



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:21 PM UTC

PDB ID : 3QS7 / pdb_00003qs7
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

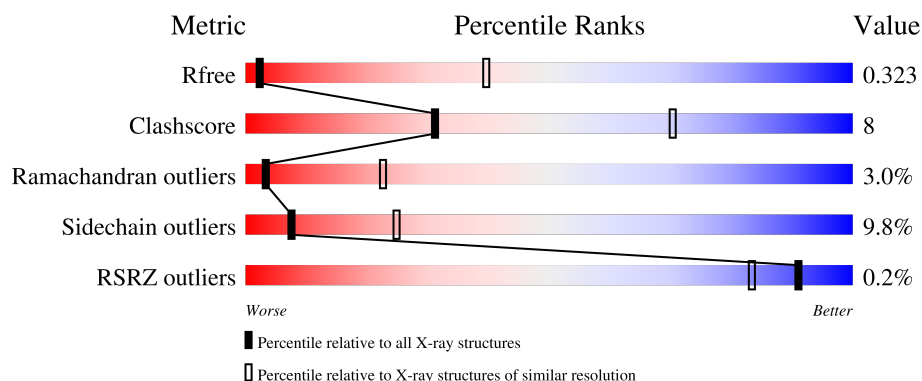
1 Overall quality at a glance

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}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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 ≥ 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	 77% 20% ..
1	B	138	 81% 15% ..
1	C	138	 81% 17% .
1	D	138	 80% 15% ..
2	E	423	 58% 17% . 22%

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Mol	Chain	Length	Quality of chain
2	F	423	59%19%•21%
2	G	423	29%9%•60%
2	H	423	45%13%•39%

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:

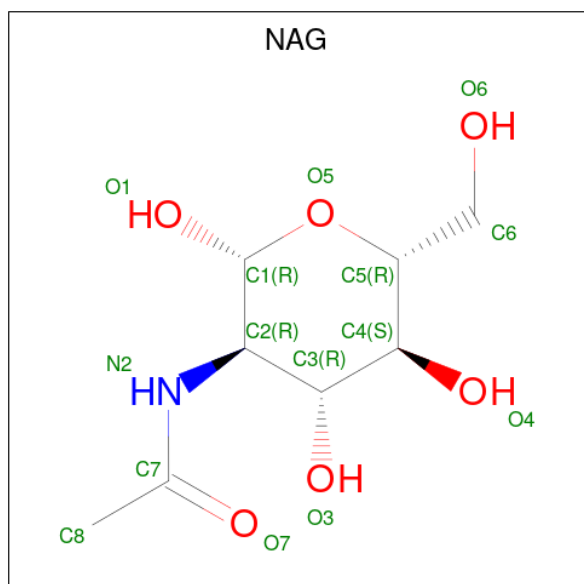
Chain	Residue	Modelled	Actual	Comment	Reference
E	24	GLU	-	expression tag	UNP P36888
E	25	THR	-	expression tag	UNP P36888
E	26	GLY	-	expression tag	UNP P36888
E	437	SER	-	expression tag	UNP P36888
E	438	GLY	-	expression tag	UNP P36888
E	439	THR	-	expression tag	UNP P36888
E	440	LYS	-	expression tag	UNP 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 (CCD ID: 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

Chain A: 



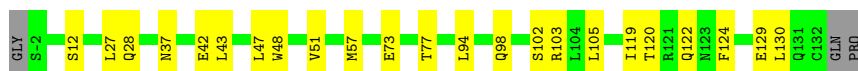
- Molecule 1: SL cytokine

Chain B: 



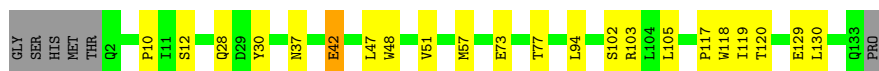
- Molecule 1: SL cytokine

Chain C: 



