



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:46 AM UTC

PDB ID : 7D85 / pdb_00007d85
Title : Crystal structure of anti-ErbB3 Fab ISU104 in complex with human ErbB3 extracellular domain 3
Authors : Yoo, Y.; Cho, H.S.
Deposited on : 2020-10-07
Resolution : 2.50 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:

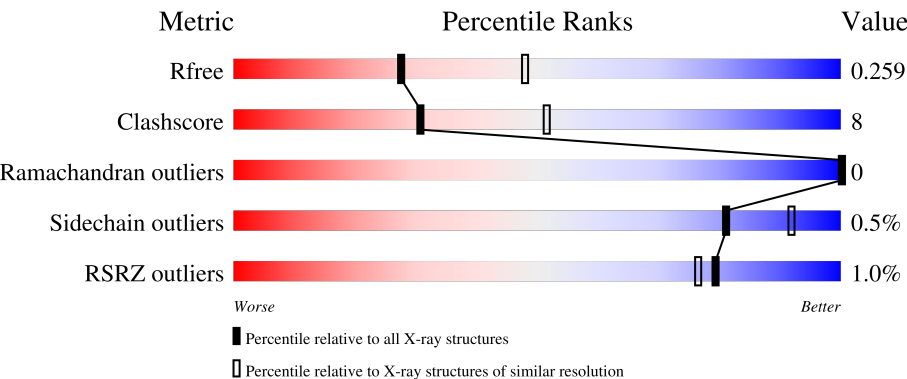
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	194	% 73% 26% ..
1	D	194	2% 82% 18% .
2	B	228	2% 79% 16% .
2	E	228	% 79% 15% 5%
3	C	216	% 81% 18% .

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Mol	Chain	Length	Quality of chain
3	F	216	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a green segment representing 77% and a yellow segment representing 21%. A small grey dot is visible at the end of the bar.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9539 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1503	945	275	273	10			
1	D	193	Total	C	N	O	S	0	0	0
			1503	945	275	273	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	GLY	-	expression tag	UNP P21860
A	308	ILE	-	expression tag	UNP P21860
D	307	GLY	-	expression tag	UNP P21860
D	308	ILE	-	expression tag	UNP P21860

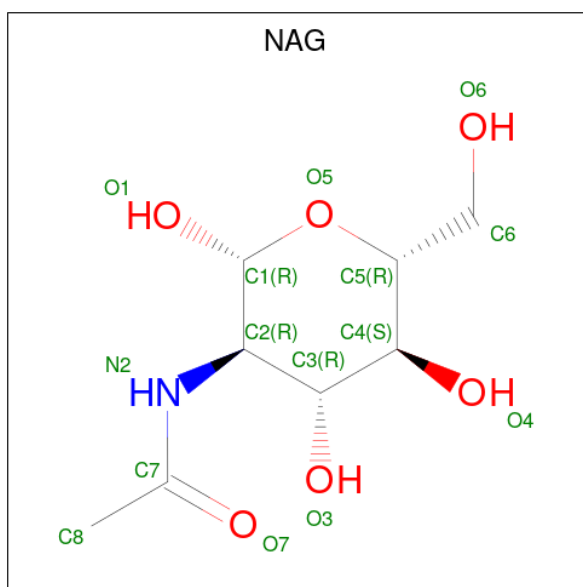
- Molecule 2 is a protein called Anti-ErbB3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1629	1028	268	326	7			
2	E	217	Total	C	N	O	S	0	0	0
			1625	1026	267	325	7			

- Molecule 3 is a protein called Anti-ErbB3 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1571	977	265	325	4			
3	F	213	Total	C	N	O	S	0	0	0
			1571	977	265	325	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

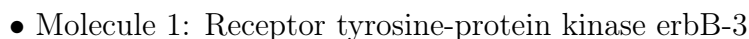
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	14	Total	O	0	0
			14	14		
5	C	7	Total	O	0	0
			7	7		
5	D	1	Total	O	0	0
			1	1		
5	E	7	Total	O	0	0
			7	7		

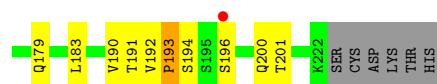
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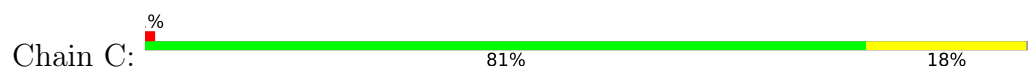
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	4	Total	O	0	0
			4	4		

