



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H3Y
Title : CRYSTAL STRUCTURE OF A HUMAN IGG1 FC-FRAGMENT,HIGH
SALT CONDITION
Authors : Krapp, S.; Mimura, Y.; Jefferis, R.; Huber, R.; Sondermann, P.
Deposited on : 2002-09-19
Resolution : 4.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

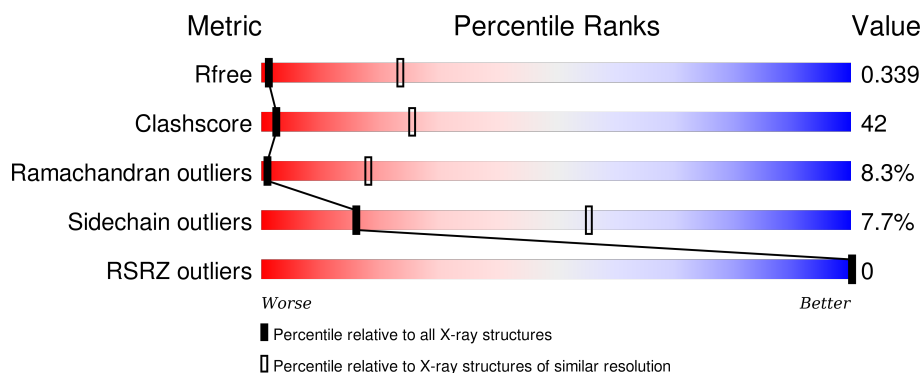
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	
1	B	223	

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
2	FUL	A	1445	-	-	X	-
2	NAG	A	1449	X	-	-	-
2	MAN	A	1451	-	-	X	-
2	NAG	A	1452	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3015 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 IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	1
			1373	848	245	274	6			
1	B	206	Total	C	N	O	S	0	0	0
			1422	886	246	283	7			

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	9	Total	C	N	O	0	0
			110	62	4	44		

- Molecule 3 is a polymer of unknown type called SUGAR (9-MER).

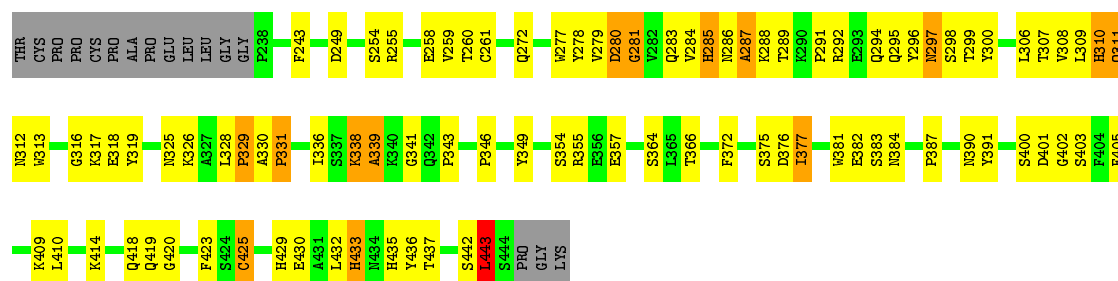
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	9	Total	C	N	O	0	0
			110	62	4	44		

3 Residue-property plots

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

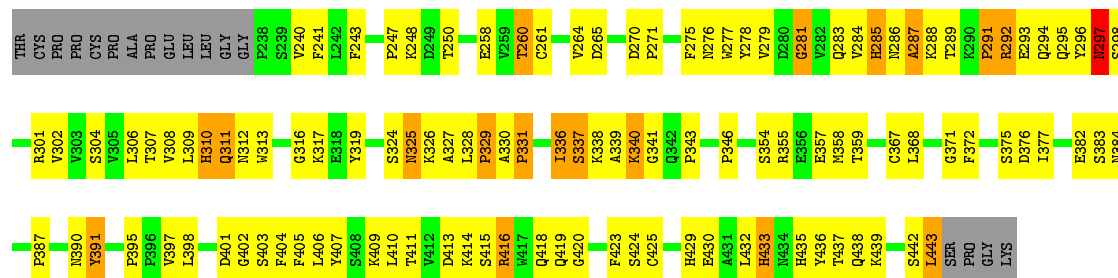
• Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain A: 



• Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.94Å 152.94Å 116.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 4.10 38.24 – 4.13	Depositor EDS
% Data completeness (in resolution range)	80.0 (50.00-4.10) 79.2 (38.24-4.13)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 4.13Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.285 , 0.349 0.275 , 0.339	Depositor DCC
R_{free} test set	285 reflections (5.78%)	DCC
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 148.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 5218 reflections	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3015	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLA, FUL, BMA, NAG, MAN

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	0.51	0/1415	0.83	1/1927 (0.1%)
1	B	0.53	0/1466	0.87	4/1988 (0.2%)
All	All	0.52	0/2881	0.85	5/3915 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	402	GLY	N-CA-C	-6.03	98.02	113.10
1	A	402	GLY	N-CA-C	-5.78	98.65	113.10
1	B	443	LEU	CA-CB-CG	-5.73	102.13	115.30
1	B	297	ASN	N-CA-CB	-5.18	101.27	110.60
1	B	395	PRO	N-CA-C	-5.11	98.81	112.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1449	NAG	C1

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	1373	0	997	88	0
1	B	1422	0	1100	114	1
2	A	110	0	94	22	0
3	B	110	0	94	13	0
All	All	3015	0	2285	221	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 42.

All (221) 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:A:1452:NAG:H83	3:B:1445:FUL:H4	1.25	1.18
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.24	1.10
1:B:325:ASN:ND2	1:B:326:LYS:H	1.52	1.06
1:A:283:GLN:HG2	1:A:285:HIS:H	1.30	0.96
3:B:1451:MAN:H2	3:B:1452:NAG:N2	1.78	0.96
1:B:308:VAL:HG13	1:B:319:TYR:OH	1.68	0.93
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.48	0.93
1:B:293:GLU:HA	1:B:302:VAL:HG22	1.52	0.92
2:A:1452:NAG:H83	3:B:1445:FUL:C4	2.02	0.88
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.04	0.88
1:B:346:PRO:CB	1:B:372:PHE:HB3	2.08	0.84
2:A:1452:NAG:C8	3:B:1445:FUL:H4	2.09	0.82
3:B:1451:MAN:H2	3:B:1452:NAG:C7	2.10	0.81
1:B:346:PRO:HB3	1:B:372:PHE:CB	2.12	0.79
1:A:277:TRP:HE1	1:A:289:THR:HG23	1.48	0.77
1:B:325:ASN:ND2	1:B:326:LYS:N	2.29	0.77
