



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:08 am GMT

PDB ID : 4WRL  
Title : Structure of the human CSF-1:CSF-1R complex  
Authors : Felix, J.; De Munck, S.; Elegheert, J.; Savvides, S.N.  
Deposited on : 2014-10-24  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

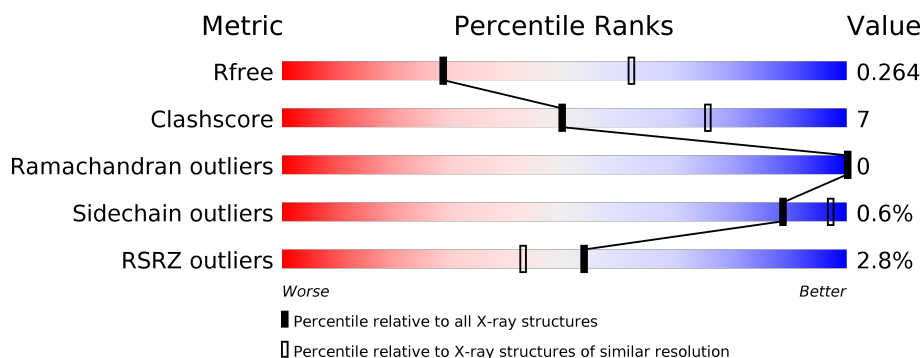
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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  $\geq 3$ , 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	286	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	286	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
2	B	170	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>12%</div> <div>17%</div> </div> </div>
2	D	170	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>11%</div> <div>17%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SIA	C	404	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6657 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 Macrophage colony-stimulating factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2074	1317	363	384	10			
1	C	277	Total	C	N	O	S	0	0	0
			2099	1333	366	390	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLN	ASN	engineered mutation	UNP P07333
A	297	GLY	-	expression tag	UNP P07333
A	298	THR	-	expression tag	UNP P07333
A	299	LYS	-	expression tag	UNP P07333
A	300	HIS	-	expression tag	UNP P07333
A	301	HIS	-	expression tag	UNP P07333
A	302	HIS	-	expression tag	UNP P07333
A	303	HIS	-	expression tag	UNP P07333
A	304	HIS	-	expression tag	UNP P07333
A	305	HIS	-	expression tag	UNP P07333
C	240	GLN	ASN	engineered mutation	UNP P07333
C	297	GLY	-	expression tag	UNP P07333
C	298	THR	-	expression tag	UNP P07333
C	299	LYS	-	expression tag	UNP P07333
C	300	HIS	-	expression tag	UNP P07333
C	301	HIS	-	expression tag	UNP P07333
C	302	HIS	-	expression tag	UNP P07333
C	303	HIS	-	expression tag	UNP P07333
C	304	HIS	-	expression tag	UNP P07333
C	305	HIS	-	expression tag	UNP P07333

- Molecule 2 is a protein called Macrophage colony-stimulating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1095	686	184	214	11			
2	D	141	Total	C	N	O	S	0	0	0
			1102	691	185	215	11			

There are 42 discrepancies between the modelled and reference sequences:

