



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2021 – 12:02 PM EDT

PDB ID : 3QS7  
Title : Crystal structure of a human Flt3 ligand-receptor ternary complex  
Authors : Verstraete, K.; Savvides, S.N.  
Deposited on : 2011-02-19  
Resolution : 4.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17.1  
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) : 2.17.1

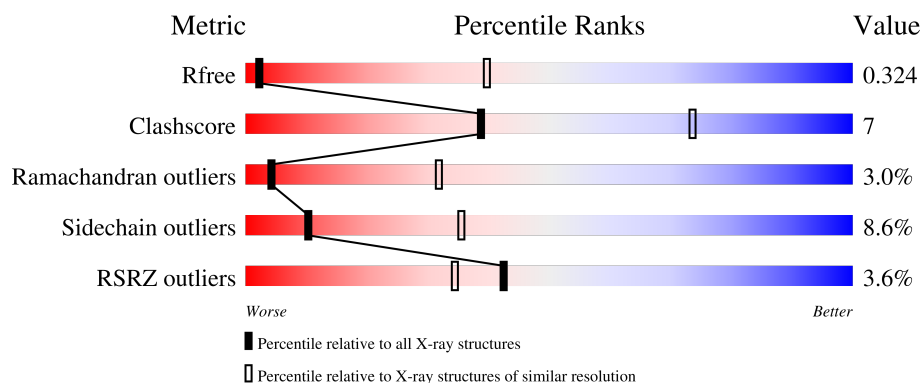
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	138	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	B	138	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	C	138	<div> <div>2%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	D	138	<div> <div>%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>
2	E	423	<div> <div>4%</div> <div>61%</div> <div>15%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	423	
2	G	423	
2	H	423	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	504	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10865 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 SL cytokine.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			984	631	163	182	8			
1	B	134	Total	C	N	O	S	0	0	0
			997	639	170	180	8			
1	C	135	Total	C	N	O	S	0	0	0
			987	629	163	187	8			
1	D	132	Total	C	N	O	S	0	0	0
			950	612	153	177	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P49771
A	-2	SER	-	expression tag	UNP P49771
A	-1	HIS	-	expression tag	UNP P49771
A	0	MET	-	expression tag	UNP P49771
B	-3	GLY	-	expression tag	UNP P49771
B	-2	SER	-	expression tag	UNP P49771
B	-1	HIS	-	expression tag	UNP P49771
B	0	MET	-	expression tag	UNP P49771
C	-3	GLY	-	expression tag	UNP P49771
C	-2	SER	-	expression tag	UNP P49771
C	-1	HIS	-	expression tag	UNP P49771
C	0	MET	-	expression tag	UNP P49771
D	-3	GLY	-	expression tag	UNP P49771
D	-2	SER	-	expression tag	UNP P49771
D	-1	HIS	-	expression tag	UNP P49771
D	0	MET	-	expression tag	UNP P49771

- Molecule 2 is a protein called FL cytokine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	328	Total	C	N	O	S	0	0	0
			2049	1334	349	352	14			
2	F	336	Total	C	N	O	S	0	0	0
			2087	1357	356	361	13			
2	G	168	Total	C	N	O	S	0	0	0
			1070	698	183	182	7			
2	H	259	Total	C	N	O	S	0	0	0
			1643	1072	278	282	11			

There are 52 discrepancies between the modelled and reference sequences:

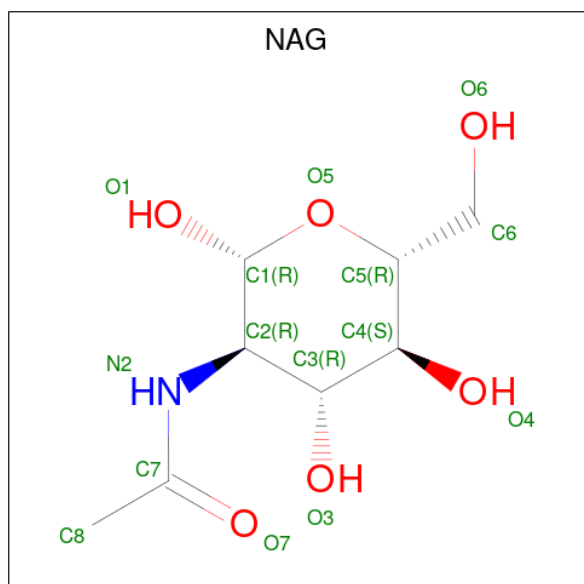
Chain	Residue	Modelled	Actual	Comment	Reference
E	24	GLU	-	expression tag	UNP P36888
E	25	THR	-	expression tag	UNP P36888
E	26	GLY	-	expression tag	UNP P36888
E	437	SER	-	expression tag	UNP P36888
E	438	GLY	-	expression tag	UNP P36888
E	439	THR	-	expression tag	UNP P36888
E	440	LYS	-	expression tag	UNP P36888
E	441	HIS	-	expression tag	UNP P36888
E	442	HIS	-	expression tag	UNP P36888
E	443	HIS	-	expression tag	UNP P36888
E	444	HIS	-	expression tag	UNP P36888
E	445	HIS	-	expression tag	UNP P36888
E	446	HIS	-	expression tag	UNP P36888
F	24	GLU	-	expression tag	UNP P36888
F	25	THR	-	expression tag	UNP P36888
F	26	GLY	-	expression tag	UNP P36888
F	437	SER	-	expression tag	UNP P36888
F	438	GLY	-	expression tag	UNP P36888
F	439	THR	-	expression tag	UNP P36888
F	440	LYS	-	expression tag	UNP P36888
F	441	HIS	-	expression tag	UNP P36888
F	442	HIS	-	expression tag	UNP P36888
F	443	HIS	-	expression tag	UNP P36888
F	444	HIS	-	expression tag	UNP P36888
F	445	HIS	-	expression tag	UNP P36888
F	446	HIS	-	expression tag	UNP P36888
G	24	GLU	-	expression tag	UNP P36888
G	25	THR	-	expression tag	UNP P36888
G	26	GLY	-	expression tag	UNP P36888
G	437	SER	-	expression tag	UNP P36888
G	438	GLY	-	expression tag	UNP P36888