1:B:241:PHE:HE1	3:B:1446:NAG:H4	1.50	0.77
2:A:1445:FUL:H3	2:A:1446:NAG:H83	1.67	0.77
1:A:297:ASN:OD1	2:A:1445:FUL:H63	1.86	0.76
1:A:280:ASP:OD1	1:A:318:GLU:N	2.15	0.76
1:A:390:ASN:O	1:A:410:LEU:HD12	1.84	0.76
1:B:346:PRO:CA	1:B:372:PHE:HB3	2.15	0.76
3:B:1451:MAN:C2	3:B:1452:NAG:N2	2.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:C	1:A:420:GLY:H	1.90	0.75
1:B:325:ASN:HD22	1:B:326:LYS:H	1.34	0.74
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.70	0.72
1:B:324:SER:OG	1:B:331:PRO:HB3	1.89	0.72
1:A:277:TRP:NE1	1:A:289:THR:HG23	2.04	0.72
1:A:325:ASN:ND2	1:A:326:LYS:H	1.87	0.72
2:A:1448:MAN:O5	2:A:1449:NAG:H82	1.89	0.71
3:B:1449:NAG:O3	3:B:1450:GLA:H2	1.90	0.71
2:A:1451:MAN:O6	2:A:1452:NAG:H82	1.89	0.71
1:B:283:GLN:HG2	1:B:285:HIS:H	1.56	0.71
2:A:1451:MAN:H4	2:A:1452:NAG:H2	1.72	0.71
1:B:418:GLN:C	1:B:420:GLY:H	1.94	0.70
1:A:432:LEU:O	1:A:435:HIS:N	2.22	0.69
1:B:401:ASP:HB2	1:B:403:SER:OG	1.93	0.69
1:B:296:TYR:CZ	1:B:301:ARG:HD3	2.30	0.67
1:A:436:TYR:CD1	1:A:437:THR:N	2.63	0.67
1:B:276:ASN:HB3	1:B:278:TYR:HE1	1.59	0.67
1:A:401:ASP:HB2	1:A:403:SER:OG	1.95	0.67
1:B:406:LEU:HD12	1:B:406:LEU:O	1.96	0.66
1:B:432:LEU:O	1:B:435:HIS:N	2.24	0.66
1:B:346:PRO:HA	1:B:372:PHE:HB3	1.78	0.65
1:A:338:LYS:HD3	1:A:376:ASP:OD2	1.96	0.65
1:B:264:VAL:O	1:B:265:ASP:HB2	1.97	0.65
1:B:436:TYR:CD1	1:B:437:THR:N	2.64	0.64
1:A:272:GLN:O	1:A:325:ASN:ND2	2.31	0.64
1:B:328:LEU:HD12	1:B:329:PRO:HD2	1.78	0.64
1:B:418:GLN:O	1:B:420:GLY:N	2.30	0.63
2:A:1445:FUL:C3	2:A:1446:NAG:H83	2.28	0.63
1:A:258:GLU:HG3	2:A:1450:GLA:H62	1.81	0.63
1:A:382:GLU:HA	1:A:387:PRO:HA	1.80	0.62
1:B:279:VAL:O	1:B:281:GLY:N	2.27	0.62
1:A:313:TRP:CZ2	1:A:338:LYS:HB2	2.34	0.62
1:B:328:LEU:HD12	1:B:329:PRO:CD	2.30	0.62
1:B:401:ASP:HB2	1:B:403:SER:CB	2.29	0.62
1:A:299:THR:OG1	1:A:300:TYR:N	2.31	0.61
1:A:418:GLN:O	1:A:420:GLY:N	2.33	0.61
1:B:413:ASP:O	1:B:416:ARG:HB2	2.01	0.61
1:B:398:LEU:HD13	1:B:404:PHE:CE1	2.36	0.60
1:B:293:GLU:HA	1:B:302:VAL:CG2	2.29	0.60
1:B:406:LEU:C	1:B:406:LEU:HD12	2.21	0.60
1:A:338:LYS:HD3	1:A:376:ASP:CG	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:SER:HA	1:B:423:PHE:HD2	1.66	0.60
1:A:308:VAL:HG13	1:A:319:TYR:OH	2.01	0.60
1:A:308:VAL:HG22	1:A:319:TYR:CE2	2.36	0.60