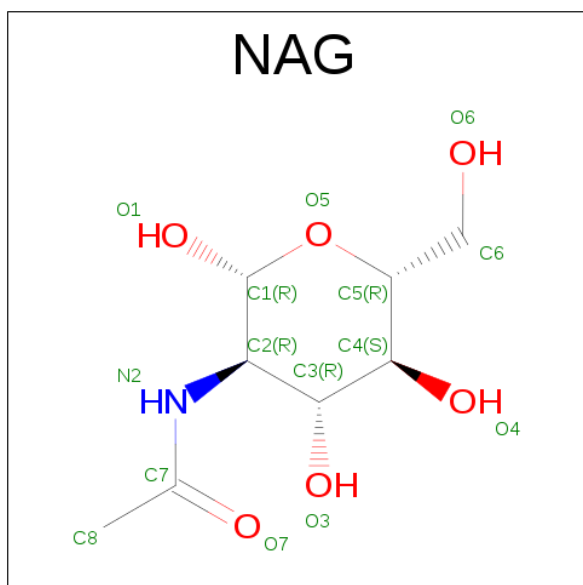
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP P09603
B	-19	GLY	-	expression tag	UNP P09603
B	-18	SER	-	expression tag	UNP P09603
B	-17	SER	-	expression tag	UNP P09603
B	-16	HIS	-	expression tag	UNP P09603
B	-15	HIS	-	expression tag	UNP P09603
B	-14	HIS	-	expression tag	UNP P09603
B	-13	HIS	-	expression tag	UNP P09603
B	-12	HIS	-	expression tag	UNP P09603
B	-11	HIS	-	expression tag	UNP P09603
B	-10	SER	-	expression tag	UNP P09603
B	-9	SER	-	expression tag	UNP P09603
B	-8	GLY	-	expression tag	UNP P09603
B	-7	LEU	-	expression tag	UNP P09603
B	-6	VAL	-	expression tag	UNP P09603
B	-5	PRO	-	expression tag	UNP P09603
B	-4	ARG	-	expression tag	UNP P09603
B	-3	GLY	-	expression tag	UNP P09603
B	-2	SER	-	expression tag	UNP P09603
B	-1	HIS	-	expression tag	UNP P09603
B	0	MET	-	expression tag	UNP P09603
D	-20	MET	-	initiating methionine	UNP P09603
D	-19	GLY	-	expression tag	UNP P09603
D	-18	SER	-	expression tag	UNP P09603
D	-17	SER	-	expression tag	UNP P09603
D	-16	HIS	-	expression tag	UNP P09603
D	-15	HIS	-	expression tag	UNP P09603
D	-14	HIS	-	expression tag	UNP P09603
D	-13	HIS	-	expression tag	UNP P09603
D	-12	HIS	-	expression tag	UNP P09603
D	-11	HIS	-	expression tag	UNP P09603
D	-10	SER	-	expression tag	UNP P09603
D	-9	SER	-	expression tag	UNP P09603
D	-8	GLY	-	expression tag	UNP P09603
D	-7	LEU	-	expression tag	UNP P09603

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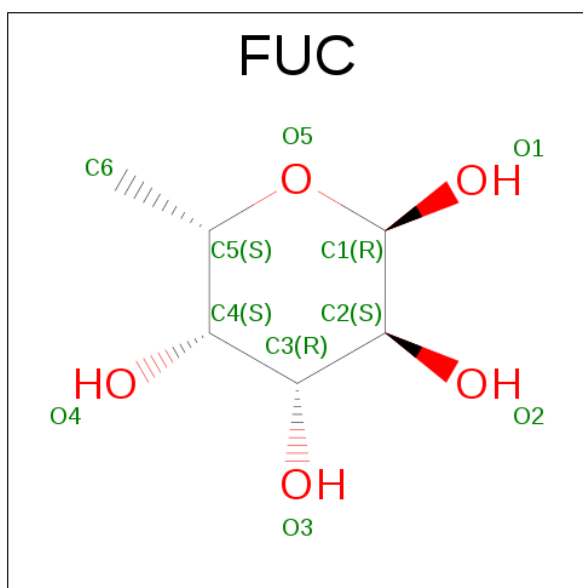
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	VAL	-	expression tag	UNP P09603
D	-5	PRO	-	expression tag	UNP P09603
D	-4	ARG	-	expression tag	UNP P09603
D	-3	GLY	-	expression tag	UNP P09603
D	-2	SER	-	expression tag	UNP P09603
D	-1	HIS	-	expression tag	UNP P09603
D	0	MET	-	expression tag	UNP P09603

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



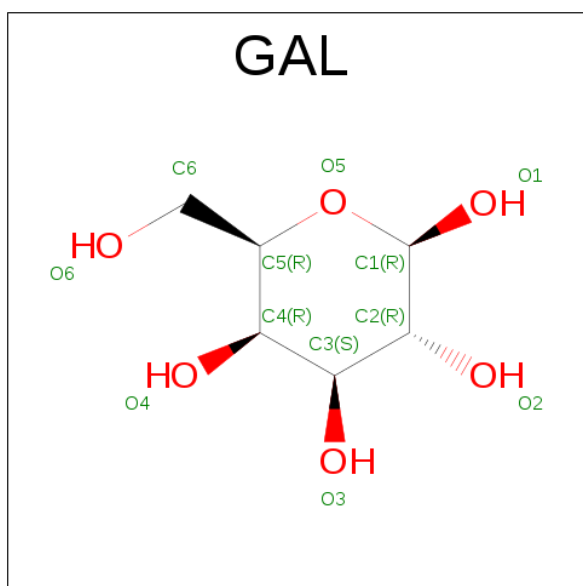
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