- Molecule 1: Receptor tyrosine-protein kinase erbB-3

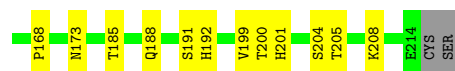
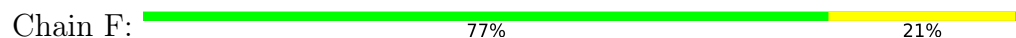




• Molecule 3: Anti-ErbB3 Fab light chain



• Molecule 3: Anti-ErbB3 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.29Å 77.78Å 93.94Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	46.63 – 2.50 46.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.63-2.50) 99.2 (46.63-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.258 0.203 , 0.259	Depositor DCC
R_{free} test set	1998 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9539	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [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	0.54	0/1539	0.70	1/2084 (0.0%)
1	D	0.42	0/1539	0.65	0/2084
2	B	0.47	0/1668	0.73	2/2272 (0.1%)
2	E	0.50	1/1664 (0.1%)	0.67	1/2267 (0.0%)
3	C	0.54	0/1610	0.71	0/2198
3	F	0.39	0/1610	0.66	0/2198
All	All	0.48	1/9630 (0.0%)	0.69	4/13103 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	193	PRO	C-O	-9.12	1.13	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	VAL	CA-C-N	6.67	129.96	120.49
2	B	12	VAL	C-N-CA	6.67	129.96	120.49
1	A	461	GLU	CB-CG-CD	5.51	121.97	112.60
2	E	191	THR	CA-CB-OG1	-5.38	101.53	109.60

