



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:27 PM UTC

PDB ID : 5TOJ / pdb_00005toj
Title : Crystal structure of the RSV F glycoprotein in complex with the neutralizing single-domain antibody F-VHH-4
Authors : Gilman, M.S.A.; Kabeche, S.C.; McLellan, J.S.
Deposited on : 2016-10-17
Resolution : 3.30 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:

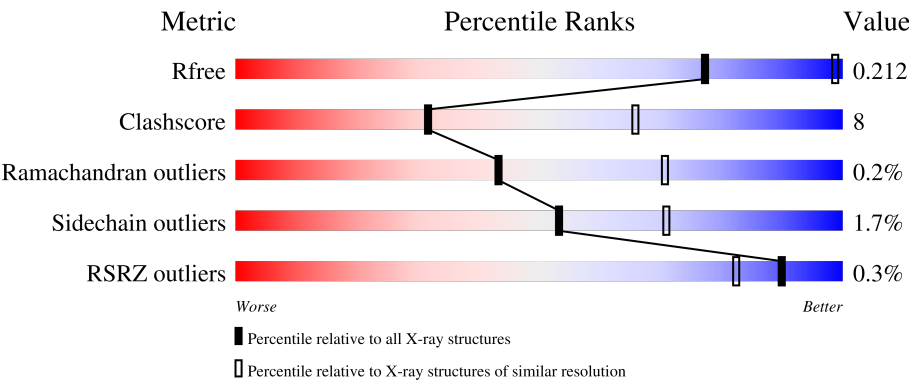
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	550	70%16%•12%
1	B	550	% 68%18%•12%
1	C	550	69%17%•13%
2	D	131	85%11%••
2	E	131	79%14%•6%

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Mol	Chain	Length	Quality of chain
2	F	131	77% 18% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14124 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 Fusion glycoprotein F0, Fibrin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3739	2368	616	732	23			
1	B	485	Total	C	N	O	S	0	0	0
			3753	2378	618	734	23			
1	C	481	Total	C	N	O	S	0	0	0
			3727	2360	614	730	23			

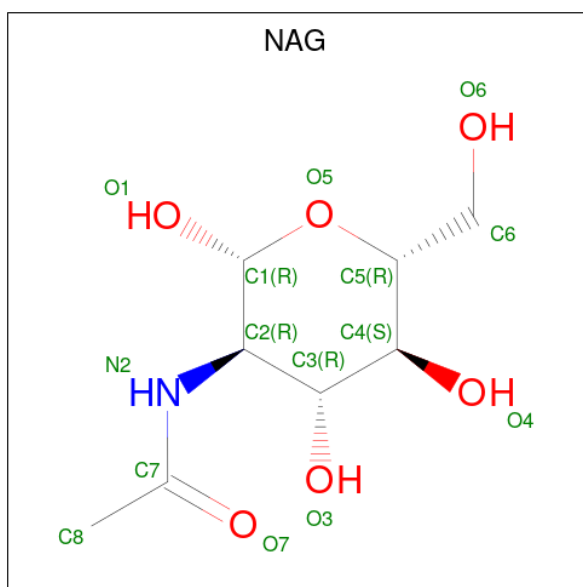
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	155	CYS	SER	engineered mutation	UNP P03420
A	190	PHE	SER	engineered mutation	UNP P03420
A	207	LEU	VAL	engineered mutation	UNP P03420
A	290	CYS	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
B	102	ALA	PRO	conflict	UNP P03420
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
C	155	CYS	SER	engineered mutation	UNP P03420
C	190	PHE	SER	engineered mutation	UNP P03420
C	207	LEU	VAL	engineered mutation	UNP P03420
C	290	CYS	SER	engineered mutation	UNP P03420
C	379	VAL	ILE	engineered mutation	UNP P03420
C	447	VAL	MET	engineered mutation	UNP P03420

- Molecule 2 is a protein called Single-domain antibody F-VHH-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	126	Total	C	N	O	S	0	0	0
			965	604	166	189	6			
2	E	123	Total	C	N	O	S	0	0	0
			943	592	161	184	6			
2	F	125	Total	C	N	O	S	0	0	0
			955	598	163	188	6			