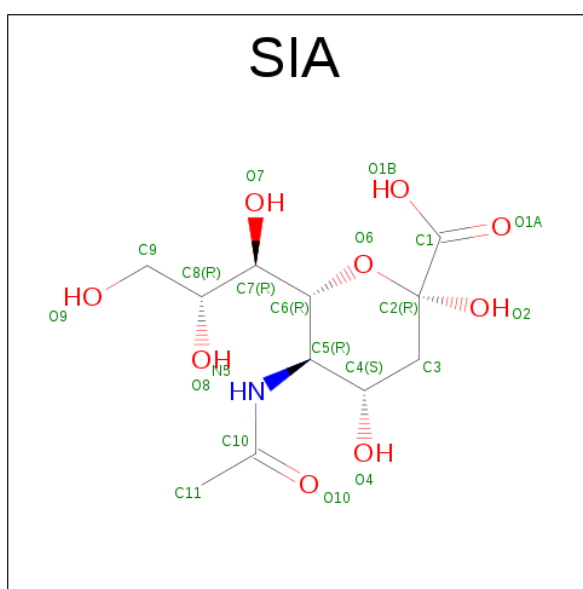
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is O-SIALIC ACID (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



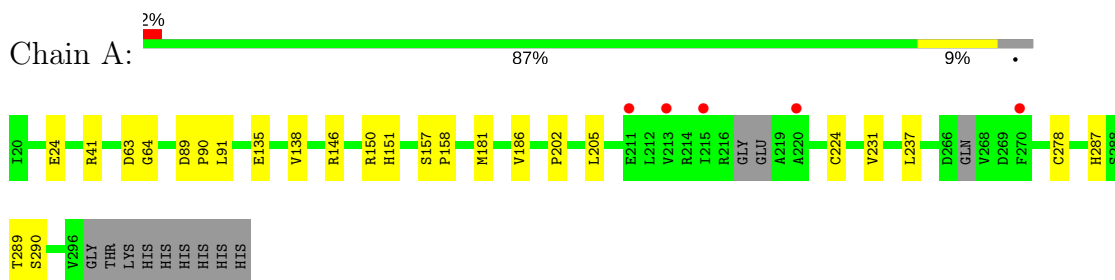
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	11	1	8		
6	A	1	Total	C	N	O	0	0
			20	11	1	8		
6	A	1	Total	C	N	O	0	0
			20	11	1	8		
6	C	1	Total	C	N	O	0	0
			20	11	1	8		
6	C	1	Total	C	N	O	0	0
			20	11	1	8		



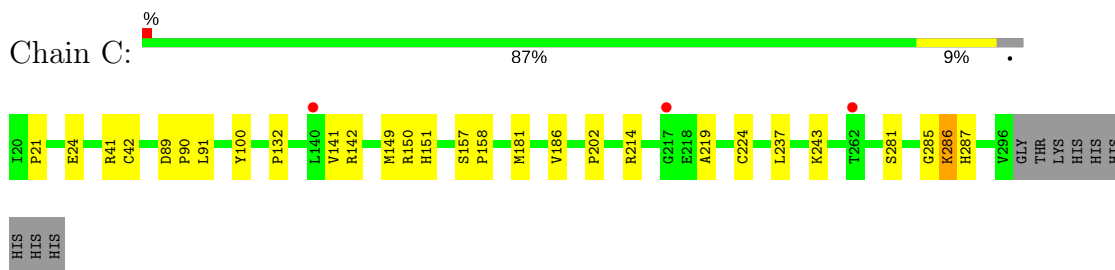
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