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	1503	0	1480	42	0
1	D	1503	0	1480	22	0
2	B	1629	0	1578	26	0
2	E	1625	0	1575	22	0
3	C	1571	0	1516	24	0
3	F	1571	0	1516	31	0
4	A	56	0	52	8	0
4	D	42	0	39	1	0
5	A	6	0	0	0	0
5	B	14	0	0	0	0
5	C	7	0	0	0	0
5	D	1	0	0	0	0
5	E	7	0	0	0	0
5	F	4	0	0	0	0
All	All	9539	0	9236	156	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 (156) 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:A:460:GLU:HG3	2:E:85:SER:HB3	1.67	0.76
2:E:193:PRO:HG2	2:E:196:SER:HB2	1.72	0.72
2:B:85:SER:HB3	1:D:460:GLU:HG2	1.73	0.70
1:A:435:ILE:HD11	1:A:455:LEU:HD11	1.74	0.68
3:C:33:SER:HB2	3:C:51:SER:HA	1.77	0.66
3:F:38:GLN:HB2	3:F:48:LEU:HD11	1.78	0.66
1:D:399:ILE:HB	1:D:430:ILE:HD13	1.76	0.66
2:E:67:ARG:NH2	2:E:90:ASP:OD2	2.29	0.65
2:B:192:VAL:HG11	2:B:202:TYR:CE2	2.32	0.64
1:A:414:MET:HG3	1:A:436:TYR:CE1	2.32	0.64
1:D:355:HIS:HB3	1:D:357:ILE:HG23	1.81	0.63
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.80	0.63
3:C:184:LEU:HG	3:C:188:GLN:HG3	1.80	0.63
1:A:414:MET:HG3	1:A:436:TYR:HE1	1.64	0.62
3:F:110:LEU:HA	3:F:144:TYR:OH	2.01	0.61
3:C:170:LYS:HE2	3:C:176:TYR:CZ	2.35	0.61
3:C:198:GLN:NE2	3:C:207:GLU:OE2	2.32	0.61
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.30	0.59
3:C:2:SER:HA	3:C:100:VAL:HG13	1.85	0.59
3:C:184:LEU:HD21	3:C:195:TYR:CZ	2.37	0.59
2:B:73:ASP:OD2	2:B:76:LYS:HG3	2.03	0.59
1:A:385:PRO:O	4:A:604:NAG:H82	2.03	0.58
3:F:123:PRO:HA	3:F:136:LEU:HD23	1.86	0.58
3:F:185:THR:HB	3:F:188:GLN:HB2	1.86	0.57
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.86	0.57
1:A:456:ARG:HH11	1:A:456:ARG:HG3	1.70	0.56
2:B:32:TYR:CD2	2:B:98:LYS:HG3	2.41	0.56
1:A:452:THR:HG22	1:A:459:THR:HB	1.87	0.56
1:D:458:PRO:O	1:D:459:THR:HB	2.05	0.56
1:A:309:PRO:HA	1:A:336:THR:HG21	1.86	0.55
2:B:124:THR:HG21	1:D:475:VAL:HG11	1.89	0.54
1:D:400:GLY:O	1:D:431:SER:HB2	2.06	0.54
3:F:121:LEU:H	3:F:208:LYS:HD2	1.73	0.54
1:A:411:LEU:HD11	1:A:413:ILE:HD11	1.90	0.54
2:E:150:VAL:HG11	2:E:158:VAL:HG11	1.90	0.54
3:F:117:PRO:HB3	3:F:143:PHE:HB3	1.89	0.54
2:E:167:LEU:HD21	2:E:190:VAL:HG21	1.89	0.53
3:C:198:GLN:HG2	3:C:207:GLU:HG3	1.91	0.53
2:B:210:PRO:HA	1:D:472:ARG:NE	2.24	0.53
3:F:146:GLY:O	3:F:168:PRO:HG2	2.09	0.53
1:A:385:PRO:C	4:A:604:NAG:H82	2.33	0.52
2:E:36:TRP:NE1	2:E:81:LEU:HB2	2.24	0.52
1:A:414:MET:HE1	2:B:101:HIS:HD2	1.75	0.52
1:A:353:PRO:HD2	1:A:354:TRP:CZ3	2.45	0.52
1:A:310:LYS:NZ	1:A:333:VAL:O	2.40	0.51