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

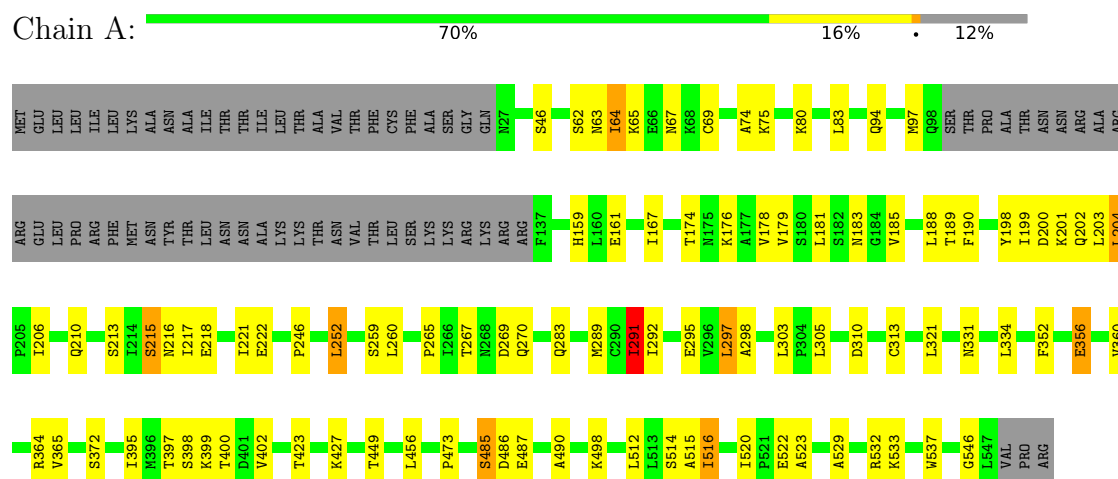


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

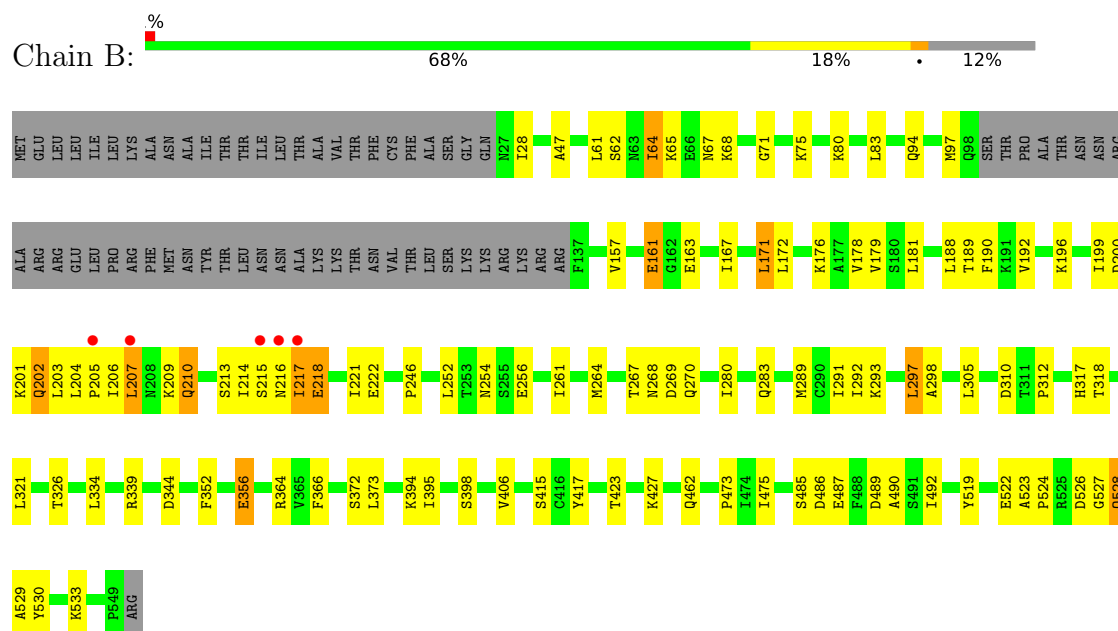
3 Residue-property plots [i](#)

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: Fusion glycoprotein F0, Fibrin chimera



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S372	Q202	ARG	MET
T400	L203	ALA	GLU
E461	L204	ARG	LEU
V402	P205	ARG	ILE
Y417	L207	LEU	LEU
T423	M208	PRO	LYS
K427	K209	ARG	ASN
M437	Q210	PHE	ALA
D448	S211	MET	ALA
T449	C212	ASN	ILE
M454	S213	TYR	THR
T485	I214	THR	ILE
L486	S215	LEU	LEU
E472	M216	ASN	THR
P473	I217	ALA	ALA
S485	E236	LYS	VAL
D486	P246	THR	THR
E487	V247	LYS	THR
A490	S248	ASN	CYS
E497	L252	VAL	PHE
S502	L260	THR	ALA
L503	L280	LEU	SER
I506	K293	SER	GLY
I516	L297	LYS	GLN
G517	T299	LYS	N27
I520	K292	ARG	I28
E521	E235	LYS	Y44
E522	L298	ARG	Y44
P524	A298	ARG	A47
A529	L305	L138	L48
Y530	D310	L141	R49
F531	L321	E163	S62
K532	T326	M166	M63
K533	F352	I167	I64
D534	E356	L171	E66
G535	Q361	K176	N67
G545	R364	L181	K68
GLY	V365	S182	C69
LEU	F366	M183	K75
VAL	G367	V185	V76
PRO	D368	T189	K77
PRO	PC	F190	K90
		M197	L96
		I198	M97
		I199	Q98
		D200	SER
		Z204	THR
			ALA
			THR
			ASN
			ASN