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Chain	Residue	Modelled	Actual	Comment	Reference
G	439	THR	-	expression tag	UNP P36888
G	440	LYS	-	expression tag	UNP P36888
G	441	HIS	-	expression tag	UNP P36888
G	442	HIS	-	expression tag	UNP P36888
G	443	HIS	-	expression tag	UNP P36888
G	444	HIS	-	expression tag	UNP P36888
G	445	HIS	-	expression tag	UNP P36888
G	446	HIS	-	expression tag	UNP P36888
H	24	GLU	-	expression tag	UNP P36888
H	25	THR	-	expression tag	UNP P36888
H	26	GLY	-	expression tag	UNP P36888
H	437	SER	-	expression tag	UNP P36888
H	438	GLY	-	expression tag	UNP P36888
H	439	THR	-	expression tag	UNP P36888
H	440	LYS	-	expression tag	UNP P36888
H	441	HIS	-	expression tag	UNP P36888
H	442	HIS	-	expression tag	UNP P36888
H	443	HIS	-	expression tag	UNP P36888
H	444	HIS	-	expression tag	UNP P36888
H	445	HIS	-	expression tag	UNP P36888
H	446	HIS	-	expression tag	UNP P36888

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

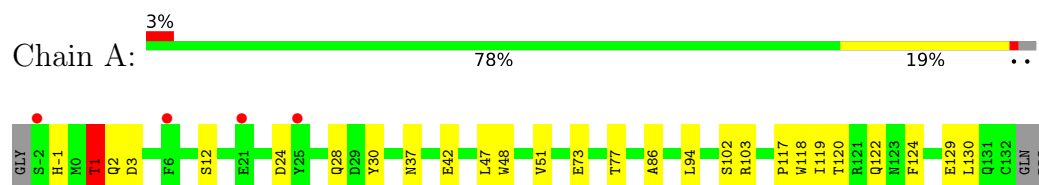


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 14	C 8	N 1	O 5	0	0
3	F	1	Total 14	C 8	N 1	O 5	0	0
3	F	1	Total 14	C 8	N 1	O 5	0	0
3	F	1	Total 14	C 8	N 1	O 5	0	0
3	G	1	Total 14	C 8	N 1	O 5	0	0
3	H	1	Total 14	C 8	N 1	O 5	0	0
3	H	1	Total 14	C 8	N 1	O 5	0	0

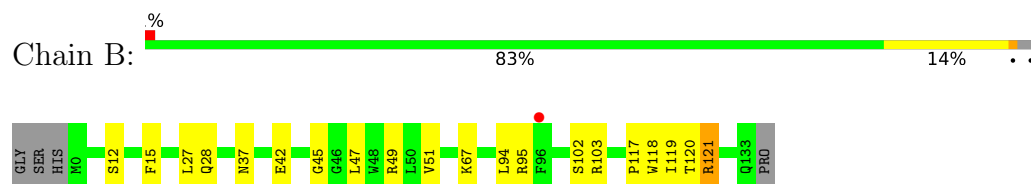
### 3 Residue-property plots [i](#)

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.