1:A:469:ARG:HH22	1:A:477:GLU:CD	2.19	0.51
2:B:51:ILE:HG13	2:B:58:ILE:HG12	1.91	0.51
1:D:436:TYR:O	1:D:437:ILE:HG13	2.10	0.51
1:A:369:ARG:NH1	4:A:602:NAG:O7	2.40	0.51
3:F:119:VAL:HG21	3:F:199:VAL:HG21	1.92	0.51
3:C:55:ARG:HD3	3:C:63:PHE:O	2.11	0.51
1:A:334:ASN:OD1	4:A:603:NAG:C1	2.59	0.50
2:E:32:TYR:O	2:E:72:ARG:NH2	2.43	0.50
3:F:112:GLN:HG3	3:F:113:PRO:HD2	1.93	0.50
3:F:121:LEU:H	3:F:208:LYS:HZ2	1.60	0.50
3:F:121:LEU:HB3	3:F:208:LYS:HD3	1.93	0.50
2:E:34:MET:HG2	2:E:72:ARG:NH2	2.27	0.50
3:C:84:GLU:OE1	3:C:170:LYS:HE3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:ASN:O	1:D:419:VAL:HG12	2.11	0.49
2:E:6:GLU:HA	2:E:21:SER:O	2.12	0.49
1:A:389:ASN:OD1	1:A:391:SER:HB3	2.12	0.49
1:A:407:ARG:HG2	3:C:92:TRP:CE3	2.47	0.49
1:A:425:ARG:HH22	4:A:602:NAG:H82	1.77	0.49
3:C:142:ASP:OD1	3:C:171:GLN:NE2	2.38	0.49
2:E:30:SER:O	2:E:53:LEU:HB2	2.13	0.49
2:E:48:VAL:HG13	2:E:64:VAL:HG11	1.95	0.49
1:A:355:HIS:HB2	1:A:357:ILE:HG12	1.95	0.49
1:A:425:ARG:NH2	4:A:602:NAG:H82	2.28	0.48
2:B:127:PRO:HD2	2:B:213:THR:HG21	1.95	0.48
3:C:146:GLY:HA2	3:C:176:TYR:CD2	2.49	0.48
1:A:414:MET:CE	2:B:101:HIS:HD2	2.26	0.47
3:F:14:PRO:HD3	3:F:110:LEU:O	2.15	0.47
3:C:140:ILE:HG22	3:C:143:PHE:CE1	2.50	0.47
2:E:34:MET:HG2	2:E:72:ARG:HH22	1.79	0.47
1:A:344:PHE:HB2	1:A:380:ILE:HA	1.96	0.47
2:B:53:LEU:HD22	2:B:101:HIS:CG	2.49	0.47
1:A:417:LEU:O	1:A:442:GLN:HG3	2.15	0.47
2:E:192:VAL:HB	2:E:193:PRO:HD2	1.95	0.47
3:F:33:SER:HB3	3:F:51:SER:HA	1.96	0.47
1:D:455:LEU:HD22	1:D:462:ARG:NH1	2.29	0.46
1:A:349:LEU:HD13	1:A:382:SER:HB3	1.98	0.46
1:D:438:SER:HA	1:D:466:LYS:O	2.16	0.46
1:A:452:THR:CG2	1:A:459:THR:HB	2.46	0.46
1:D:437:ILE:O	1:D:465:ILE:HA	2.16	0.46
1:A:473:ASP:O	1:A:477:GLU:HG3	2.16	0.45
3:C:112:GLN:HG3	3:C:113:PRO:HD2	1.99	0.45
1:A:414:MET:CE	2:B:101:HIS:CD2	3.00	0.45
1:A:447:HIS:CG	1:A:471:ARG:HG3	2.50	0.45
1:A:449:LEU:HD22	1:A:451:TRP:CZ2	2.52	0.45
2:E:73:ASP:OD2	2:E:76:LYS:HG3	2.16	0.45
2:B:147:GLY:HA2	2:B:162:TRP:CH2	2.51	0.45
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.98	0.45
1:D:372:ARG:HH22	4:D:602:NAG:H62	1.80	0.45
2:B:152:ASP:HB3	2:B:183:LEU:HD13	1.98	0.45
1:D:364:LYS:O	1:D:367:VAL:HG22	2.18	0.44
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.99	0.44
2:B:151:LYS:HA	2:B:185:SER:OG	2.17	0.44
3:F:26:SER:O	3:F:31:SER:OG	2.28	0.44
1:A:414:MET:HE1	2:B:101:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:84:GLU:HB2	3:F:109:VAL:HG23	1.99	0.44