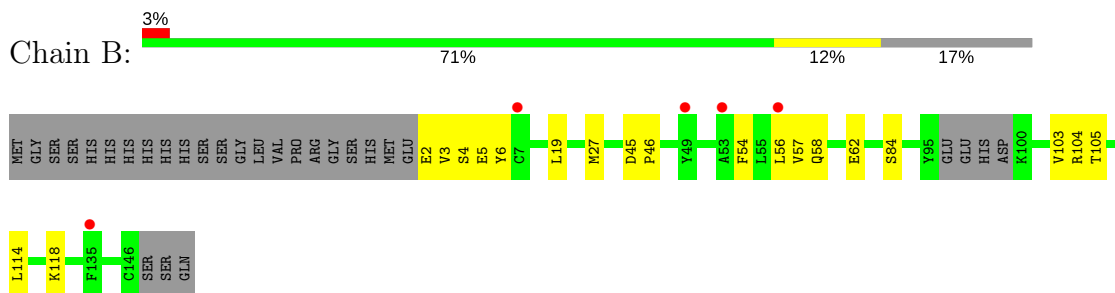
- Molecule 1: Macrophage colony-stimulating factor 1 receptor



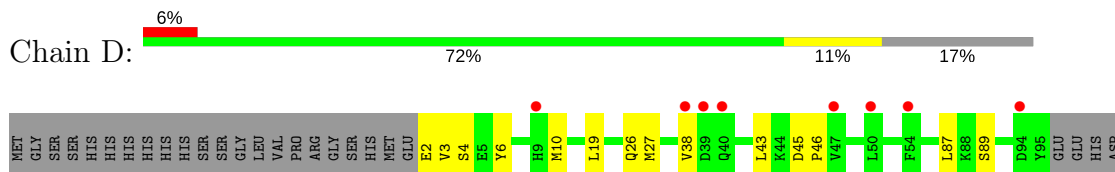
- Molecule 1: Macrophage colony-stimulating factor 1 receptor

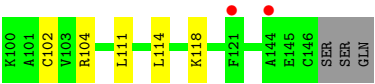


- Molecule 2: Macrophage colony-stimulating factor 1



- Molecule 2: Macrophage colony-stimulating factor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.00Å 143.00Å 138.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.80 49.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.71-2.80) 99.8 (49.71-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.223 , 0.261 0.229 , 0.264	Depositor DCC
$R_{free}$ test set	1705 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h 0.013 for -l,-k,-h 0.012 for -h,-l,-k 0.007 for -h,l,k 0.418 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SIA, GAL, NAG, FUC

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	0.32	0/2126	0.44	0/2905
1	C	0.29	0/2152	0.44	0/2942
2	B	0.23	0/1111	0.39	0/1504
2	D	0.25	0/1118	0.39	0/1513
All	All	0.28	0/6507	0.42	0/8864