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|-------|
| Q1 |
| V2 |
| G26 |
| F27 |
| T28 |
| L29 |
| T34 |
| A40 |
| K43 |
| Y58 |
| R71 |
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| R96 |
| Y100F |
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|----|----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Q1 | V2 | F27 | T28 | A40 | K43 | E44 | | Y58 | R71 | D72 | N73 | M82 | L82C | X83 | P84 | A93 | R96 | S97 | S98 | Y100F | W103 | V111 | SER | SER | HIS | HIS | HIS | HIS | HIS | HIS | HIS |
|----|----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-------|------|------|------|-----|-----|-----|-----|-----|-----|
| Q1 | V2 | E6 | L11 | G15 | S21 | G26 | F27 | T28 | L29 | I34 | A40 | K43 | R71 | D72 | N73 | V78 | M82 | R82A | S82B | L82C | K83 | P84 | R85 | R96 | Y100F | V111 | S112 | S113 | HIS | HIS | HIS | HIS | HIS | HIS |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-------|------|------|------|-----|-----|-----|-----|-----|-----|

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.19Å 173.19Å 153.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.96 – 3.30 37.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.96-3.30) 99.9 (37.96-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.234 (Not available) , 0.212	Depositor DCC
R_{free} test set	2023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14124	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	0.37	0/3796	0.87	9/5143 (0.2%)
1	B	0.39	0/3811	0.95	12/5165 (0.2%)
1	C	0.39	0/3784	0.94	10/5127 (0.2%)
2	D	0.39	0/989	0.85	3/1339 (0.2%)
2	E	0.32	0/966	0.80	2/1308 (0.2%)
2	F	0.34	0/978	0.87	4/1324 (0.3%)
All	All	0.38	0/14324	0.90	40/19406 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	LEU	N-CA-C	9.98	125.54	113.16
1	C	517	GLY	N-CA-C	8.85	124.40	114.67
1	C	64	ILE	N-CA-C	7.82	117.96	106.85
1	B	217	ILE	N-CA-C	7.79	120.82	111.09
1	A	201	LYS	N-CA-C	7.40	122.41	113.23
1	C	204	LEU	CA-C-N	-7.37	111.18	119.28
1	C	204	LEU	C-N-CA	-7.37	111.18	119.28
1	B	71	GLY	N-CA-C	7.29	119.89	111.36
2	D	26	GLY	N-CA-C	6.77	124.67	115.32
1	C	64	ILE	CB-CA-C	-6.76	102.75	111.53
1	B	210	GLN	N-CA-C	-6.70	103.66	110.97
1	B	209	LYS	N-CA-C	-6.65	98.92	109.23
1	C	28	ILE	N-CA-C	6.63	117.45	108.17
1	A	546	GLY	N-CA-C	-6.58	106.36	114.92
1	B	171	LEU	N-CA-C	6.36	119.97	112.72
1	A	516	ILE	N-CA-C	-6.33	104.11	111.00
1	B	201	LYS	N-CA-C	6.27	121.00	113.23
2	F	27	PHE	CA-C-N	-6.12	113.02	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	27	PHE	C-N-CA	-6.12	113.02	122.87
1	B	64	ILE	CB-CA-C	-6.08	101.33	111.29
1	B	268	ASN	N-CA-C	6.04	117.86	111.28
2	D	27	PHE	CA-C-N	-6.01	114.71	123.00
2	D	27	PHE	C-N-CA	-6.01	114.71	123.00
1	A	291	ILE	N-CA-C	5.75	115.42	108.06
1	C	201	LYS	N-CA-C	5.71	120.31	113.23
1	A	210	GLN	N-CA-C	-5.69	104.08	111.02
2	E	27	PHE	CA-C-N	-5.56	113.91	122.87
2	E	27	PHE	C-N-CA	-5.56	113.91	122.87
2	F	26	GLY	N-CA-C	5.47	122.87	115.32
1	B	218	GLU	N-CA-C	-5.46	105.48	111.82
1	C	163	GLU	N-CA-C	5.27	116.83	111.14
1	A	64	ILE	CB-CA-C	-5.26	102.67	111.29
1	A	485	SER	N-CA-C	5.21	119.62	113.16
1	A	204	LEU	CA-C-N	-5.20	113.56	119.28
1	A	204	LEU	C-N-CA	-5.20	113.56	119.28
1	C	485	SER	N-CA-C	5.18	119.58	113.16
2	F	2	VAL	N-CA-C	5.16	115.65	108.84
1	B	217	ILE	CB-CA-C	-5.14	103.94	112.26
1	C	207	LEU	N-CA-C	5.07	119.45	113.16
1	B	222	GLU	N-CA-C	-5.03	105.79	111.28