2:E:200:GLN:HG3	2:E:201:THR:N	2.32	0.44
2:E:67:ARG:HB3	2:E:84:ASN:O	2.18	0.44
1:A:428:LYS:O	1:A:456:ARG:NH1	2.51	0.44
1:A:456:ARG:HG3	1:A:456:ARG:NH1	2.33	0.43
3:C:4:LEU:HB2	3:C:102:GLY:HA2	2.00	0.43
3:F:121:LEU:H	3:F:208:LYS:CD	2.31	0.43
1:D:344:PHE:HB2	1:D:380:ILE:HA	2.00	0.43
3:F:34:VAL:HG12	3:F:52:ASP:HA	2.01	0.43
3:F:200:THR:HA	3:F:204:SER:O	2.18	0.43
3:C:136:LEU:HD12	3:C:182:LEU:HD23	2.01	0.43
2:E:67:ARG:HH22	2:E:90:ASP:CG	2.24	0.43
3:F:188:GLN:O	3:F:191:SER:HB3	2.18	0.43
3:F:200:THR:HG22	3:F:205:THR:OG1	2.18	0.43
1:A:334:ASN:OD1	4:A:603:NAG:O5	2.36	0.43
3:F:119:VAL:HG21	3:F:199:VAL:CG2	2.48	0.43
2:B:189:VAL:HB	3:C:139:LEU:HD13	2.01	0.43
3:F:82:GLU:OE2	3:F:82:GLU:N	2.50	0.43
3:F:154:ALA:HB1	3:F:192:HIS:CD2	2.53	0.43
1:A:341:ASN:OD1	1:A:376:GLY:HA3	2.19	0.43
2:E:67:ARG:HH21	2:E:87:ARG:HG3	1.84	0.43
3:C:124:PRO:HD3	3:C:136:LEU:HD23	2.00	0.42
3:F:148:VAL:HG22	3:F:201:HIS:HD2	1.84	0.42
3:C:134:ALA:HB3	3:C:184:LEU:O	2.20	0.42
2:B:127:PRO:HB3	2:B:153:TYR:HB3	2.02	0.42
3:C:3:VAL:HG12	3:C:3:VAL:O	2.19	0.42
2:B:128:SER:HB3	2:B:130:PHE:CE2	2.53	0.42
3:C:193:LYS:HA	3:C:193:LYS:HD2	1.85	0.42
2:E:98:LYS:HE3	2:E:110:TYR:HB3	2.01	0.42
2:B:210:PRO:HG3	1:D:472:ARG:NH2	2.34	0.42
2:E:179:GLN:HG3	2:E:183:LEU:O	2.20	0.42
1:D:443:LEU:O	1:D:469:ARG:HB3	2.20	0.41
1:D:473:ASP:O	1:D:477:GLU:HG3	2.20	0.41
2:B:91:THR:HA	2:B:117:VAL:O	2.21	0.41
3:C:34:VAL:HG23	3:C:67:LYS:HD3	2.02	0.41
1:A:449:LEU:HD22	1:A:451:TRP:CE2	2.55	0.41
4:A:603:NAG:C1	4:A:603:NAG:O7	2.68	0.41
3:F:173:ASN:OD1	3:F:173:ASN:N	2.48	0.41
1:A:332:PHE:HA	1:A:335:CYS:SG	2.61	0.41
1:A:379:ASN:OD1	1:A:412:LEU:HD22	2.20	0.41
1:D:436:TYR:C	1:D:437:ILE:HG13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:120:THR:HA	3:F:208:LYS:HZ2	1.85	0.41
1:A:481:CYS:SG	1:A:490:CYS:N	2.94	0.41
1:D:325:ASP:OD1	1:D:327:SER:OG	2.30	0.41
1:D:389:ASN:OD1	1:D:391:SER:HB2	2.21	0.40
1:A:436:TYR:CD2	2:B:102:MET:HE3	2.57	0.40
3:C:36:TRP:CE2	3:C:74:LEU:HB2	2.56	0.40
3:C:153:LYS:HB2	3:C:196:SER:HB2	2.03	0.40
3:F:7:PRO:HA	3:F:8:PRO:HD3	1.97	0.40
3:F:28:ASN:HA	3:F:92:TRP:O	2.20	0.40
3:F:32:ASN:O	3:F:67:LYS:NZ	2.54	0.40
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.90	0.40
1:A:434:ARG:HG2	1:A:462:ARG:HA	2.03	0.40
1:D:355:HIS:O	1:D:356:LYS:HG2	2.22	0.40
3:F:56:PRO:HD2	3:F:59:VAL:HG21	2.03	0.40
3:F:121:LEU:HB3	3:F:208:LYS:CD	2.52	0.40