1:A:443:LEU:O	1:A:443:LEU:HD23	2.03	0.59
1:A:279:VAL:O	1:A:281:GLY:N	2.33	0.58
1:B:405:PHE:CD1	1:B:405:PHE:C	2.75	0.58
1:A:429:HIS:CG	1:A:430:GLU:N	2.72	0.58
1:B:383:SER:HB2	1:B:423:PHE:HE2	1.69	0.58
1:B:276:ASN:HB3	1:B:278:TYR:CE1	2.39	0.58
1:A:410:LEU:O	1:A:410:LEU:HG	2.03	0.57
1:B:308:VAL:HG13	1:B:319:TYR:CZ	2.39	0.57
2:A:1445:FUL:O3	2:A:1446:NAG:H82	2.04	0.57
1:B:258:GLU:HG3	3:B:1450:GLA:H61	1.86	0.56
1:A:381:TRP:CH2	1:A:425:CYS:HB3	2.41	0.56
1:A:243:PHE:CD2	2:A:1449:NAG:H62	2.41	0.56
1:A:346:PRO:HB3	1:A:372:PHE:CB	2.15	0.56
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.41	0.55
1:A:294:GLN:CB	1:A:296:TYR:HE1	2.18	0.55
1:A:383:SER:HB2	1:A:423:PHE:CE2	2.41	0.55
1:A:259:VAL:HG23	1:A:308:VAL:CG2	2.37	0.55
1:B:390:ASN:O	1:B:410:LEU:HD12	2.07	0.55
1:A:338:LYS:HD3	1:A:376:ASP:OD1	2.07	0.54
1:A:284:VAL:O	1:A:287:ALA:HB2	2.06	0.54
1:B:383:SER:HB2	1:B:423:PHE:CE2	2.43	0.53
1:B:368:LEU:HB2	1:B:407:TYR:CE2	2.44	0.53
1:A:249:ASP:HA	1:A:255:ARG:HD3	1.90	0.53
1:B:240:VAL:O	1:B:241:PHE:CD2	2.61	0.53
1:B:240:VAL:O	1:B:241:PHE:HD2	1.90	0.53
1:B:429:HIS:CG	1:B:430:GLU:N	2.77	0.53
1:B:310:HIS:O	1:B:311:GLN:C	2.47	0.53
1:A:338:LYS:NZ	1:A:339:ALA:HB2	2.23	0.53
1:B:339:ALA:O	1:B:340:LYS:O	2.26	0.53
1:A:258:GLU:O	2:A:1450:GLA:H61	2.09	0.52
1:B:354:SER:O	1:B:355:ARG:C	2.46	0.52
1:B:346:PRO:HD3	1:B:429:HIS:HD2	1.75	0.52
1:B:312:ASN:HB3	1:B:317:LYS:HG3	1.91	0.52
1:B:337:SER:O	1:B:338:LYS:C	2.47	0.52
1:B:278:TYR:CD1	1:B:278:TYR:N	2.79	0.51
1:A:366:THR:HG21	1:B:407:TYR:CE2	2.46	0.51
1:A:338:LYS:O	1:A:339:ALA:O	2.29	0.51
1:B:288:LYS:O	1:B:289:THR:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:CE1	3:B:1446:NAG:H4	2.39	0.50
2:A:1445:FUL:H3	2:A:1446:NAG:C8	2.40	0.50
1:B:436:TYR:HD1	1:B:437:THR:N	2.08	0.50
1:B:250:THR:O	1:B:310:HIS:HD2	1.95	0.50
1:A:381:TRP:CZ3	1:A:425:CYS:HB3	2.47	0.50
3:B:1451:MAN:O3	3:B:1452:NAG:C1	2.60	0.49
2:A:1445:FUL:C3	2:A:1446:NAG:C8	2.90	0.49
1:A:308:VAL:HG22	1:A:319:TYR:HE2	1.77	0.49
1:B:325:ASN:HD22	1:B:326:LYS:N	2.00	0.49
1:A:283:GLN:HG2	1:A:285:HIS:N	2.12	0.49
1:A:375:SER:O	1:A:377:ILE:HG22	2.13	0.49
1:B:436:TYR:HE1	1:B:438:GLN:HB2	1.78	0.48
1:B:247:PRO:O	1:B:250:THR:OG1	2.31	0.48
1:B:306:LEU:HD12	1:B:307:THR:N	2.28	0.48