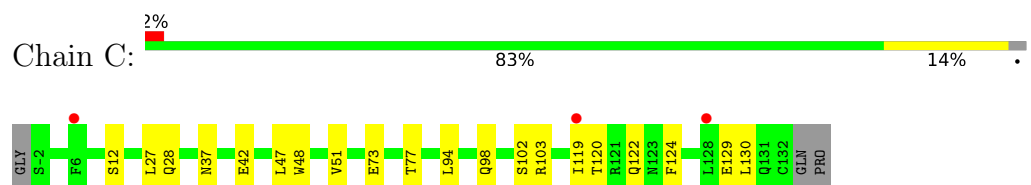
- Molecule 1: SL cytokine



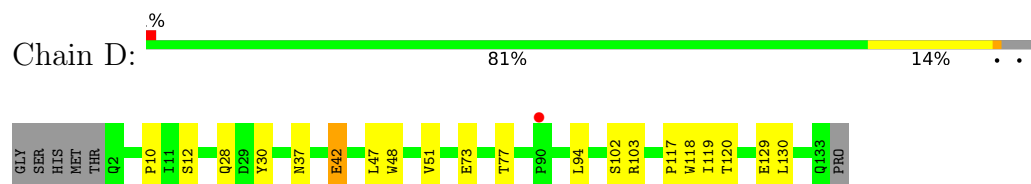
- Molecule 1: SL cytokine



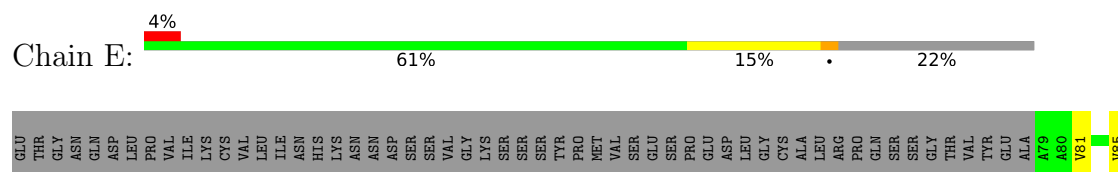
- Molecule 1: SL cytokine



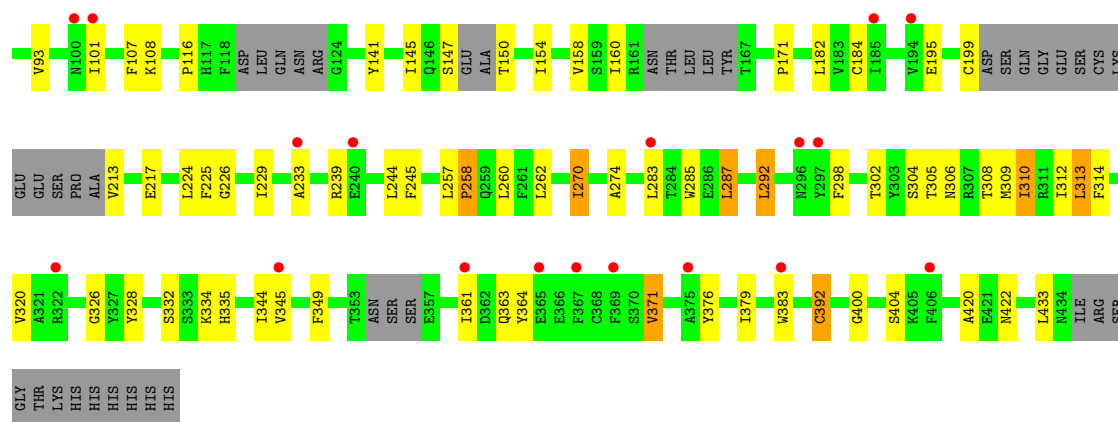
- Molecule 1: SL cytokine



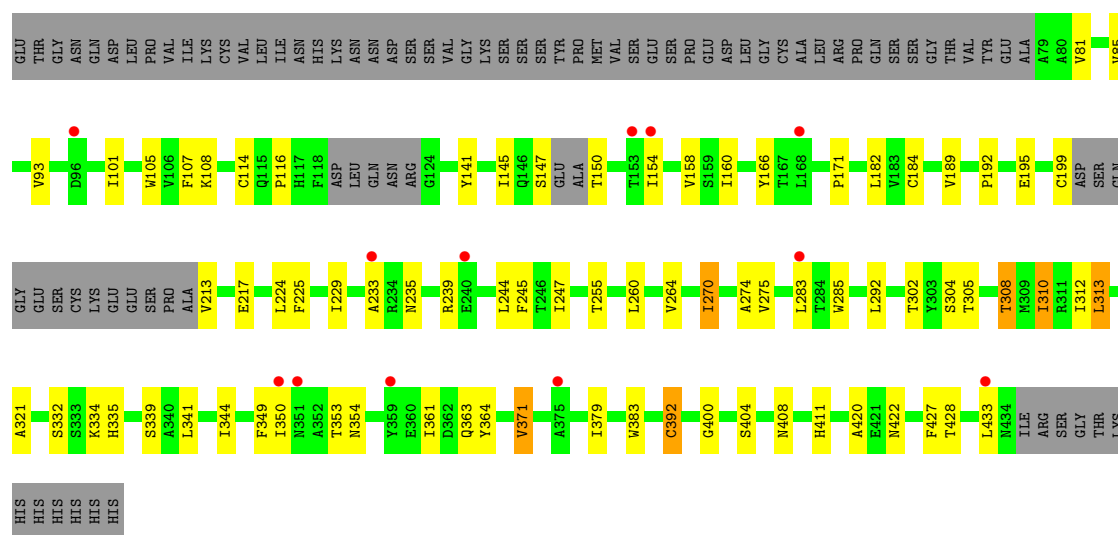
- Molecule 2: FL cytokine receptor



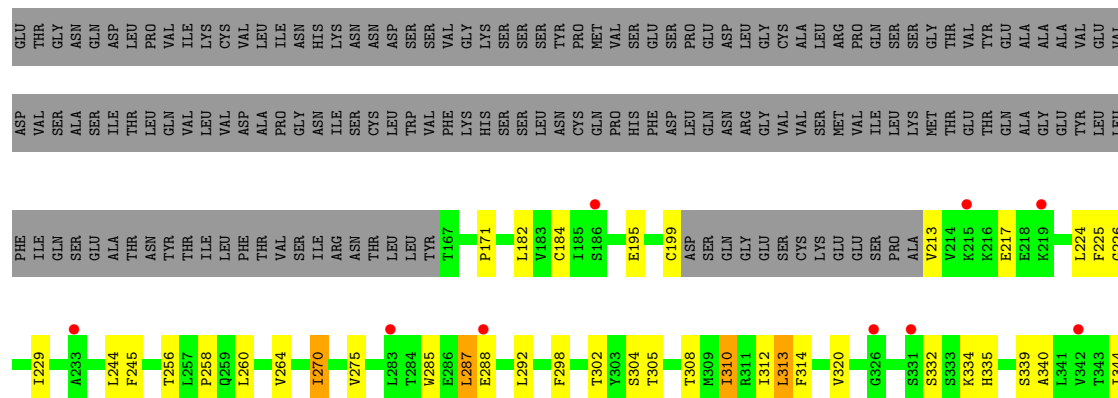




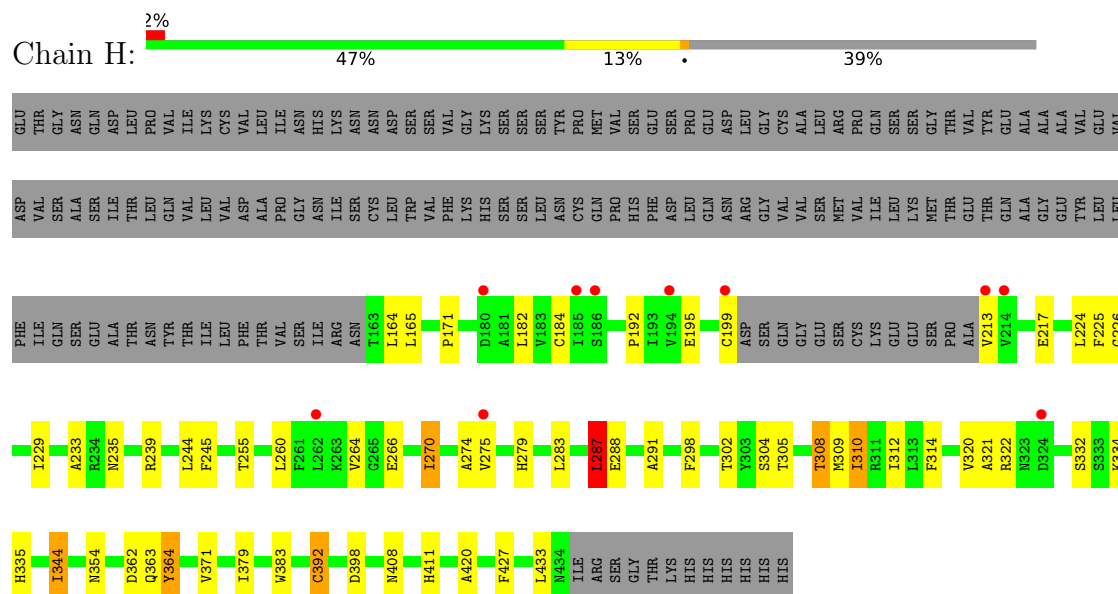
• Molecule 2: FL cytokine receptor



• Molecule 2: FL cytokine receptor



- Molecule 2: FL cytokine receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.89Å 146.26Å 105.95Å 90.00° 109.66° 90.00°	Depositor
Resolution (Å)	39.04 – 4.30 39.04 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.04-4.30) 93.2 (39.04-4.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 4.28Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, $R_{free}$	0.260 , 0.281 0.287 , 0.324	Depositor DCC
$R_{free}$ test set	1010 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	161.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 303.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	10865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/1005	0.57	1/1380 (0.1%)
1	B	0.37	0/1018	0.52	0/1392
1	C	0.36	0/1006	0.53	0/1379
1	D	0.37	0/970	0.52	0/1334
2	E	0.53	0/2089	0.69	0/2886
2	F	0.51	0/2129	0.69	0/2950
2	G	0.49	0/1093	0.69	0/1515
2	H	0.54	0/1684	0.71	0/2331
All	All	0.47	0/10994	0.64	1/15167 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	THR	C-N-CA	5.54	135.56	121.70

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	984	0	898	13	0
1	B	997	0	935	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	987	0	904	10	0
1	D	950	0	861	12	0
2	E	2049	0	1534	31	0
2	F	2087	0	1552	33	0
2	G	1070	0	844	19	0
2	H	1643	0	1207	27	0
3	E	14	0	13	0	0
3	F	42	0	39	2	0
3	G	14	0	13	0	0
3	H	28	0	26	0	0
All	All	10865	0	8826	147	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 7.