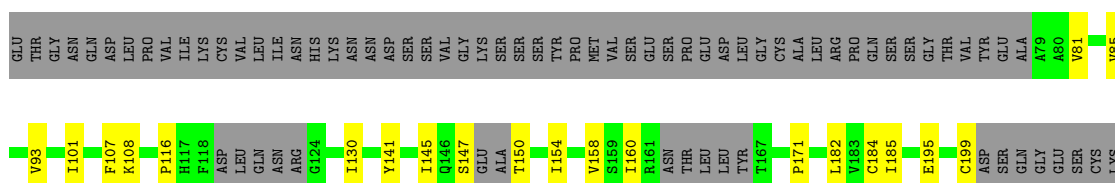
- Molecule 1: SL cytokine

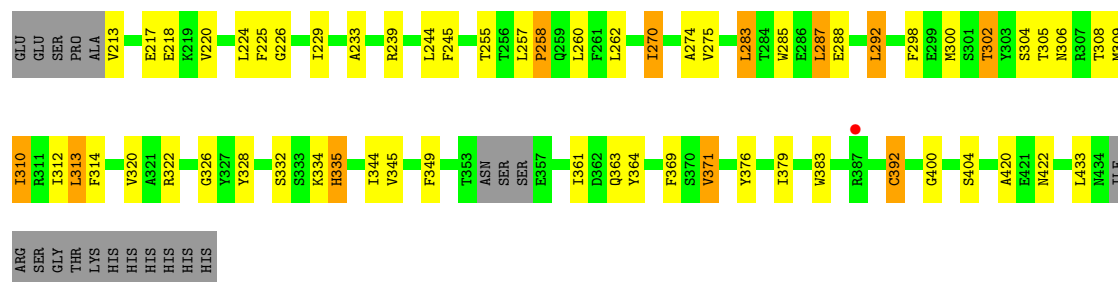
Chain D: 



- Molecule 2: FL cytokine receptor

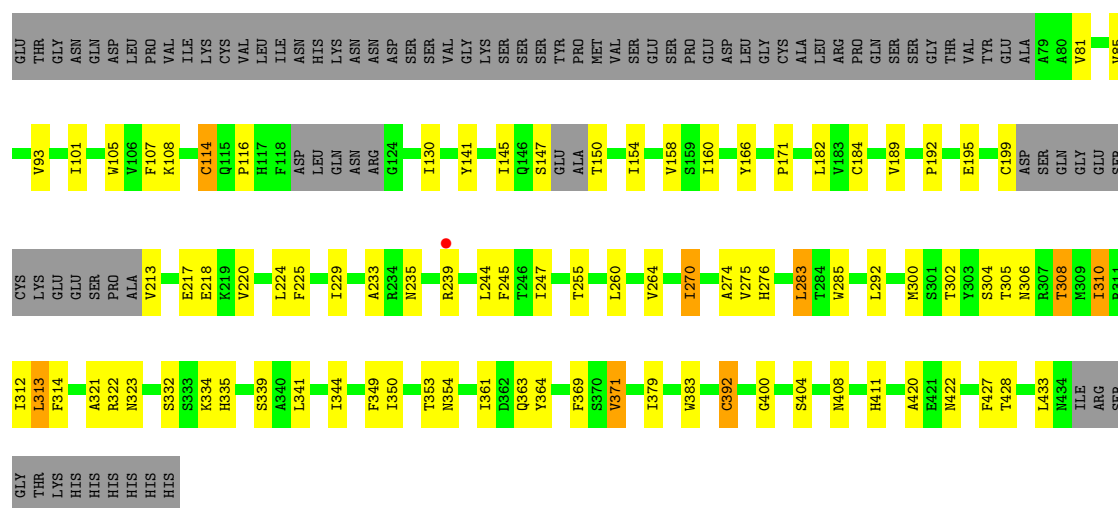
Chain E: 