1:B:243:PHE:HB2	1:B:260:THR:HB	1.95	0.48
2:A:1451:MAN:C4	2:A:1452:NAG:H2	2.43	0.48
1:B:416:ARG:CZ	1:B:416:ARG:HA	2.44	0.48
1:B:283:GLN:CG	1:B:285:HIS:H	2.26	0.48
1:B:336:ILE:HG23	1:B:336:ILE:O	2.14	0.48
1:A:418:GLN:C	1:A:420:GLY:N	2.59	0.48
1:A:310:HIS:O	1:A:311:GLN:C	2.52	0.48
1:A:401:ASP:HB2	1:A:403:SER:CB	2.43	0.47
2:A:1451:MAN:H4	2:A:1452:NAG:C7	2.43	0.47
1:A:280:ASP:N	1:A:318:GLU:O	2.44	0.47
1:A:429:HIS:ND1	1:A:430:GLU:N	2.57	0.47
1:B:284:VAL:O	1:B:287:ALA:HB2	2.15	0.47
1:A:278:TYR:HA	1:A:283:GLN:HA	1.97	0.47
1:B:401:ASP:HB2	1:B:403:SER:HB3	1.96	0.47
1:B:295:GLN:C	1:B:296:TYR:HD1	2.17	0.47
1:A:432:LEU:O	1:A:433:HIS:C	2.52	0.47
1:B:328:LEU:CD1	1:B:329:PRO:HD2	2.43	0.47
1:A:341:GLY:O	1:A:343:PRO:HD3	2.14	0.47
1:B:382:GLU:HA	1:B:387:PRO:HA	1.97	0.47
1:B:424:SER:HB3	1:B:439:LYS:O	2.15	0.47
1:B:310:HIS:O	1:B:313:TRP:N	2.48	0.47
1:A:354:SER:O	1:A:355:ARG:C	2.53	0.47
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.50	0.47
1:A:306:LEU:HD12	1:A:307:THR:N	2.29	0.47
1:A:325:ASN:CG	1:A:326:LYS:H	2.18	0.46
2:A:1451:MAN:H4	2:A:1452:NAG:C2	2.42	0.46
1:B:296:TYR:CE2	1:B:301:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:THR:O	1:B:310:HIS:CD2	2.68	0.46
1:B:294:GLN:CB	1:B:296:TYR:HE1	2.28	0.46
1:B:243:PHE:N	1:B:260:THR:O	2.45	0.45
1:A:297:ASN:HB2	1:A:298:SER:H	1.58	0.45
1:B:286:ASN:O	1:B:288:LYS:N	2.49	0.45
1:B:418:GLN:C	1:B:420:GLY:N	2.63	0.45
1:B:339:ALA:C	1:B:340:LYS:O	2.55	0.45
1:A:286:ASN:O	1:A:288:LYS:N	2.50	0.45
1:B:326:LYS:HB2	1:B:326:LYS:HE2	1.77	0.45
1:B:375:SER:O	1:B:376:ASP:C	2.55	0.45
2:A:1448:MAN:O3	2:A:1449:NAG:C1	2.65	0.45
1:B:283:GLN:HG2	1:B:285:HIS:N	2.28	0.45
1:B:354:SER:O	1:B:357:GLU:N	2.50	0.45
1:B:313:TRP:CH2	1:B:338:LYS:N	2.85	0.45
1:A:405:PHE:CE1	1:B:409:LYS:NZ	2.85	0.45
2:A:1451:MAN:O6	2:A:1452:NAG:C8	2.63	0.44
1:B:309:LEU:HA	1:B:309:LEU:HD12	1.83	0.44
1:B:328:LEU:HA	1:B:329:PRO:HD3	1.73	0.44
1:A:316:GLY:O	1:A:317:LYS:C	2.55	0.44
1:B:330:ALA:O	1:B:331:PRO:C	2.56	0.44
1:A:319:TYR:N	1:A:319:TYR:CD1	2.85	0.44
1:B:301:ARG:O	1:B:301:ARG:HG2	2.17	0.44
1:B:316:GLY:O	1:B:317:LYS:C	2.55	0.44
1:B:270:ASP:HB2	1:B:327:ALA:HB2	1.99	0.44
1:B:291:PRO:HD3	1:B:304:SER:OG	2.17	0.44
1:B:297:ASN:HB3	1:B:298:SER:H	1.28	0.44