There are no symmetry-related clashes.

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	191/194 (98%)	181 (95%)	10 (5%)	0	100	100
1	D	191/194 (98%)	179 (94%)	12 (6%)	0	100	100
2	B	214/228 (94%)	209 (98%)	5 (2%)	0	100	100
2	E	213/228 (93%)	209 (98%)	4 (2%)	0	100	100
3	C	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
3	F	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
All	All	1231/1276 (96%)	1188 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/168 (100%)	167 (99%)	1 (1%)	78	91
1	D	168/168 (100%)	168 (100%)	0	100	100
2	B	183/193 (95%)	181 (99%)	2 (1%)	65	84
2	E	183/193 (95%)	182 (100%)	1 (0%)	81	92
3	C	179/182 (98%)	178 (99%)	1 (1%)	78	91
3	F	179/182 (98%)	179 (100%)	0	100	100
All	All	1060/1086 (98%)	1055 (100%)	5 (0%)	81	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLU
2	B	98	LYS
2	B	217	LYS
3	C	25	SER
2	E	194	SER

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	322	GLN
1	A	350	ASN
1	A	442	GLN
2	B	13	GLN
1	D	322	GLN
1	D	467	HIS
2	E	39	GLN
2	E	82	GLN
3	F	38	GLN
3	F	39	GLN
3	F	201	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
4	NAG	A	601	1	14,14,15	0.59	0	17,19,21	0.88	1 (5%)
4	NAG	A	604	1	14,14,15	1.00	0	17,19,21	1.91	5 (29%)
4	NAG	D	601	1	14,14,15	1.54	4 (28%)	17,19,21	1.82	5 (29%)
4	NAG	A	602	1	14,14,15	0.90	1 (7%)	17,19,21	0.70	0
4	NAG	A	603	-	14,14,15	0.87	0	17,19,21	1.20	2 (11%)
4	NAG	D	603	1	14,14,15	1.39	2 (14%)	17,19,21	2.12	8 (47%)
4	NAG	D	602	1	14,14,15	1.40	1 (7%)	17,19,21	1.75	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	601	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	4/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	-	-	5/6/23/26	0/1/1/1
4	NAG	D	603	1	-	2/6/23/26	0/1/1/1
4	NAG	D	602	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	NAG	O5-C1	-3.24	1.38	1.43
4	D	603	NAG	C1-C2	-3.14	1.48	1.52
4	A	602	NAG	C1-C2	2.97	1.56	1.52
4	D	602	NAG	O5-C5	-2.93	1.37	1.43
4	D	601	NAG	O5-C5	-2.76	1.38	1.43
4	D	601	NAG	C2-N2	-2.26	1.42	1.46
4	D	603	NAG	O5-C1	-2.10	1.40	1.43
4	D	601	NAG	O7-C7	-2.02	1.18	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	NAG	C1-O5-C5	-5.69	104.56	112.19
4	D	603	NAG	C2-N2-C7	-3.97	117.58	122.90
4	D	602	NAG	C4-C3-C2	-3.87	105.34	111.02
4	D	603	NAG	O5-C1-C2	-3.59	105.73	111.29
4	D	601	NAG	C1-O5-C5	-3.54	107.45	112.19
4	D	602	NAG	C2-N2-C7	-3.33	118.44	122.90
4	D	603	NAG	C1-C2-N2	-3.17	105.44	110.43
4	D	601	NAG	C3-C4-C5	-3.15	104.52	110.23
4	A	604	NAG	C4-C3-C2	2.85	115.20	111.02
4	A	601	NAG	C1-O5-C5	2.85	116.00	112.19
4	D	603	NAG	C3-C4-C5	-2.79	105.17	110.23
4	D	603	NAG	O4-C4-C3	2.68	116.70	110.38
4	D	601	NAG	O5-C1-C2	-2.65	107.19	111.29
4	D	603	NAG	O5-C5-C6	2.40	112.34	107.66
4	D	601	NAG	C1-C2-N2	-2.40	106.66	110.43
4	D	603	NAG	O6-C6-C5	-2.39	103.21	111.33
4	D	602	NAG	O3-C3-C4	-2.38	104.77	110.38
4	A	603	NAG	C3-C4-C5	-2.31	106.05	110.23
4	D	603	NAG	O4-C4-C5	-2.27	103.74	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	NAG	C6-C5-C4	2.13	118.24	113.02
4	A	604	NAG	O5-C5-C6	2.13	111.80	107.66
4	A	604	NAG	C3-C4-C5	2.11	114.06	110.23
4	A	604	NAG	O4-C4-C3	-2.06	105.52	110.38
4	D	602	NAG	C1-O5-C5	2.06	114.94	112.19
4	A	603	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	NAG	C1-C2-N2-C7
4	A	604	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6
4	D	603	NAG	C8-C7-N2-C2
4	A	603	NAG	C4-C5-C6-O6
4	D	601	NAG	C8-C7-N2-C2
4	D	601	NAG	O7-C7-N2-C2
4	D	603	NAG	O7-C7-N2-C2
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	D	602	NAG	C8-C7-N2-C2
4	D	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	D	602	NAG	O7-C7-N2-C2
4	D	601	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	NAG	2	0
4	A	602	NAG	3	0
4	A	603	NAG	3	0
4	D	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	193/194 (99%)	0.17	1 (0%) 87 85	27, 39, 53, 73	0
1	D	193/194 (99%)	0.20	4 (2%) 63 59	28, 41, 60, 78	0
2	B	218/228 (95%)	-0.05	4 (1%) 67 64	22, 32, 61, 79	0
2	E	217/228 (95%)	-0.11	2 (0%) 81 78	23, 33, 53, 74	0
3	C	213/216 (98%)	-0.03	2 (0%) 81 78	27, 35, 47, 68	0
3	F	213/216 (98%)	0.09	0 100 100	24, 38, 58, 68	0
All	All	1247/1276 (97%)	0.04	13 (1%) 79 76	22, 36, 56, 79	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	3	VAL	4.0
1	D	354	TRP	3.5
3	C	2	SER	3.5
1	A	354	TRP	3.1
1	D	308	ILE	3.0
2	B	143	THR	2.9
2	B	136	SER	2.9
2	B	135	SER	2.7
1	D	356	LYS	2.6
2	E	135	SER	2.5
2	B	142	GLY	2.4
1	D	472	ARG	2.0
2	E	196	SER	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($\text{\AA}^2$)	Q<0.9
4	NAG	A	603	14/15	0.62	0.13	51,72,78,81	0
4	NAG	D	603	14/15	0.72	0.14	54,63,70,72	0
4	NAG	A	604	14/15	0.78	0.11	45,60,67,69	0
4	NAG	D	602	14/15	0.79	0.12	53,59,65,70	0
4	NAG	A	602	14/15	0.80	0.12	49,57,64,69	0
4	NAG	D	601	14/15	0.80	0.10	45,49,54,54	0
4	NAG	A	601	14/15	0.89	0.09	39,43,48,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.