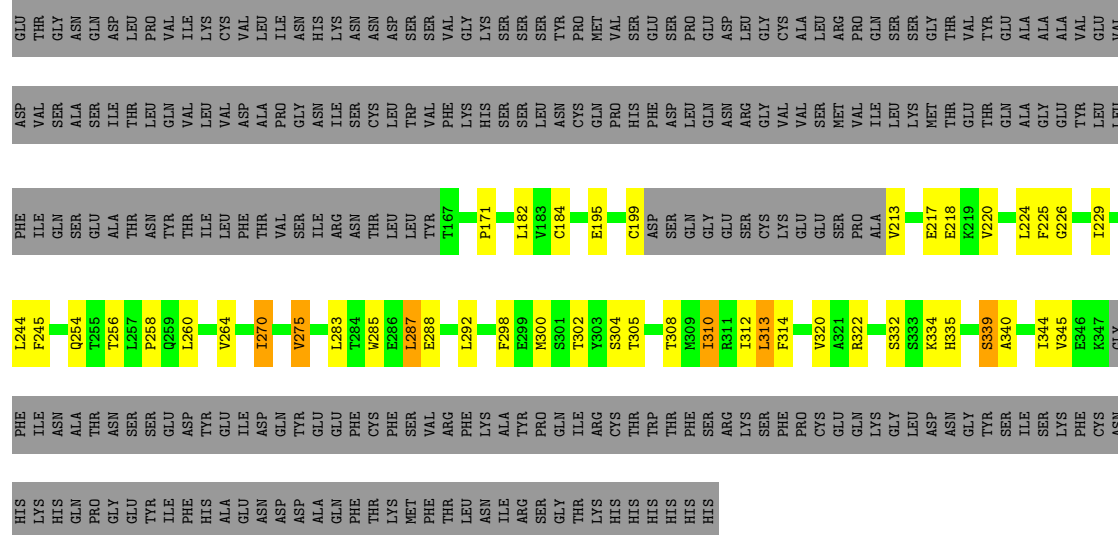
- Molecule 2: FL cytokine receptor

Chain F: 59% 19% 21%



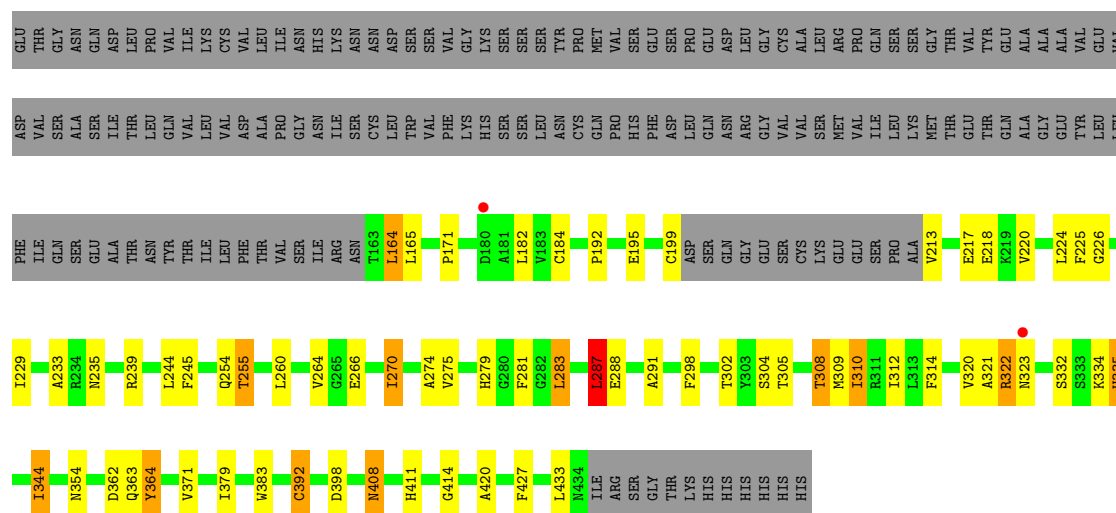
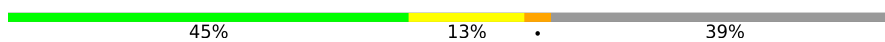
- Molecule 2: FL cytokine receptor