2:A:1445:FUL:O3	2:A:1446:NAG:C8	2.65	0.44
1:A:288:LYS:O	1:A:289:THR:C	2.55	0.44
1:B:432:LEU:O	1:B:433:HIS:C	2.57	0.44
1:B:339:ALA:O	1:B:340:LYS:C	2.55	0.44
1:B:275:PHE:CE2	1:B:304:SER:HB3	2.53	0.43
1:B:414:LYS:O	1:B:415:SER:C	2.56	0.43
1:A:259:VAL:CG2	1:A:308:VAL:HG21	2.42	0.43
1:B:355:ARG:O	1:B:358:MET:HG2	2.18	0.43
1:A:277:TRP:CD1	1:A:289:THR:CG2	3.02	0.43
1:B:243:PHE:CD1	3:B:1449:NAG:H5	2.54	0.43
1:B:443:LEU:HD12	1:B:443:LEU:HA	1.55	0.43
1:B:241:PHE:CE1	3:B:1447:BMA:C1	3.01	0.43
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.33	0.43
1:B:286:ASN:O	1:B:287:ALA:C	2.56	0.43
1:B:382:GLU:O	1:B:424:SER:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLN:C	1:B:296:TYR:CD1	2.92	0.43
1:A:375:SER:O	1:A:376:ASP:C	2.56	0.43
1:A:308:VAL:HG12	1:A:309:LEU:N	2.33	0.43
1:A:391:TYR:HA	1:A:409:LYS:O	2.18	0.43
1:B:429:HIS:CG	1:B:430:GLU:H	2.33	0.43
1:A:258:GLU:HG3	2:A:1450:GLA:C6	2.46	0.43
1:A:330:ALA:O	1:A:331:PRO:C	2.57	0.43
1:A:325:ASN:CG	1:A:326:LYS:N	2.72	0.43
1:A:381:TRP:O	1:A:387:PRO:HA	2.18	0.43
1:A:442:SER:O	1:A:443:LEU:O	2.37	0.43
1:B:291:PRO:HB2	1:B:292:ARG:H	1.62	0.43
1:A:243:PHE:N	1:A:260:THR:O	2.52	0.42
1:A:391:TYR:HB2	1:A:409:LYS:O	2.19	0.42
1:B:397:VAL:HG12	1:B:398:LEU:N	2.34	0.42
1:B:391:TYR:HB2	1:B:409:LYS:O	2.19	0.42
1:B:391:TYR:CD2	1:B:391:TYR:C	2.92	0.42
1:A:286:ASN:O	1:A:287:ALA:C	2.57	0.42
1:A:295:GLN:C	1:A:296:TYR:CD1	2.93	0.42
1:A:308:VAL:CG1	1:A:309:LEU:N	2.82	0.42
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.84	0.41
1:B:247:PRO:O	1:B:248:LYS:C	2.59	0.41
1:A:357:GLU:OE1	1:A:364:SER:N	2.52	0.41
1:B:391:TYR:HA	1:B:409:LYS:O	2.21	0.41
1:B:325:ASN:CG	1:B:326:LYS:N	2.74	0.41
1:B:409:LYS:CB	1:B:409:LYS:NZ	2.83	0.41
1:A:349:TYR:CE2	1:B:357:GLU:HG3	2.56	0.41
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.63	0.41
1:A:338:LYS:HZ1	1:A:339:ALA:HB2	1.86	0.41
1:A:354:SER:O	1:A:357:GLU:N	2.54	0.41
1:B:341:GLY:O	1:B:343:PRO:N	2.54	0.40
1:B:371:GLY:HA2	1:B:403:SER:HB2	2.03	0.40
1:A:295:GLN:C	1:A:296:TYR:HD1	2.25	0.40
1:A:277:TRP:NE1	1:A:289:THR:CG2	2.80	0.40
1:A:338:LYS:HE3	1:A:338:LYS:C	2.42	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:B:309:LEU:CD1	1:B:309:LEU:CD1[9_765]	1.59	0.61

