS	3.2
1	A	204	PRO	3.1
1	A	202	SER	3.1
2	H	110	THR	3.1
3	Y	1564	GLU	3.1
1	L	12	SER	3.1
2	B	172	SER	3.1
1	L	171	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	156	SER	3.0
1	L	146	VAL	3.0
1	L	78	LEU	3.0
1	A	157	GLY	3.0
2	H	151	THR	3.0
1	L	108	ARG	3.0
2	H	92	CYS	2.9
2	H	115	SER	2.9
1	A	140	TYR	2.9
1	L	53	PHE	2.9
1	L	94	THR	2.9
1	L	5	THR	2.9
3	Y	1611	ALA	2.9
2	H	107	THR	2.8
1	L	183	LYS	2.8
1	L	168	SER	2.8
1	L	127	SER	2.8
3	Y	1464	CYS	2.8
1	L	18	ARG	2.8
2	H	147	PRO	2.7
1	L	193	ALA	2.7
1	L	209	PHE	2.7
1	A	110	VAL	2.7
2	H	196	CYS	2.7
3	X	1567	PRO	2.7
2	H	141	LEU	2.7
2	H	201	LYS	2.7
1	L	126	LYS	2.6
2	H	161	SER	2.6
1	L	136	LEU	2.6
3	Y	1463	VAL	2.6
2	B	129	LYS	2.6
2	H	73	THR	2.6
3	Y	1673	ARG	2.6
1	L	194	CYS	2.6
1	L	103	LYS	2.6
2	H	207	VAL	2.6
1	L	114	SER	2.5
1	A	153	ALA	2.5
1	A	205	VAL	2.5
3	X	1566	VAL	2.5
1	L	77	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	100	GLN	2.5
2	B	1	GLU	2.5
1	L	190	LYS	2.5
2	H	172	SER	2.5
2	H	157	GLY	2.5
1	L	74	THR	2.5
1	L	161	GLU	2.4
2	B	61	ASP	2.4
3	Y	1467	GLN	2.4
3	Y	1565	HIS	2.4
1	L	152	ASN	2.4
1	L	35	TRP	2.4
1	L	123	GLU	2.3
1	A	41	GLY	2.3
1	L	134	CYS	2.3
3	Y	1546	CYS	2.3
2	H	114	ALA	2.3
2	H	197	ASN	2.3
1	L	7	SER	2.3
2	H	153	SER	2.3
2	H	169	VAL	2.3
2	B	133	GLY	2.2
2	B	174	GLY	2.2
2	H	25	SER	2.2
2	H	191	THR	2.2
1	L	19	VAL	2.2
1	L	135	LEU	2.2
2	H	80	LEU	2.2
1	L	186	TYR	2.2
3	X	1454	GLU	2.2
3	X	1691	SER	2.2
2	H	84	ALA	2.2
2	H	202	PRO	2.2
3	Y	1528	GLN	2.1
3	Y	1572	ALA	2.1
2	H	159	LEU	2.1
2	H	122	PHE	2.1
1	L	52	SER	2.1
1	A	107	LYS	2.1
1	L	184	ALA	2.1
1	L	106	ILE	2.1
2	B	100(J)	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	148	GLU	2.0
1	L	175	LEU	2.0
2	H	82(C)	LEU	2.0
2	H	188	SER	2.0
1	L	13	ALA	2.0
2	H	61	ASP	2.0
1	A	199	GLN	2.0
1	L	173	TYR	2.0
2	H	100(J)	VAL	2.0
1	L	170	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	X	2004	14/15	0.91	0.14	0.71	31,40,50,50	0
6	NAG	X	2005	14/15	0.84	0.21	-	53,56,61,64	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. 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
5	CA	Y	2001	1/1	0.86	0.42	3.46	67,67,67,67	0
5	CA	X	2001	1/1	0.97	0.18	1.68	43,43,43,43	0
5	CA	Y	2003	1/1	0.99	0.06	-1.69	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	Y	2002	1/1	0.99	0.06	-1.77	21,21,21,21	0
4	SO4	B	222	5/5	0.99	0.06	-2.07	31,32,32,33	0
5	CA	X	2002	1/1	1.00	0.03	-3.31	13,13,13,13	0
5	CA	X	2003	1/1	0.99	0.03	-4.91	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.