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	2074	0	1999	17	0
1	C	2099	0	2038	22	0
2	B	1095	0	1018	17	1
2	D	1102	0	1033	14	1
3	A	56	0	48	1	0
3	C	56	0	49	2	0
4	A	10	0	10	0	0
4	C	10	0	10	0	0
5	A	33	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	22	0	18	3	0
6	A	60	0	51	6	0
6	C	40	0	34	13	0
All	All	6657	0	6335	87	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (87) 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)
2:D:3:VAL:HG22	2:D:89:SER:O	1.73	0.88
5:A:406:GAL:O4	6:A:407:SIA:O1A	1.92	0.87
1:C:90:PRO:O	1:C:91:LEU:HB2	1.74	0.86
1:C:281:SER:CB	1:C:286:LYS:HG3	2.11	0.81
6:C:404:SIA:H113	6:C:404:SIA:H4	1.61	0.81
1:C:286:LYS:HD2	1:C:286:LYS:N	1.96	0.80
1:A:90:PRO:O	1:A:91:LEU:HB2	1.83	0.77
2:B:104:ARG:HD2	2:B:105:THR:N	2.00	0.76
1:C:281:SER:HB3	1:C:286:LYS:HG3	1.68	0.75
6:C:404:SIA:HN5	6:C:404:SIA:H91	1.53	0.73
3:C:405:NAG:O3	3:C:405:NAG:H82	1.91	0.70
6:C:404:SIA:H6	6:C:404:SIA:C11	2.22	0.69
6:C:404:SIA:H91	6:C:404:SIA:N5	2.08	0.69
2:B:104:ARG:NE	2:B:105:THR:O	2.26	0.68
1:A:90:PRO:O	1:A:91:LEU:CB	2.43	0.65
1:C:89:ASP:OD1	1:C:90:PRO:HD2	1.96	0.64
1:C:281:SER:HB2	1:C:286:LYS:HG3	1.81	0.63
1:C:281:SER:HB2	1:C:286:LYS:HE2	1.79	0.63
1:A:89:ASP:OD1	1:A:90:PRO:HD2	1.98	0.63
2:B:104:ARG:HD2	2:B:105:THR:H	1.64	0.62
6:C:404:SIA:H112	6:C:404:SIA:H6	1.84	0.60
1:C:214:ARG:NH1	1:C:219:ALA:O	2.34	0.59
6:C:409:SIA:O1B	6:C:409:SIA:H6	2.02	0.59
3:C:401:NAG:H61	5:C:403:GAL:H2	1.85	0.59
1:A:89:ASP:OD1	1:A:90:PRO:CD	2.51	0.58
1:C:90:PRO:O	1:C:91:LEU:CB	2.46	0.58
1:A:290:SER:OG	3:A:409:NAG:O7	2.14	0.57
1:C:224:CYS:HB2	1:C:237:LEU:HD13	1.88	0.56
1:C:202:PRO:HB2	1:C:287:HIS:HB2	1.88	0.56
2:B:4:SER:HG	2:B:6:TYR:HD2	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:411:SIA:O1B	6:A:411:SIA:H4	2.06	0.55
6:C:404:SIA:H5	6:C:404:SIA:C9	2.35	0.55
1:C:89:ASP:OD1	1:C:90:PRO:CD	2.55	0.55
6:C:404:SIA:H91	6:C:404:SIA:C5	2.38	0.54
2:B:56:LEU:HD11	2:B:103:VAL:HG11	1.92	0.52
1:A:224:CYS:HB2	1:A:237:LEU:HD13	1.92	0.52
2:B:104:ARG:CD	2:B:105:THR:N	2.73	0.51
1:A:202:PRO:HB2	1:A:287:HIS:HB2	1.93	0.51
5:A:406:GAL:HO4	6:A:407:SIA:C1	2.17	0.51