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	3739	0	3777	71	0
1	B	3753	0	3793	82	0
1	C	3727	0	3763	68	1
2	D	965	0	912	11	0
2	E	943	0	895	15	0
2	F	955	0	905	13	0
3	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	C	14	0	13	0	0
All	All	14124	0	14084	229	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 8.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HD11	1:B:199:ILE:HG21	1.49	0.94
1:B:75:LYS:HD2	1:B:216:ASN:HA	1.50	0.92
1:C:423:THR:OG1	2:E:96:ARG:NH1	2.08	0.87
1:C:64:ILE:HD11	1:C:199:ILE:HG21	1.57	0.86
1:A:334:LEU:HD11	1:A:395:ILE:HD12	1.61	0.83
1:A:64:ILE:HD11	1:A:199:ILE:HG21	1.60	0.82
1:B:206:ILE:HG13	1:B:207:LEU:HG	1.61	0.82
1:A:423:THR:OG1	2:F:96:ARG:NH1	2.12	0.81
1:A:218:GLU:HG3	1:C:217:ILE:HD13	1.60	0.80
1:B:75:LYS:HG2	1:B:217:ILE:HG23	1.68	0.75
1:B:423:THR:OG1	2:D:96:ARG:NH1	2.19	0.75
1:B:206:ILE:HG22	1:B:213:SER:O	1.88	0.73
1:B:519:TYR:OH	1:C:516:ILE:O	2.05	0.73
1:A:67:ASN:HD22	1:A:83:LEU:HD23	1.56	0.69
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.72	0.69
1:B:334:LEU:HD11	1:B:395:ILE:HD12	1.72	0.69
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.73	0.69
1:C:215:SER:OG	1:C:216:ASN:N	2.24	0.68
1:A:94:GLN:HA	1:A:97:MET:HE2	1.77	0.67
1:A:221:ILE:HD12	1:C:217:ILE:HD11	1.76	0.67
1:B:161:GLU:CD	1:B:161:GLU:H	2.03	0.67
1:C:190:PHE:CE2	1:C:260:LEU:HG	2.30	0.66
1:B:200:ASP:HA	1:B:204:LEU:HD12	1.77	0.65
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.80	0.64
2:D:29:LEU:HD12	2:D:71:ARG:HE	1.63	0.63
1:C:503:LEU:HD23	1:C:506:ILE:HD11	1.81	0.62
1:B:269:ASP:OD1	1:B:270:GLN:N	2.32	0.62
1:B:214:ILE:CG2	1:B:215:SER:H	2.12	0.62
1:A:398:SER:HA	1:A:485:SER:O	2.00	0.62
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.83	0.60
1:A:269:ASP:OD1	1:A:270:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.82	0.60
1:B:202:GLN:HB3	1:B:203:LEU:HD12	1.84	0.59
2:F:84:PRO:HA	2:F:111:VAL:HB	1.83	0.59
1:A:427:LYS:O	2:F:100(F):TYR:HA	2.03	0.58
1:A:216:ASN:HB2	1:A:218:GLU:OE1	2.02	0.58
2:E:43:LYS:NZ	2:E:44:GLU:O	2.37	0.58
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.84	0.58
1:B:524:PRO:HG2	1:B:530:TYR:CZ	2.39	0.58
1:A:97:MET:HE1	1:A:292:ILE:HB	1.86	0.57
1:A:520:ILE:HD11	1:B:522:GLU:HA	1.86	0.57
1:B:97:MET:HE1	1:B:292:ILE:HB	1.86	0.57
1:B:427:LYS:O	2:D:100(F):TYR:HA	2.04	0.57
2:D:40:ALA:HB3	2:D:43:LYS:HE3	1.86	0.57
1:C:423:THR:HG1	2:E:96:ARG:HH12	1.51	0.57
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.87	0.56
1:A:486:ASP:OD1	1:A:486:ASP:N	2.38	0.56
2:E:84:PRO:HA	2:E:111:VAL:HB	1.86	0.56
1:C:206:ILE:HG13	1:C:207:LEU:HG	1.88	0.56
1:B:202:GLN:O	1:B:205:PRO:HD2	2.06	0.56
1:C:138:LEU:HB3	1:C:141:LEU:HD12	1.86	0.56
1:A:399:LYS:NZ	1:C:497:GLU:OE1	2.37	0.55
1:B:267:THR:HA	2:E:58:TYR:HB2	1.88	0.55
1:B:67:ASN:HB3	1:B:80:LYS:HE3	1.88	0.55
1:C:200:ASP:HA	1:C:204:LEU:HG	1.89	0.54
1:B:487:GLU:HB3	1:B:490:ALA:HB2	1.90	0.54
1:A:190:PHE:CE2	1:A:260:LEU:HG	2.41	0.54
1:A:529:ALA:HA	1:C:533:LYS:HB2	1.90	0.53
1:C:69:CYS:O	1:C:80:LYS:NZ	2.37	0.53
1:C:183:ASN:OD1	1:C:185:VAL:HG12	2.09	0.53
2:E:40:ALA:HB3	2:E:43:LYS:HE3	1.89	0.53
1:C:427:LYS:O	2:E:100(F):TYR:HA	2.09	0.53
1:B:157:VAL:HG11	1:B:181:LEU:HB3	1.91	0.52
1:A:218:GLU:HG2	1:C:75:LYS:HG3	1.92	0.52
1:B:310:ASP:OD1	1:B:364:ARG:NH1	2.30	0.52
1:A:97:MET:SD	1:A:291:ILE:HA	2.51	0.51
1:C:454:ASN:HA	2:E:98:SER:HB2	1.93	0.51
1:A:203:LEU:O	1:A:206:ILE:HG12	2.10	0.51
1:B:533:LYS:HB2	1:C:529:ALA:HA	1.93	0.51
1:A:533:LYS:HB2	1:B:529:ALA:HA	1.90	0.51
1:B:167:ILE:HD13	1:B:179:VAL:HG21	1.92	0.51