All (147) 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:H:287:LEU:HD23	2:H:288:GLU:H	1.38	0.89
2:F:147:SER:HG	2:F:150:THR:N	1.84	0.76
2:H:304:SER:HB2	2:H:310:ILE:HD11	1.71	0.72
2:F:304:SER:HB2	2:F:310:ILE:HD11	1.73	0.70
2:H:322:ARG:HA	2:H:344:ILE:HG21	1.71	0.69
1:A:1:THR:CB	1:A:86:ALA:HB2	2.23	0.69
2:E:147:SER:HG	2:E:150:THR:N	1.92	0.68
2:E:304:SER:HB2	2:E:310:ILE:HD11	1.76	0.66
2:H:379:ILE:HD13	2:H:420:ALA:HB1	1.78	0.64
2:E:345:VAL:HG21	2:E:349:PHE:CD2	2.35	0.62
2:E:182:LEU:HB2	2:E:224:LEU:HD21	1.82	0.62
1:A:119:ILE:HG23	1:A:120:THR:HG23	1.82	0.62
1:C:122:GLN:HB2	1:C:124:PHE:CZ	2.35	0.62
2:G:182:LEU:HB2	2:G:224:LEU:HD21	1.83	0.61
2:F:349:PHE:CE1	3:F:504:NAG:H82	2.35	0.61
2:H:182:LEU:HB2	2:H:224:LEU:HD21	1.84	0.60
1:A:122:GLN:HB2	1:A:124:PHE:CZ	2.37	0.60
2:E:171:PRO:HB3	2:E:184:CYS:SG	2.43	0.59
2:F:379:ILE:HD13	2:F:420:ALA:HB1	1.84	0.59
1:D:28:GLN:HG3	1:D:102:SER:HB3	1.84	0.59
1:B:119:ILE:HG23	1:B:120:THR:HG23	1.85	0.59
2:G:320:VAL:HB	2:G:344:ILE:HD13	1.84	0.59
2:H:332:SER:CB	2:H:335:HIS:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:PRO:HB3	2:H:184:CYS:SG	2.43	0.58
1:C:119:ILE:HG23	1:C:120:THR:HG23	1.86	0.58
2:H:320:VAL:HB	2:H:344:ILE:HD11	1.85	0.58
2:E:225:PHE:HA	2:E:312:ILE:HD11	1.85	0.58
1:D:119:ILE:HG23	1:D:120:THR:HG23	1.86	0.57
2:G:304:SER:HB2	2:G:310:ILE:HD11	1.86	0.56
1:C:28:GLN:HG3	1:C:102:SER:HB3	1.88	0.56
2:F:166:TYR:HA	2:F:189:VAL:HB	1.88	0.56
2:E:199:CYS:HA	2:E:213:VAL:HA	1.87	0.56
2:E:345:VAL:HG21	2:E:349:PHE:HD2	1.71	0.56
2:H:245:PHE:HD2	2:H:270:ILE:HG23	1.71	0.55
1:A:28:GLN:HG3	1:A:102:SER:HB3	1.88	0.55
2:F:182:LEU:HB2	2:F:224:LEU:HD21	1.88	0.55
2:G:195:GLU:HA	2:G:217:GLU:HA	1.89	0.55
2:E:379:ILE:HD13	2:E:420:ALA:HB1	1.89	0.54
2:F:428:THR:H	3:F:503:NAG:H82	1.72	0.54
1:B:12:SER:HB2	2:F:302:THR:HA	1.90	0.54
2:F:233:ALA:O	2:F:239:ARG:HA	2.07	0.54
2:F:354:ASN:HB2	2:F:427:PHE:CE1	2.43	0.53
2:H:199:CYS:HA	2:H:213:VAL:HA	1.90	0.53
1:B:117:PRO:HG2	1:B:118:TRP:CD1	2.44	0.53
2:F:101:ILE:HG12	2:F:147:SER:HA	1.91	0.53
2:G:199:CYS:HA	2:G:213:VAL:HA	1.91	0.53
1:B:28:GLN:HG3	1:B:102:SER:HB3	1.90	0.52
2:E:371:VAL:HG23	2:E:404:SER:HB3	1.91	0.52
2:G:225:PHE:HA	2:G:312:ILE:HD11	1.90	0.52
2:F:199:CYS:HA	2:F:213:VAL:HA	1.91	0.52
2:E:81:VAL:HB	2:E:158:VAL:HA	1.91	0.51
1:D:10:PRO:HB3	2:H:279:HIS:CE1	2.45	0.51
2:H:298:PHE:HB3	2:H:314:PHE:CE1	2.46	0.51
2:F:81:VAL:HB	2:F:158:VAL:HA	1.93	0.51
2:H:287:LEU:CD2	2:H:288:GLU:H	2.16	0.51
2:H:225:PHE:HA	2:H:312:ILE:HD11	1.92	0.51
2:E:101:ILE:HG12	2:E:147:SER:HA	1.93	0.51
2:E:320:VAL:HB	2:E:344:ILE:HD13	1.93	0.51
1:B:121:ARG:HH11	1:B:121:ARG:HB2	1.76	0.50
1:C:27:LEU:HD13	1:D:30:TYR:CE1	2.47	0.50
2:F:171:PRO:HB3	2:F:184:CYS:SG	2.51	0.50
2:H:245:PHE:CD2	2:H:270:ILE:HG23	2.46	0.50
2:F:225:PHE:HA	2:F:312:ILE:HD11	1.93	0.50
1:A:47:LEU:O	1:A:51:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:GLU:HA	2:F:217:GLU:HA	1.94	0.50
1:D:117:PRO:HG2	1:D:118:TRP:CD1	2.47	0.50
1:B:47:LEU:O	1:B:51:VAL:HG23	2.12	0.49
1:C:47:LEU:O	1:C:51:VAL:HG23	2.12	0.49
1:A:117:PRO:HG2	1:A:118:TRP:CD1	2.47	0.49
2:E:298:PHE:HB3	2:E:314:PHE:CE1	2.46	0.49
1:D:47:LEU:O	1:D:51:VAL:HG23	2.13	0.49
2:E:285:TRP:CD1	2:E:313:LEU:HD23	2.48	0.49
2:F:245:PHE:CD2	2:F:270:ILE:HG23	2.48	0.49
1:A:30:TYR:CD1	1:B:27:LEU:HD13	2.48	0.48
1:C:12:SER:HB2	2:G:302:THR:HA	1.95	0.48
1:A:24:ASP:O	1:B:67:LYS:CB	2.62	0.48
2:H:264:VAL:HG13	2:H:321:ALA:HA	1.95	0.48
2:F:192:PRO:HB3	2:F:235:ASN:HB3	1.96	0.48
2:E:262:LEU:HA	2:E:376:TYR:CZ	2.48	0.48