Chain G: 29% 9% 60%



- Molecule 2: FL cytokine receptor

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 , 0.323	Depositor DCC
R_{free} test set	1010 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	161.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 939.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10865	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.69	0/1005	1.11	2/1380 (0.1%)
1	B	0.64	0/1018	1.06	0/1392
1	C	0.64	0/1006	1.06	0/1379
1	D	0.65	0/970	1.04	0/1334
2	E	1.01	1/2089 (0.0%)	1.28	9/2886 (0.3%)
2	F	0.97	0/2129	1.27	10/2950 (0.3%)
2	G	0.94	0/1093	1.28	4/1515 (0.3%)
2	H	1.01	0/1684	1.32	10/2331 (0.4%)
All	All	0.88	1/10994 (0.0%)	1.21	35/15167 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	185	ILE	CA-CB	5.24	1.60	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	254	GLN	CA-C-N	8.98	132.69	120.38
2	G	254	GLN	C-N-CA	8.98	132.69	120.38
2	E	306	ASN	CA-CB-CG	8.15	120.75	112.60
1	A	1	THR	CA-C-N	7.34	135.56	121.54
1	A	1	THR	C-N-CA	7.34	135.56	121.54
2	F	323	ASN	CA-CB-CG	6.94	119.54	112.60
2	E	322	ARG	CA-C-N	6.51	129.00	120.28
2	E	322	ARG	C-N-CA	6.51	129.00	120.28
2	F	322	ARG	CA-C-N	6.51	129.29	120.38
2	F	322	ARG	C-N-CA	6.51	129.29	120.38
2	H	164	LEU	CA-C-N	6.27	133.52	121.54
2	H	164	LEU	C-N-CA	6.27	133.52	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	322	ARG	CA-C-N	6.08	128.71	120.38
2	G	322	ARG	C-N-CA	6.08	128.71	120.38
2	H	335	HIS	N-CA-C	5.99	115.20	108.25
2	F	276	HIS	CA-C-N	5.88	128.05	120.70
2	F	276	HIS	C-N-CA	5.88	128.05	120.70
2	H	323	ASN	CA-CB-CG	5.88	118.48	112.60
2	H	322	ARG	CA-C-N	5.85	128.40	120.38
2	H	322	ARG	C-N-CA	5.85	128.40	120.38
2	E	369	PHE	CA-CB-CG	5.84	119.64	113.80
2	E	255	THR	CA-C-N	5.80	130.40	122.34
2	E	255	THR	C-N-CA	5.80	130.40	122.34
2	H	281	PHE	CA-CB-CG	5.45	119.25	113.80
2	H	414	GLY	N-CA-C	5.34	118.40	110.60
2	F	369	PHE	CA-CB-CG	5.27	119.07	113.80
2	F	114	CYS	CA-C-N	5.23	128.01	122.26
2	F	114	CYS	C-N-CA	5.23	128.01	122.26
2	F	306	ASN	CA-C-N	5.17	129.46	122.07
2	F	306	ASN	C-N-CA	5.17	129.46	122.07
2	E	335	HIS	N-CA-C	5.14	114.21	108.25
2	E	288	GLU	CA-C-N	5.09	129.63	122.46
2	E	288	GLU	C-N-CA	5.09	129.63	122.46
2	H	408	ASN	CA-C-N	5.07	127.48	120.29
2	H	408	ASN	C-N-CA	5.07	127.48	120.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	15	0
1	B	997	0	935	14	0
1	C	987	0	904	11	0
1	D	950	0	861	13	0
2	E	2049	0	1534	33	0
2	F	2087	0	1552	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1070	0	844	21	0
2	H	1643	0	1207	29	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	161	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 8.

All (161) 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	1.87	0.72
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	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:300:MET:HE2	2:G:314:PHE:HE2	1.69	0.57
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
2:E:300:MET:HE2	2:E:314:PHE:HE2	1.69	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:F:300:MET:HE2	2:F:314:PHE:HE2	1.72	0.54
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
2:F:195:GLU:HA	2:F:217:GLU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:257:LEU:O	2:E:258:PRO:C	2.58	0.46
2:G:245:PHE:HZ	2:G:258:PRO:HB3	1.81	0.46
1:A:57:MET:HE1	1:A:105:LEU:CD2	2.46	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
2:H:254:GLN:O	2:H:255:THR:C	2.60	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
1:D:57:MET:HE1	1:D:105:LEU:CD2	2.48	0.44
2:H:274:ALA:HB3	2:H:283:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:218:GLU:C	2:E:220:VAL:H	2.27	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
2:F:218:GLU:C	2:F:220:VAL:H	2.27	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
1:B:57:MET:HE1	1:B:105:LEU:HD21	2.01	0.42
1:B:57:MET:HE1	1:B:105:LEU:CD2	2.49	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:A:57:MET:HE1	1:A:105:LEU:HD21	2.01	0.42
1:C:27:LEU:HD13	1:D:30:TYR:CD1	2.54	0.42
2:H:218:GLU:C	2:H:220:VAL:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:MET:HE1	1:C:105:LEU:CD2	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:G:218:GLU:C	2:G:220:VAL:H	2.29	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
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%)	2	19
1	B	132/138 (96%)	123 (93%)	8 (6%)	1 (1%)	16	52
1	C	133/138 (96%)	126 (95%)	6 (4%)	1 (1%)	16	52
1	D	130/138 (94%)	121 (93%)	8 (6%)	1 (1%)	16	52
2	E	316/423 (75%)	273 (86%)	32 (10%)	11 (4%)	3	20
2	F	328/423 (78%)	282 (86%)	34 (10%)	12 (4%)	2	20
2	G	164/423 (39%)	137 (84%)	23 (14%)	4 (2%)	4	27
2	H	255/423 (60%)	215 (84%)	27 (11%)	13 (5%)	1	15
All	All	1591/2244 (71%)	1398 (88%)	145 (9%)	48 (3%)	3	22

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
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