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	205/223 (92%)	165 (80%)	22 (11%)	18 (9%)	1	17
1	B	204/223 (92%)	159 (78%)	29 (14%)	16 (8%)	1	20
All	All	409/446 (92%)	324 (79%)	51 (12%)	34 (8%)	1	18

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ALA
1	A	377	ILE
1	A	443	LEU
1	B	297	ASN
1	B	377	ILE
1	A	281	GLY
1	A	287	ALA
1	A	292	ARG
1	A	419	GLN
1	A	433	HIS
1	B	287	ALA
1	B	292	ARG
1	B	340	LYS
1	B	419	GLN
1	A	291	PRO
1	A	336	ILE
1	B	281	GLY
1	B	291	PRO
1	B	311	GLN
1	A	297	ASN
1	A	310	HIS
1	A	311	GLN
1	A	331	PRO
1	A	384	ASN
1	B	384	ASN

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Mol	Chain	Res	Type
1	A	285	HIS
1	A	329	PRO
1	A	414	LYS
1	B	285	HIS
1	B	310	HIS
1	B	329	PRO
1	B	336	ILE
1	B	331	PRO
1	B	433	HIS

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	108/206 (52%)	101 (94%)	7 (6%)	21	61
1	B	127/206 (62%)	116 (91%)	11 (9%)	13	49
All	All	235/412 (57%)	217 (92%)	18 (8%)	16	55

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	280	ASP
1	A	312	ASN
1	A	338	LYS
1	A	400	SER
1	A	425	CYS
1	A	443	LEU
1	B	260	THR
1	B	271	PRO
1	B	325	ASN
1	B	337	SER
1	B	359	THR
1	B	367	CYS
1	B	391	TYR

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Mol	Chain	Res	Type
1	B	411	THR
1	B	416	ARG
1	B	425	CYS
1	B	442	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	283	GLN
1	A	295	GLN
1	A	325	ASN
1	A	418	GLN
1	A	434	ASN
1	B	312	ASN
1	B	325	ASN
1	B	342	GLN
1	B	438	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 ⓘ

18 carbohydrates 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
2	NAG	A	1444	1,2	14,14,15	1.13	2 (14%)	15,19,21	1.47	2 (13%)
2	FUL	A	1445	2	10,10,11	0.64	0	14,14,16	0.78	1 (7%)
2	NAG	A	1446	2	14,14,15	0.98	1 (7%)	15,19,21	1.63	3 (20%)
2	MAN	A	1447	2	11,11,12	0.72	0	14,15,17	1.89	2 (14%)
2	MAN	A	1448	2	11,11,12	0.99	0	14,15,17	0.83	0
2	NAG	A	1449	2	14,14,15	1.29	3 (21%)	15,19,21	2.23	4 (26%)
2	GLA	A	1450	2	11,11,12	1.35	2 (18%)	14,15,17	1.03	0
2	MAN	A	1451	2	11,11,12	0.88	0	14,15,17	1.42	2 (14%)
2	NAG	A	1452	2	14,14,15	1.24	2 (14%)	15,19,21	1.26	2 (13%)
3	NAG	B	1444	1,3	14,14,15	0.75	0	15,19,21	1.78	3 (20%)
3	FUL	B	1445	3	10,10,11	0.93	0	14,14,16	0.93	0
3	NAG	B	1446	3	14,14,15	0.75	0	15,19,21	1.22	1 (6%)
3	BMA	B	1447	3	11,11,12	1.20	1 (9%)	14,15,17	0.80	0
3	MAN	B	1448	3	11,11,12	1.02	1 (9%)	14,15,17	1.43	2 (14%)
3	NAG	B	1449	3	14,14,15	0.95	1 (7%)	15,19,21	1.63	3 (20%)
3	GLA	B	1450	3	11,11,12	0.80	0	14,15,17	1.21	2 (14%)
3	MAN	B	1451	3	11,11,12	1.18	1 (9%)	14,15,17	2.51	3 (21%)
3	NAG	B	1452	3	14,14,15	0.88	0	15,19,21	1.14	1 (6%)