2:E:287:LEU:HG	2:E:328:TYR:CZ	2.48	0.48
2:F:245:PHE:HD2	2:F:270:ILE:HG23	1.78	0.48
2:F:285:TRP:CD1	2:F:313:LEU:HD23	2.49	0.48
2:E:107:PHE:HA	2:E:141:TYR:HD2	1.78	0.47
2:F:247:ILE:HD12	2:F:285:TRP:HH2	1.79	0.47
2:G:171:PRO:HB3	2:G:184:CYS:SG	2.53	0.47
2:F:105:TRP:HD1	2:F:114:CYS:HB3	1.79	0.47
2:G:245:PHE:HZ	2:G:258:PRO:CB	2.27	0.47
1:B:45:GLY:O	1:B:49:ARG:HG3	2.14	0.47
2:F:304:SER:HB3	2:F:308:THR:HB	1.97	0.47
2:G:245:PHE:HZ	2:G:258:PRO:HB3	1.81	0.46
2:H:192:PRO:HB3	2:H:235:ASN:HB3	1.98	0.46
2:E:287:LEU:HD21	2:E:326:GLY:HA3	1.97	0.46
2:E:332:SER:CB	2:E:335:HIS:HB2	2.46	0.45
2:G:275:VAL:HG22	2:G:310:ILE:HG23	1.98	0.45
2:H:266:GLU:O	2:H:320:VAL:HG22	2.15	0.45
1:D:28:GLN:HG3	1:D:102:SER:CB	2.47	0.45
2:F:107:PHE:HA	2:F:141:TYR:HD2	1.81	0.45
1:B:37:ASN:OD1	1:B:94:LEU:HD12	2.17	0.45
1:A:12:SER:HB2	2:E:302:THR:HA	1.99	0.44
2:H:233:ALA:O	2:H:239:ARG:HA	2.17	0.44
1:D:12:SER:HB2	2:H:302:THR:HA	1.99	0.44
2:H:274:ALA:HB3	2:H:283:LEU:HD11	1.99	0.44
1:A:73:GLU:O	1:A:77:THR:HG23	2.17	0.44
2:G:264:VAL:HA	2:G:320:VAL:HG23	1.99	0.44
1:A:24:ASP:HB3	1:B:67:LYS:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:SER:O	1:B:15:PHE:HD2	2.01	0.44
2:F:379:ILE:HG22	2:F:422:ASN:HB3	1.99	0.44
2:G:245:PHE:HD2	2:G:270:ILE:HG23	1.83	0.44
2:F:383:TRP:HD1	2:F:392:CYS:HB3	1.83	0.43
1:A:37:ASN:OD1	1:A:94:LEU:HD12	2.18	0.43
2:E:233:ALA:O	2:E:239:ARG:HA	2.18	0.43
2:E:379:ILE:HG22	2:E:422:ASN:HB3	2.01	0.43
2:F:332:SER:CB	2:F:335:HIS:HB2	2.49	0.43
2:G:285:TRP:CD1	2:G:313:LEU:HD23	2.54	0.43
1:C:37:ASN:OD1	1:C:94:LEU:HD12	2.19	0.43
1:C:73:GLU:O	1:C:77:THR:HG23	2.19	0.42
1:D:37:ASN:OD1	1:D:94:LEU:HD12	2.19	0.42
2:E:195:GLU:HA	2:E:217:GLU:HA	2.01	0.42
2:G:258:PRO:HG2	2:G:339:SER:O	2.19	0.42
2:E:262:LEU:HA	2:E:376:TYR:CE2	2.54	0.42
2:H:195:GLU:HA	2:H:217:GLU:HA	2.01	0.42
2:F:350:ILE:HG12	2:F:379:ILE:HG21	2.01	0.42
2:H:362:ASP:O	2:H:364:TYR:N	2.53	0.42
2:E:274:ALA:HB3	2:E:283:LEU:HD11	2.01	0.42
2:F:275:VAL:HG22	2:F:310:ILE:HG23	2.00	0.42
2:G:298:PHE:HB3	2:G:314:PHE:CE1	2.55	0.42
2:H:354:ASN:HB3	2:H:427:PHE:CE1	2.54	0.42
2:F:264:VAL:HG13	2:F:321:ALA:HA	2.02	0.42
2:G:258:PRO:HB2	2:G:340:ALA:CB	2.49	0.42
2:E:383:TRP:CD1	2:E:392:CYS:HB3	2.55	0.42
2:F:383:TRP:CD1	2:F:392:CYS:HB3	2.55	0.42
1:C:27:LEU:HD13	1:D:30:TYR:CD1	2.54	0.42
2:E:257:LEU:O	2:E:258:PRO:C	2.58	0.42
2:E:245:PHE:HD2	2:E:270:ILE:HG23	1.85	0.41
2:F:371:VAL:HG23	2:F:404:SER:HB3	2.02	0.41
2:H:383:TRP:CD1	2:H:392:CYS:HB3	2.56	0.41
1:D:48:TRP:CD1	1:D:130:LEU:HG	2.55	0.41
2:H:275:VAL:HG22	2:H:310:ILE:HG23	2.02	0.41
2:G:287:LEU:HB3	2:G:288:GLU:H	1.77	0.41
2:G:332:SER:CB	2:G:335:HIS:HB2	2.50	0.41
1:C:48:TRP:CD1	1:C:130:LEU:HG	2.55	0.41
2:E:245:PHE:CD2	2:E:270:ILE:HG23	2.56	0.41
1:A:48:TRP:CD1	1:A:130:LEU:HG	2.56	0.41
2:F:274:ALA:HB3	2:F:283:LEU:HD11	2.03	0.41
2:H:304:SER:HB3	2:H:308:THR:HB	2.02	0.41
1:D:73:GLU:O	1:D:77:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:383:TRP:HD1	2:E:392:CYS:HB3	1.86	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	133/138 (96%)	121 (91%)	7 (5%)	5 (4%)	3	27
1	B	132/138 (96%)	123 (93%)	8 (6%)	1 (1%)	19	60
1	C	133/138 (96%)	126 (95%)	6 (4%)	1 (1%)	19	60
1	D	130/138 (94%)	121 (93%)	8 (6%)	1 (1%)	19	60
2	E	316/423 (75%)	273 (86%)	32 (10%)	11 (4%)	3	29
2	F	328/423 (78%)	282 (86%)	34 (10%)	12 (4%)	3	28
2	G	164/423 (39%)	137 (84%)	23 (14%)	4 (2%)	6	36
2	H	255/423 (60%)	215 (84%)	27 (11%)	13 (5%)	2	22
All	All	1591/2244 (71%)	1398 (88%)	145 (9%)	48 (3%)	4	32