1:C:167:ILE:HG23	1:C:189:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ARG:HE	1:C:368:ASP:CG	2.19	0.51
1:B:318:THR:OG1	1:B:339:ARG:HD3	2.11	0.50
1:A:183:ASN:OD1	1:A:185:VAL:HG12	2.12	0.50
1:A:75:LYS:HD2	1:A:215:SER:O	2.11	0.50
1:B:526:ASP:C	1:B:528:GLN:H	2.19	0.50
1:C:76:VAL:HG23	1:C:214:ILE:HG23	1.92	0.50
1:A:178:VAL:HG22	1:A:188:LEU:HD23	1.92	0.50
1:B:261:ILE:HA	1:B:264:MET:HE3	1.93	0.50
1:A:487:GLU:HB3	1:A:490:ALA:HB2	1.94	0.50
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	1.93	0.50
1:B:526:ASP:O	1:B:528:GLN:N	2.43	0.49
2:F:29:LEU:HD12	2:F:71:ARG:NH2	2.27	0.49
1:A:69:CYS:HB3	1:A:80:LYS:HZ1	1.77	0.49
1:A:174:THR:HG22	1:A:176:LYS:H	1.77	0.49
1:B:94:GLN:HA	1:B:97:MET:HE2	1.94	0.49
1:C:66:GLU:OE2	1:C:68:LYS:HE2	2.12	0.49
2:F:71:ARG:HH21	2:F:73:ASN:HA	1.78	0.49
1:C:137:PHE:CD1	1:C:137:PHE:C	2.91	0.49
1:B:267:THR:HG23	1:B:269:ASP:OD1	2.13	0.49
1:A:200:ASP:HA	1:A:204:LEU:HB2	1.95	0.48
1:C:310:ASP:OD1	1:C:364:ARG:NH1	2.38	0.48
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.49	0.47
1:A:498:LYS:NZ	1:B:486:ASP:OD1	2.35	0.47
1:C:208:ASN:O	1:C:209:LYS:HG3	2.14	0.47
1:C:522:GLU:HG3	1:C:523:ALA:O	2.14	0.47
1:A:356:GLU:CD	1:A:356:GLU:H	2.22	0.47
1:C:215:SER:OG	1:C:216:ASN:OD1	2.32	0.47
1:A:62:SER:OG	1:A:64:ILE:HG13	2.13	0.47
1:B:356:GLU:CD	1:B:356:GLU:H	2.21	0.47
1:A:260:LEU:HD13	1:A:303:LEU:HD11	1.96	0.47
1:B:214:ILE:HG22	1:B:215:SER:H	1.79	0.47
1:C:62:SER:HB2	1:C:196:LYS:HA	1.95	0.47
1:A:267:THR:OG1	1:A:269:ASP:OD1	2.30	0.47
1:A:360:VAL:HG22	1:A:365:VAL:HG22	1.97	0.47
1:B:394:LYS:NZ	1:C:400:THR:HG21	2.29	0.47
1:B:398:SER:HA	1:B:485:SER:O	2.14	0.47
2:F:11:LEU:HD11	2:F:112:SER:HB3	1.95	0.47
1:B:178:VAL:HG22	1:B:188:LEU:HD23	1.96	0.47
1:B:217:ILE:O	1:B:221:ILE:HG13	2.15	0.47
1:C:171:LEU:HD11	1:C:189:THR:HG22	1.97	0.47
1:B:394:LYS:NZ	1:B:489:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:LYS:HZ2	1:C:400:THR:HG21	1.80	0.47
1:C:198:TYR:O	1:C:202:GLN:HB2	2.15	0.47
1:B:62:SER:OG	1:B:64:ILE:HG13	2.14	0.46
1:C:236:GLU:OE2	1:C:248:SER:OG	2.29	0.46
1:C:524:PRO:HG2	1:C:530:TYR:CZ	2.50	0.46
2:E:71:ARG:NH1	2:E:73:ASN:OD1	2.48	0.46
2:F:40:ALA:HB3	2:F:43:LYS:HE3	1.96	0.46
1:B:334:LEU:HB2	1:B:475:ILE:HD13	1.95	0.46
1:B:47:ALA:HB2	1:B:364:ARG:HD2	1.97	0.46
1:C:212:CYS:O	1:C:214:ILE:HG13	2.16	0.46
1:C:427:LYS:N	1:C:448:ASP:OD2	2.45	0.46
1:B:62:SER:HB3	1:B:199:ILE:HD12	1.97	0.46
1:A:289:MET:HE1	1:A:297:LEU:HD13	1.97	0.46
1:C:176:LYS:HG2	1:C:190:PHE:CE1	2.51	0.46
1:C:352:PHE:CE2	1:C:372:SER:HB3	2.51	0.46
1:B:214:ILE:CG2	1:B:215:SER:N	2.77	0.46
1:B:207:LEU:HD23	1:B:207:LEU:HA	1.69	0.46
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.50	0.46
1:A:532:ARG:O	1:B:530:TYR:N	2.44	0.45
1:C:47:ALA:HB2	1:C:364:ARG:HD2	1.99	0.45
1:C:202:GLN:O	1:C:205:PRO:HD2	2.16	0.45
1:A:159:HIS:CE1	1:A:291:ILE:HG23	2.51	0.45
1:B:214:ILE:HG22	1:B:215:SER:N	2.32	0.45
1:B:395:ILE:HD13	1:B:492:ILE:HD13	1.98	0.45
1:C:28:ILE:HD13	1:C:44:TYR:CZ	2.51	0.45
1:A:206:ILE:HB	1:A:213:SER:O	2.16	0.45
1:A:512:LEU:O	1:A:516:ILE:HG13	2.17	0.45
1:B:297:LEU:HD12	1:B:298:ALA:N	2.31	0.45
1:A:167:ILE:HD13	1:A:179:VAL:HG21	1.98	0.45
1:B:67:ASN:ND2	1:B:83:LEU:HD23	2.32	0.45
1:B:176:LYS:HE2	1:B:190:PHE:CE2	2.52	0.45
1:C:289:MET:HE1	1:C:297:LEU:HD13	1.99	0.45
1:C:280:ILE:HG21	1:C:366:PHE:CG	2.52	0.45
1:A:222:GLU:OE1	1:C:77:LYS:NZ	2.48	0.45
1:C:198:TYR:CE1	1:C:202:GLN:HG3	2.52	0.45
1:B:522:GLU:HG3	1:B:523:ALA:O	2.17	0.45
1:B:289:MET:HE1	1:B:297:LEU:HD13	1.98	0.45
2:E:93:ALA:HB2	2:E:103:TRP:CE3	2.52	0.45
1:C:185:VAL:HG23	2:F:100(F):TYR:CZ	2.52	0.44