2:D:4:SER:OG	2:D:6:TYR:CD2	2.64	0.50
5:A:406:GAL:O4	6:A:407:SIA:C1	2.60	0.50
2:B:2:GLU:O	2:B:3:VAL:C	2.48	0.50
2:B:114:LEU:HD21	2:D:27:MET:HE1	1.94	0.50
2:B:104:ARG:CD	2:B:105:THR:O	2.60	0.49
1:C:150:ARG:HG2	1:C:151:HIS:CD2	2.47	0.49
6:C:404:SIA:C9	6:C:404:SIA:C5	2.90	0.49
6:A:404:SIA:O10	6:A:404:SIA:O4	2.31	0.48
1:C:285:GLY:C	1:C:286:LYS:HD2	2.33	0.48
1:A:181:MET:HE2	1:A:186:VAL:HG11	1.95	0.48
1:A:205:LEU:HD13	1:A:289:THR:HG22	1.96	0.47
5:A:410:GAL:H3	6:A:411:SIA:H32	1.35	0.47
1:A:150:ARG:HG2	1:A:151:HIS:CD2	2.50	0.46
2:B:4:SER:OG	2:B:5:GLU:N	2.47	0.46
1:A:89:ASP:HA	1:A:90:PRO:HD3	1.84	0.46
2:D:10:MET:HE3	2:D:87:LEU:HD23	1.96	0.46
2:B:27:MET:HE1	2:D:114:LEU:HD21	1.98	0.46
2:D:2:GLU:HB3	2:D:89:SER:HB2	1.97	0.46
1:A:63:ASP:OD1	1:A:64:GLY:N	2.49	0.45
2:D:19:LEU:HD13	2:D:118:LYS:HA	1.99	0.45
2:B:19:LEU:HD13	2:B:118:LYS:HA	1.99	0.45
1:C:286:LYS:CD	1:C:286:LYS:N	2.73	0.45
1:C:181:MET:HE2	1:C:186:VAL:HG21	1.99	0.44
1:C:24:GLU:OE2	1:C:41:ARG:NH1	2.41	0.43
2:D:26:GLN:HB2	2:D:111:LEU:HD21	2.00	0.43
2:B:58:GLN:HE22	2:B:84:SER:HB3	1.83	0.43
5:C:408:GAL:O2	6:C:409:SIA:H31	2.19	0.43
2:B:104:ARG:HD2	2:B:105:THR:O	2.19	0.42
1:A:157:SER:HA	1:A:158:PRO:HD3	1.87	0.42
1:C:142:ARG:NH2	2:B:62:GLU:OE1	2.30	0.42
1:C:141:VAL:HG22	1:C:142:ARG:H	1.85	0.42
2:D:43:LEU:HD11	2:D:102:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:TYR:CD1	1:C:132:PRO:HD3	2.55	0.42
2:B:45:ASP:HA	2:B:46:PRO:HD2	1.93	0.42
1:C:21:PRO:HB2	1:C:42:CYS:SG	2.60	0.41
2:D:38:VAL:HG23	2:D:43:LEU:HD13	2.02	0.41
1:A:24:GLU:OE1	1:A:41:ARG:NH1	2.44	0.41
2:B:54:PHE:O	2:B:57:VAL:HG22	2.20	0.41
1:C:157:SER:HA	1:C:158:PRO:HD3	1.89	0.41
5:C:403:GAL:H3	6:C:404:SIA:O1A	2.07	0.41
1:A:135:GLU:O	1:A:138:VAL:HG22	2.21	0.41
1:A:231:VAL:HG11	2:D:10:MET:SD	2.61	0.41
6:C:409:SIA:O1B	6:C:409:SIA:H4	2.20	0.41
2:D:45:ASP:HA	2:D:46:PRO:HD2	1.93	0.41
6:C:404:SIA:H6	6:C:404:SIA:H113	1.98	0.41
2:D:4:SER:HG	2:D:6:TYR:HD2	1.63	0.41
1:A:278:CYS:N	1:A:289:THR:O	2.44	0.41
2:D:2:GLU:HG2	2:D:2:GLU:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ARG:CG	2:D:104:ARG:NH2[4_554]	2.03	0.17