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
2	E	85	VAL
2	E	334	LYS
2	F	85	VAL
2	F	334	LYS
2	F	363	GLN
2	G	334	LYS
2	H	165	LEU
2	H	255	THR

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Mol	Chain	Res	Type
2	H	305	THR
2	H	334	LYS
2	H	363	GLN
2	E	258	PRO
2	E	292	LEU
2	E	363	GLN
2	F	255	THR
2	F	305	THR
2	G	305	THR
2	H	164	LEU
2	H	291	ALA
1	A	-1	HIS
1	A	1	THR
1	A	42	GLU
1	C	42	GLU
1	D	42	GLU
2	E	305	THR
2	E	364	TYR
2	F	108	LYS
2	F	353	THR
2	F	364	TYR
2	H	226	GLY
2	H	364	TYR
1	B	42	GLU
2	E	108	LYS
2	E	226	GLY
2	F	408	ASN
2	G	256	THR
2	H	398	ASP
2	H	408	ASN
1	A	3	ASP
2	E	116	PRO
2	H	411	HIS
2	E	400	GLY
2	F	116	PRO
2	F	411	HIS
2	H	287	LEU
2	F	400	GLY
2	G	226	GLY

### 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	99/127 (78%)	97 (98%)	2 (2%)	55	73
1	B	101/127 (80%)	98 (97%)	3 (3%)	41	64
1	C	101/127 (80%)	98 (97%)	3 (3%)	41	64
1	D	95/127 (75%)	92 (97%)	3 (3%)	39	62
2	E	126/383 (33%)	107 (85%)	19 (15%)	3	17
2	F	127/383 (33%)	108 (85%)	19 (15%)	3	17
2	G	74/383 (19%)	64 (86%)	10 (14%)	4	20
2	H	103/383 (27%)	91 (88%)	12 (12%)	5	23
All	All	826/2040 (40%)	755 (91%)	71 (9%)	10	35

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	129	GLU
1	B	95	ARG
1	B	103	ARG
1	B	121	ARG
1	C	98	GLN
1	C	103	ARG
1	C	129	GLU
1	D	42	GLU
1	D	103	ARG
1	D	129	GLU
2	E	93	VAL
2	E	145	ILE
2	E	154	ILE
2	E	160	ILE
2	E	229	ILE
2	E	244	LEU
2	E	260	LEU
2	E	270	ILE

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Mol	Chain	Res	Type
2	E	287	LEU
2	E	292	LEU
2	E	306	ASN
2	E	308	THR
2	E	309	MET
2	E	310	ILE
2	E	313	LEU
2	E	361	ILE
2	E	371	VAL
2	E	392	CYS
2	E	433	LEU
2	F	93	VAL
2	F	145	ILE
2	F	154	ILE
2	F	160	ILE
2	F	229	ILE
2	F	244	LEU
2	F	260	LEU
2	F	270	ILE
2	F	292	LEU
2	F	308	THR
2	F	310	ILE
2	F	313	LEU
2	F	339	SER
2	F	341	LEU
2	F	344	ILE
2	F	361	ILE
2	F	371	VAL
2	F	392	CYS
2	F	433	LEU
2	G	229	ILE
2	G	244	LEU
2	G	260	LEU
2	G	270	ILE
2	G	287	LEU
2	G	292	LEU
2	G	308	THR
2	G	310	ILE
2	G	313	LEU
2	G	345	VAL
2	H	229	ILE
2	H	244	LEU

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Mol	Chain	Res	Type
2	H	260	LEU
2	H	270	ILE
2	H	287	LEU
2	H	308	THR
2	H	309	MET
2	H	310	ILE
2	H	344	ILE
2	H	371	VAL
2	H	392	CYS
2	H	433	LEU