1:C:297:LEU:HD12	1:C:298:ALA:N	2.32	0.44
2:F:34:ILE:HG21	2:F:78:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD21	1:A:260:LEU:HD12	1.99	0.44
1:C:166:LYS:NZ	1:C:182:SER:HB3	2.31	0.44
2:D:84:PRO:HA	2:D:111:VAL:HB	2.00	0.44
1:B:317:HIS:HB3	1:B:406:VAL:HG11	1.99	0.44
2:D:2:VAL:HG13	2:D:27:PHE:CD2	2.52	0.44
1:A:198:TYR:O	1:A:202:GLN:HB2	2.17	0.44
1:B:68:LYS:HB3	1:B:210:GLN:HA	2.00	0.44
1:A:423:THR:HG1	2:F:96:ARG:HH12	1.53	0.44
1:A:97:MET:SD	1:A:289:MET:HE3	2.58	0.44
1:B:427:LYS:HB3	1:B:427:LYS:HE3	1.86	0.44
1:A:217:ILE:HD13	1:B:217:ILE:HD12	2.00	0.43
1:B:61:LEU:O	1:B:196:LYS:HB2	2.17	0.43
1:B:83:LEU:HD22	1:B:207:LEU:HD13	2.00	0.43
2:F:6:GLU:HA	2:F:21:SER:O	2.18	0.43
2:F:15:GLY:HA2	2:F:82(B):SER:HA	2.00	0.43
1:A:97:MET:HE3	1:A:97:MET:HB2	1.74	0.43
1:A:331:ASN:O	1:A:399:LYS:HG2	2.17	0.43
1:C:137:PHE:C	1:C:137:PHE:HD1	2.26	0.43
2:D:27:PHE:HE1	2:D:29:LEU:HD23	1.83	0.43
2:E:43:LYS:HE3	2:E:43:LYS:HB3	1.87	0.43
2:E:82:MET:HB3	2:E:82(C):LEU:HD21	2.00	0.43
1:B:68:LYS:HD2	1:B:210:GLN:HG3	1.99	0.43
1:B:312:PRO:HG2	1:B:344:ASP:OD2	2.19	0.43
1:C:291:ILE:HD11	1:C:293:LYS:HE2	2.00	0.43
1:A:64:ILE:O	1:A:64:ILE:HG22	2.18	0.43
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.31	0.43
1:B:291:ILE:HD11	1:B:293:LYS:HE2	1.99	0.43
1:B:64:ILE:O	1:B:64:ILE:HG22	2.18	0.42
1:A:400:THR:HG22	1:A:402:VAL:HG23	2.01	0.42
1:C:62:SER:OG	1:C:64:ILE:HG13	2.19	0.42
1:C:487:GLU:HB3	1:C:490:ALA:HB2	2.01	0.42
1:A:46:SER:HB3	1:A:313:CYS:SG	2.59	0.42
1:A:63:ASN:HB2	1:A:295:GLU:HG2	2.02	0.42
1:A:74:ALA:HB1	1:B:218:GLU:HB3	2.02	0.42
1:A:181:LEU:HD12	1:A:185:VAL:HG13	2.02	0.42
1:B:28:ILE:HD12	1:B:462:GLN:NE2	2.34	0.42
2:D:43:LYS:HE3	2:D:43:LYS:HB3	1.83	0.42
1:A:522:GLU:HG3	1:A:523:ALA:O	2.18	0.42
1:B:64:ILE:HD11	1:B:199:ILE:HD13	2.02	0.42
1:B:97:MET:SD	1:B:291:ILE:HA	2.59	0.42
1:B:192:VAL:HG13	1:B:256:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:SER:HB3	1:B:417:TYR:CE2	2.54	0.42
1:A:217:ILE:O	1:A:221:ILE:HG13	2.19	0.42
1:A:265:PRO:HA	2:D:58:TYR:CE1	2.54	0.42
1:C:76:VAL:HG21	1:C:214:ILE:HG12	2.02	0.42
2:D:27:PHE:CE1	2:D:29:LEU:HD23	2.55	0.42
2:E:2:VAL:HG13	2:E:27:PHE:CD2	2.55	0.41
1:A:334:LEU:CD1	1:A:397:THR:HG22	2.50	0.41
1:A:449:THR:HB	1:A:456:LEU:HD11	2.02	0.41
1:A:514:SER:O	1:A:515:ALA:HB3	2.20	0.41
1:B:97:MET:SD	1:B:289:MET:HE3	2.60	0.41
1:B:172:LEU:HA	1:B:172:LEU:HD12	1.80	0.41
1:C:417:TYR:HA	1:C:437:ASN:OD1	2.20	0.41
1:B:373:LEU:HD13	1:C:402:VAL:HG21	2.00	0.41
1:A:67:ASN:O	1:A:80:LYS:HE3	2.20	0.41
1:A:176:LYS:HZ3	1:A:259:SER:HB3	1.84	0.41
1:A:537:TRP:HZ2	1:C:520:ILE:HD13	1.86	0.41
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.74	0.41
1:B:171:LEU:HD11	1:B:189:THR:HG22	2.02	0.41
1:A:297:LEU:HD12	1:A:298:ALA:N	2.35	0.41
1:B:280:ILE:HG21	1:B:366:PHE:CG	2.55	0.41
1:C:449:THR:HB	1:C:456:LEU:HD11	2.01	0.41
1:C:502:SER:O	1:C:506:ILE:HG12	2.20	0.41
2:D:29:LEU:HD22	2:D:34:ILE:HD11	2.03	0.41
1:A:334:LEU:HD12	1:A:397:THR:HG22	2.02	0.41
1:C:181:LEU:HD12	1:C:185:VAL:HG13	2.03	0.41
1:C:454:ASN:CA	2:E:98:SER:HB2	2.51	0.41
1:B:206:ILE:CG1	1:B:207:LEU:HG	2.41	0.40
1:C:96:LEU:HD23	1:C:96:LEU:HA	1.77	0.40
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.74	0.40
1:C:532:ARG:NH1	1:C:535:GLY:O	2.55	0.40
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.73	0.40
1:C:66:GLU:HG2	1:C:67:ASN:N	2.37	0.40
1:B:157:VAL:HG12	1:B:163:GLU:HG2	2.04	0.40
2:E:43:LYS:HG2	2:E:44:GLU:N	2.37	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)
1:C:209:LYS:NZ	1:C:211:SER:O[4_557]	2.08	0.12