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/286 (94%)	258 (96%)	10 (4%)	0	100	100
1	C	275/286 (96%)	259 (94%)	16 (6%)	0	100	100
2	B	137/170 (81%)	132 (96%)	5 (4%)	0	100	100
2	D	137/170 (81%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	817/912 (90%)	781 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/249 (91%)	225 (100%)	1 (0%)	93	98
1	C	230/249 (92%)	227 (99%)	3 (1%)	73	93
2	B	120/160 (75%)	120 (100%)	0	100	100
2	D	122/160 (76%)	122 (100%)	0	100	100
All	All	698/818 (85%)	694 (99%)	4 (1%)	89	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	C	149	MET
1	C	243	LYS
1	C	286	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	401	1,5,4	14,14,15	0.78	1 (7%)	15,19,21	1.21	3 (20%)
4	FUC	A	402	3	9,10,11	0.64	0	13,14,16	0.96	1 (7%)
5	GAL	A	403	3,6	11,11,12	0.82	1 (9%)	13,15,17	2.53	4 (30%)
6	SIA	A	404	5	17,20,21	0.25	0	19,28,31	0.50	0
3	NAG	A	405	1,5	14,14,15	1.14	1 (7%)	15,19,21	0.95	0
5	GAL	A	406	3	11,11,12	2.49	3 (27%)	13,15,17	1.79	4 (30%)
6	SIA	A	407	-	17,20,21	0.24	0	19,28,31	0.50	0
3	NAG	A	408	1	14,14,15	0.32	0	15,19,21	0.48	0
3	NAG	A	409	1,5	14,14,15	0.46	0	15,19,21	1.63	3 (20%)
5	GAL	A	410	3,6	11,11,12	0.80	0	13,15,17	1.40	2 (15%)
6	SIA	A	411	5	17,20,21	0.24	0	19,28,31	0.51	0
3	NAG	C	401	1,5,4	14,14,15	0.46	0	15,19,21	1.35	2 (13%)
4	FUC	C	402	3	9,10,11	0.73	0	13,14,16	1.10	1 (7%)
5	GAL	C	403	3,6	11,11,12	1.42	2 (18%)	13,15,17	2.06	3 (23%)
6	SIA	C	404	5	17,20,21	0.25	0	19,28,31	0.50	0
3	NAG	C	405	1	14,14,15	0.35	0	15,19,21	1.56	3 (20%)
3	NAG	C	406	1	14,14,15	0.27	0	15,19,21	0.40	0
3	NAG	C	407	1,5	14,14,15	0.41	0	15,19,21	0.95	1 (6%)
5	GAL	C	408	3,6	11,11,12	1.35	1 (9%)	13,15,17	1.75	3 (23%)
6	SIA	C	409	5	17,20,21	0.25	0	19,28,31	0.50	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
3	NAG	A	401	1,5,4	-	0/6/23/26	0/1/1/1
4	FUC	A	402	3	-	0/0/17/20	0/1/1/1
5	GAL	A	403	3,6	-	0/2/19/22	0/1/1/1
6	SIA	A	404	5	-	0/14/34/38	0/1/1/1
3	NAG	A	405	1,5	-	0/6/23/26	0/1/1/1
5	GAL	A	406	3	-	0/2/19/22	0/1/1/1
6	SIA	A	407	-	-	0/14/34/38	0/1/1/1
3	NAG	A	408	1	-	0/6/23/26	0/1/1/1
3	NAG	A	409	1,5	-	0/6/23/26	0/1/1/1
5	GAL	A	410	3,6	-	0/2/19/22	0/1/1/1
6	SIA	A	411	5	-	0/14/34/38	0/1/1/1
3	NAG	C	401	1,5,4	-	0/6/23/26	0/1/1/1
4	FUC	C	402	3	-	0/0/17/20	0/1/1/1
5	GAL	C	403	3,6	-	0/2/19/22	0/1/1/1
6	SIA	C	404	5	-	0/14/34/38	0/1/1/1
3	NAG	C	405	1	-	1/6/23/26	0/1/1/1
3	NAG	C	406	1	-	0/6/23/26	0/1/1/1
3	NAG	C	407	1,5	-	0/6/23/26	0/1/1/1
5	GAL	C	408	3,6	-	0/2/19/22	0/1/1/1
6	SIA	C	409	5	-	0/14/34/38	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	NAG	O5-C1	-3.88	1.37	1.43
5	C	403	GAL	C2-C3	-3.03	1.48	1.52
5	A	403	GAL	C2-C3	-2.21	1.49	1.52
5	C	403	GAL	O3-C3	2.20	1.48	1.43
3	A	401	NAG	C1-C2	2.79	1.56	1.52
5	C	408	GAL	C2-C3	3.26	1.56	1.52
5	A	406	GAL	C2-C3	3.84	1.57	1.52
5	A	406	GAL	O3-C3	4.51	1.53	1.43
5	A	406	GAL	C4-C3	5.50	1.66	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	GAL	O3-C3-C2	-4.30	102.20	110.02
5	C	408	GAL	O3-C3-C4	-3.16	103.49	110.36
3	C	405	NAG	C4-C3-C2	-2.72	107.04	111.02
3	C	405	NAG	O5-C1-C2	-2.37	108.17	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C3-C4-C5	-2.34	106.10	110.22
5	C	403	GAL	C3-C4-C5	-2.29	106.18	110.22