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

7 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	G	500	2	14,14,15	1.08	1 (7%)	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	H	503	2	14,14,15	1.01	1 (7%)	17,19,21	0.70	0
3	NAG	F	503	2	14,14,15	1.05	1 (7%)	17,19,21	0.68	0
3	NAG	F	501	2	14,14,15	1.05	1 (7%)	17,19,21	0.70	0
3	NAG	E	501	2	14,14,15	1.05	1 (7%)	17,19,21	0.70	0
3	NAG	F	504	2	14,14,15	1.07	1 (7%)	17,19,21	0.70	0
3	NAG	H	504	2	14,14,15	1.04	1 (7%)	17,19,21	0.68	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	G	500	2	-	0/6/23/26	0/1/1/1
3	NAG	H	503	2	-	0/6/23/26	0/1/1/1
3	NAG	F	503	2	-	0/6/23/26	0/1/1/1
3	NAG	F	501	2	-	0/6/23/26	0/1/1/1
3	NAG	E	501	2	-	1/6/23/26	0/1/1/1
3	NAG	F	504	2	-	1/6/23/26	0/1/1/1
3	NAG	H	504	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	500	NAG	C1-C2	2.80	1.56	1.52
3	F	504	NAG	C1-C2	2.78	1.56	1.52
3	E	501	NAG	C1-C2	2.72	1.56	1.52
3	F	503	NAG	C1-C2	2.68	1.56	1.52
3	H	504	NAG	C1-C2	2.62	1.56	1.52
3	F	501	NAG	C1-C2	2.57	1.56	1.52
3	H	503	NAG	C1-C2	2.48	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	504	NAG	O5-C5-C6-O6
3	E	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	504	NAG	O5-C5-C6-O6
3	H	504	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	503	NAG	1	0
3	F	504	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	135/138 (97%)	0.14	4 (2%)	50	39	122, 154, 189, 193	0
1	B	134/138 (97%)	0.10	1 (0%)	87	82	123, 147, 172, 179	0
1	C	135/138 (97%)	0.17	3 (2%)	62	52	129, 166, 189, 196	0
1	D	132/138 (95%)	0.05	1 (0%)	86	79	138, 152, 184, 190	0
2	E	328/423 (77%)	0.25	18 (5%)	25	22	135, 184, 235, 243	0
2	F	336/423 (79%)	0.07	12 (3%)	42	34	133, 179, 221, 237	0
2	G	168/423 (39%)	0.38	10 (5%)	21	18	155, 179, 202, 208	0
2	H	259/423 (61%)	0.12	10 (3%)	39	31	122, 152, 175, 187	0
All	All	1627/2244 (72%)	0.16	59 (3%)	42	34	122, 168, 218, 243	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	233	ALA	7.6
2	G	326	GLY	6.5
2	E	365	GLU	5.5
2	H	199	CYS	4.9
2	G	219	LYS	4.5
2	E	345	VAL	4.5
2	F	350	ILE	4.3
2	G	233	ALA	3.5
2	E	240	GLU	3.4
2	H	214	VAL	3.3
1	C	119	ILE	3.3
2	H	324	ASP	3.3
1	A	25	TYR	3.1
2	E	369	PHE	3.1
1	A	-2	SER	3.1
2	E	367	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	297	TYR	2.9
2	G	345	VAL	2.9
2	G	215	LYS	2.9
2	E	185	ILE	2.9
2	G	283	LEU	2.8
2	F	153	THR	2.8
2	G	331	SER	2.7
2	G	342	VAL	2.6
2	F	168	LEU	2.6
2	H	213	VAL	2.5
2	E	406	PHE	2.5
2	F	351	ASN	2.5
2	H	186	SER	2.5
2	F	240	GLU	2.4
2	G	186	SER	2.4
2	H	185	ILE	2.4
1	C	128	LEU	2.4
2	F	96	ASP	2.4
2	F	233	ALA	2.4
2	E	283	LEU	2.4
2	H	194	VAL	2.4
1	B	96	PHE	2.3
2	E	322	ARG	2.3
2	G	288	GLU	2.3
2	E	375	ALA	2.3
2	H	180	ASP	2.3
2	F	154	ILE	2.2
1	A	6	PHE	2.2
2	H	262	LEU	2.2
2	F	359	TYR	2.1
2	E	383	TRP	2.1
2	E	296	ASN	2.1
2	H	275	VAL	2.1
2	E	100	ASN	2.1
1	D	90	PRO	2.1
2	F	433	LEU	2.1
1	A	21	GLU	2.1
2	F	375	ALA	2.1
2	E	194	VAL	2.1
2	E	101	ILE	2.1
2	F	283	LEU	2.0
1	C	6	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	361	ILE	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	F	504	14/15	0.46	0.61	192,192,192,192	0
3	NAG	H	504	14/15	0.70	0.23	173,173,173,173	0
3	NAG	H	503	14/15	0.75	0.23	178,178,178,178	0
3	NAG	F	501	14/15	0.76	0.33	186,186,186,186	0
3	NAG	F	503	14/15	0.80	0.35	201,201,201,201	0
3	NAG	G	500	14/15	0.81	0.22	173,173,173,173	0
3	NAG	E	501	14/15	0.91	0.18	194,194,194,194	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.