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	479/550 (87%)	465 (97%)	13 (3%)	1 (0%)	43	71
1	B	481/550 (88%)	467 (97%)	12 (2%)	2 (0%)	30	60
1	C	477/550 (87%)	454 (95%)	22 (5%)	1 (0%)	43	71
2	D	124/131 (95%)	118 (95%)	6 (5%)	0	100	100
2	E	121/131 (92%)	118 (98%)	3 (2%)	0	100	100
2	F	123/131 (94%)	120 (98%)	3 (2%)	0	100	100
All	All	1805/2043 (88%)	1742 (96%)	59 (3%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	B	65	LYS
1	C	65	LYS
1	B	527	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	435/494 (88%)	429 (99%)	6 (1%)	59	73
1	B	437/494 (88%)	429 (98%)	8 (2%)	51	70
1	C	434/494 (88%)	427 (98%)	7 (2%)	55	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	103/108 (95%)	101 (98%)	2 (2%)	50	68
2	E	100/108 (93%)	98 (98%)	2 (2%)	48	68
2	F	102/108 (94%)	100 (98%)	2 (2%)	48	68
All	All	1611/1806 (89%)	1584 (98%)	27 (2%)	53	71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLU
1	A	215	SER
1	A	252	LEU
1	A	291	ILE
1	A	297	LEU
1	A	356	GLU
1	B	161	GLU
1	B	202	GLN
1	B	252	LEU
1	B	254	ASN
1	B	297	LEU
1	B	326	THR
1	B	356	GLU
1	B	528	GLN
1	C	137	PHE
1	C	252	LEU
1	C	297	LEU
1	C	326	THR
1	C	356	GLU
1	C	361	GLN
1	C	472	GLU
2	D	1	GLN
2	D	28	THR
2	E	1	GLN
2	E	28	THR
2	F	1	GLN
2	F	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	225	GLN
1	A	277	ASN
1	A	380	ASN
1	A	460	ASN
1	B	197	ASN
1	B	216	ASN
1	B	317	HIS
1	C	268	ASN
1	C	528	GLN
2	D	81	GLN