5	A	406	GAL	O5-C1-C2	-2.00	107.65	110.79
3	A	401	NAG	C1-O5-C5	2.02	114.94	112.17
4	A	402	FUC	C1-O5-C5	2.03	116.87	112.39
3	A	401	NAG	O4-C4-C5	2.04	114.42	109.28
4	C	402	FUC	C1-O5-C5	2.12	117.08	112.39
3	C	407	NAG	C2-N2-C7	2.16	126.09	122.94
3	A	409	NAG	C2-N2-C7	2.31	126.32	122.94
3	C	401	NAG	C1-O5-C5	2.37	115.43	112.17
5	A	406	GAL	C2-C3-C4	2.39	115.05	110.88
5	C	408	GAL	C1-O5-C5	2.43	115.52	112.17
5	A	403	GAL	O5-C1-C2	2.68	114.99	110.79
5	A	410	GAL	C1-O5-C5	2.70	115.89	112.17
5	C	403	GAL	O3-C3-C2	2.76	115.05	110.02
3	A	409	NAG	O4-C4-C3	2.99	116.87	110.36
5	A	406	GAL	O3-C3-C4	3.26	117.45	110.36
5	A	406	GAL	O4-C4-C3	3.34	117.63	110.36
5	A	410	GAL	C1-C2-C3	3.40	113.95	109.65
3	A	409	NAG	C1-O5-C5	3.67	117.22	112.17
3	C	405	NAG	C2-N2-C7	3.78	128.46	122.94
3	C	401	NAG	O4-C4-C5	3.90	119.11	109.28
5	C	408	GAL	C1-C2-C3	4.53	115.39	109.65
5	A	403	GAL	C1-O5-C5	4.66	118.59	112.17
5	C	403	GAL	C1-O5-C5	4.79	118.77	112.17
5	A	403	GAL	C1-C2-C3	5.33	116.41	109.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	405	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	404	SIA	1	0
5	A	406	GAL	3	0
6	A	407	SIA	3	0
3	A	409	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	410	GAL	1	0
6	A	411	SIA	2	0
3	C	401	NAG	1	0
5	C	403	GAL	2	0
6	C	404	SIA	10	0
3	C	405	NAG	1	0
5	C	408	GAL	1	0
6	C	409	SIA	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/286 (95%)	0.08	5 (1%) 69 60	48, 83, 146, 188	0
1	C	277/286 (96%)	0.02	3 (1%) 80 74	44, 84, 137, 168	0
2	B	141/170 (82%)	0.12	5 (3%) 44 33	50, 104, 168, 217	0
2	D	141/170 (82%)	0.32	10 (7%) 17 9	53, 102, 169, 189	0
All	All	833/912 (91%)	0.11	23 (2%) 53 43	44, 92, 157, 217	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ALA	5.8
2	B	135	PHE	4.6
2	B	53	ALA	3.5
2	D	9	HIS	3.4
2	D	47	VAL	3.4
1	A	211	GLU	3.1
2	D	144	ALA	3.0
1	A	215	ILE	2.9
1	C	262	THR	2.7
1	C	217	GLY	2.6
1	A	213	VAL	2.5
2	D	94	ASP	2.5
2	D	54	PHE	2.5
1	A	270	PHE	2.4
2	B	56	LEU	2.3
2	B	7	CYS	2.3
1	C	140	LEU	2.2
2	D	39	ASP	2.2
2	D	50	LEU	2.2
2	D	40	GLN	2.1
2	D	121	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	38	VAL	2.1
2	B	49	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	409	14/15	0.85	0.17	-0.38	146,151,162,179	0
5	GAL	A	403	11/12	0.72	0.14	-	130,150,161,173	0
3	NAG	C	401	14/15	0.90	0.16	-	98,107,134,136	0
3	NAG	C	406	14/15	0.78	0.23	-	123,140,142,145	0
3	NAG	A	401	14/15	0.91	0.15	-	113,120,145,155	0
4	FUC	C	402	10/11	0.88	0.16	-	137,147,151,160	0
6	SIA	A	404	20/21	0.62	0.20	-	152,169,185,190	0
6	SIA	C	404	20/21	0.66	0.25	-	151,180,189,191	0
3	NAG	A	405	14/15	0.76	0.15	-	130,153,158,166	0
4	FUC	A	402	10/11	0.88	0.16	-	124,133,141,145	0
5	GAL	C	403	11/12	0.73	0.18	-	124,144,161,172	0
3	NAG	A	408	14/15	0.64	0.19	-	150,162,168,170	0
3	NAG	C	407	14/15	0.69	0.19	-	138,151,169,170	0
6	SIA	C	409	20/21	0.73	0.28	-	179,210,225,232	0
5	GAL	C	408	11/12	0.82	0.12	-	134,142,186,189	0
6	SIA	A	411	20/21	0.70	0.23	-	163,182,200,201	0
5	GAL	A	410	11/12	0.83	0.14	-	184,203,208,208	0
5	GAL	A	406	11/12	0.63	0.15	-	181,198,224,227	0
6	SIA	A	407	20/21	0.73	0.13	-	182,203,218,221	0
3	NAG	C	405	14/15	0.77	0.16	-	145,154,167,175	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.