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Mol	Chain	Res	Type
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%)	48	66
1	B	101/127 (80%)	98 (97%)	3 (3%)	36	57
1	C	101/127 (80%)	97 (96%)	4 (4%)	28	49
1	D	95/127 (75%)	92 (97%)	3 (3%)	34	56
2	E	126/383 (33%)	104 (82%)	22 (18%)	2	11
2	F	127/383 (33%)	106 (84%)	21 (16%)	2	12
2	G	74/383 (19%)	61 (82%)	13 (18%)	2	11
2	H	103/383 (27%)	90 (87%)	13 (13%)	4	18
All	All	826/2040 (40%)	745 (90%)	81 (10%)	7	25

All (81) 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	43	LEU
1	C	98	GLN
1	C	103	ARG
1	C	129	GLU
1	D	42	GLU

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Mol	Chain	Res	Type
1	D	103	ARG
1	D	129	GLU
2	E	93	VAL
2	E	130	ILE
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
2	E	275	VAL
2	E	283	LEU
2	E	287	LEU
2	E	292	LEU
2	E	302	THR
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	130	ILE
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	283	LEU
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

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Mol	Chain	Res	Type
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	275	VAL
2	G	283	LEU
2	G	287	LEU
2	G	292	LEU
2	G	308	THR
2	G	310	ILE
2	G	313	LEU
2	G	339	SER
2	G	345	VAL
2	H	229	ILE
2	H	244	LEU
2	H	260	LEU
2	H	270	ILE
2	H	283	LEU
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. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	39	GLN
1	B	39	GLN
1	B	111	GLN
1	C	39	GLN
1	D	39	GLN
1	D	111	GLN
2	E	351	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 ⓘ

There are no oligosaccharides 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	1.14	1 (7%)	17,19,21	0.74	0
3	NAG	H	503	2	14,14,15	1.06	1 (7%)	17,19,21	0.72	0
3	NAG	H	504	2	14,14,15	1.09	1 (7%)	17,19,21	0.70	0
3	NAG	F	503	2	14,14,15	1.11	1 (7%)	17,19,21	0.69	0
3	NAG	F	501	2	14,14,15	1.10	1 (7%)	17,19,21	0.71	0
3	NAG	F	504	2	14,14,15	1.13	1 (7%)	17,19,21	0.72	0
3	NAG	E	501	2	14,14,15	1.11	1 (7%)	17,19,21	0.71	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	504	2	-	2/6/23/26	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	F	504	2	-	1/6/23/26	0/1/1/1
3	NAG	E	501	2	-	1/6/23/26	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	3.07	1.56	1.52
3	F	504	NAG	C1-C2	3.04	1.56	1.52
3	E	501	NAG	C1-C2	2.97	1.56	1.52
3	F	503	NAG	C1-C2	2.93	1.56	1.52
3	H	504	NAG	C1-C2	2.87	1.56	1.52
3	F	501	NAG	C1-C2	2.81	1.56	1.52
3	H	503	NAG	C1-C2	2.72	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
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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	135/138 (97%)	-0.68	0	100 100	122, 154, 189, 193	0
1	B	134/138 (97%)	-0.69	0	100 100	123, 147, 172, 179	0
1	C	135/138 (97%)	-0.71	0	100 100	129, 166, 189, 196	0
1	D	132/138 (95%)	-0.77	0	100 100	138, 152, 184, 190	0
2	E	328/423 (77%)	-0.51	1 (0%)	90 80	135, 184, 235, 243	0
2	F	336/423 (79%)	-0.54	1 (0%)	90 80	133, 179, 221, 237	0
2	G	168/423 (39%)	-0.50	0	100 100	155, 179, 202, 208	0
2	H	259/423 (61%)	-0.71	2 (0%)	82 68	122, 152, 175, 187	0
All	All	1627/2244 (72%)	-0.61	4 (0%)	91 83	122, 168, 218, 243	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	323	ASN	3.1
2	E	387	ARG	2.4
2	H	180	ASP	2.4
2	F	239	ARG	2.3

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	501	14/15	0.93	0.11	194,194,194,194	0
3	NAG	F	503	14/15	0.96	0.06	201,201,201,201	0
3	NAG	F	501	14/15	0.97	0.09	186,186,186,186	0
3	NAG	H	504	14/15	0.97	0.10	173,173,173,173	0
3	NAG	G	500	14/15	0.98	0.06	173,173,173,173	0
3	NAG	H	503	14/15	0.98	0.07	178,178,178,178	0
3	NAG	F	504	14/15	0.98	0.06	192,192,192,192	0

6.5 Other polymers [i](#)

There are no such residues in this entry.