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 ⓘ

3 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	C	800	1	14,14,15	0.39	0	17,19,21	0.60	0
3	NAG	A	800	1	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	B	800	1	14,14,15	0.23	0	17,19,21	0.61	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	C	800	1	-	0/6/23/26	0/1/1/1
3	NAG	A	800	1	-	0/6/23/26	0/1/1/1
3	NAG	B	800	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	800	NAG	O5-C5-C6-O6
3	B	800	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	483/550 (87%)	-0.40	0	100	100	49, 78, 165, 238	0
1	B	485/550 (88%)	-0.38	5 (1%)	79	63	48, 84, 170, 264	0
1	C	481/550 (87%)	-0.42	0	100	100	50, 82, 159, 239	0
2	D	126/131 (96%)	-0.42	0	100	100	58, 77, 109, 151	0
2	E	123/131 (93%)	-0.25	0	100	100	80, 128, 167, 175	0
2	F	125/131 (95%)	-0.34	0	100	100	62, 98, 137, 188	0
All	All	1823/2043 (89%)	-0.39	5 (0%)	90	82	48, 84, 163, 264	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	SER	5.4
1	B	217	ILE	2.5
1	B	205	PRO	2.4
1	B	207	LEU	2.3
1	B	216	ASN	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 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	B	800	14/15	0.77	0.09	109,118,126,126	0
3	NAG	C	800	14/15	0.91	0.07	81,92,99,100	0
3	NAG	A	800	14/15	0.95	0.06	71,78,85,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.