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
2	NAG	A	1444	1,2	-	1/6/23/26	0/1/1/1
2	FUL	A	1445	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1446	2	-	0/6/23/26	0/1/1/1
2	MAN	A	1447	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1448	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1449	2	1/1/5/7	0/6/23/26	0/1/1/1
2	GLA	A	1450	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1451	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1452	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1444	1,3	-	0/6/23/26	0/1/1/1
3	FUL	B	1445	3	-	0/0/17/20	0/1/1/1
3	NAG	B	1446	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1447	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1448	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1449	3	-	0/6/23/26	0/1/1/1
3	GLA	B	1450	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1451	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1452	3	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1444	NAG	C1-C2	-2.26	1.49	1.52
3	B	1449	NAG	C1-C2	-2.01	1.49	1.52
2	A	1450	GLA	C2-C3	2.02	1.55	1.52
2	A	1452	NAG	O5-C1	2.11	1.47	1.43
2	A	1449	NAG	O5-C5	2.12	1.48	1.43
2	A	1446	NAG	O4-C4	2.17	1.48	1.43
2	A	1449	NAG	O5-C1	2.35	1.47	1.43
2	A	1444	NAG	C4-C5	2.50	1.58	1.53
3	B	1448	MAN	C1-C2	2.69	1.58	1.52
2	A	1450	GLA	C1-C2	2.76	1.58	1.52
2	A	1452	NAG	C1-C2	3.17	1.56	1.52
2	A	1449	NAG	C1-C2	3.21	1.56	1.52
3	B	1451	MAN	C2-C3	3.41	1.57	1.52
3	B	1447	BMA	C2-C3	3.53	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1449	NAG	C4-C3-C2	-5.38	102.86	111.23
3	B	1444	NAG	C2-N2-C7	-4.49	117.27	123.04
2	A	1451	MAN	C1-C2-C3	-3.87	104.97	109.54
3	B	1449	NAG	C4-C3-C2	-3.67	105.53	111.23
3	B	1444	NAG	C4-C3-C2	-3.66	105.53	111.23
2	A	1449	NAG	C2-N2-C7	-3.62	118.39	123.04
3	B	1446	NAG	C2-N2-C7	-3.61	118.40	123.04
2	A	1444	NAG	C2-N2-C7	-3.54	118.50	123.04
3	B	1449	NAG	C2-N2-C7	-3.41	118.65	123.04
2	A	1446	NAG	C2-N2-C7	-3.36	118.72	123.04
2	A	1446	NAG	C4-C3-C2	-3.19	106.27	111.23
2	A	1452	NAG	C2-N2-C7	-2.98	119.20	123.04
2	A	1449	NAG	C3-C4-C5	-2.93	105.08	110.20
3	B	1451	MAN	C3-C4-C5	-2.11	106.53	110.20
2	A	1452	NAG	O7-C7-C8	-2.02	118.36	122.06
2	A	1445	FUL	C1-O5-C5	2.18	115.74	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1449	NAG	C1-O5-C5	2.26	115.12	112.25
3	B	1450	GLA	C1-O5-C5	2.36	115.24	112.25
2	A	1451	MAN	C1-O5-C5	2.51	115.43	112.25
2	A	1447	MAN	C2-C3-C4	2.52	115.32	111.04
2	A	1446	NAG	C1-O5-C5	2.54	115.47	112.25
3	B	1448	MAN	O5-C1-C2	2.57	115.03	110.86
3	B	1452	NAG	C3-C4-C5	2.69	114.89	110.20
2	A	1444	NAG	C3-C4-C5	3.01	115.44	110.20
3	B	1444	NAG	C1-O5-C5	3.14	116.24	112.25
3	B	1450	GLA	C1-C2-C3	3.24	113.37	109.54
3	B	1448	MAN	C1-O5-C5	3.64	116.87	112.25
3	B	1451	MAN	C1-O5-C5	3.88	117.18	112.25
2	A	1449	NAG	C1-O5-C5	3.95	117.26	112.25
2	A	1447	MAN	C1-C2-C3	5.80	116.41	109.54
3	B	1451	MAN	C1-C2-C3	7.82	118.79	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1449	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1444	NAG	O7-C7-N2-C2

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1445	FUL	7	0
2	A	1446	NAG	6	0
2	A	1448	MAN	2	0
2	A	1449	NAG	3	0
2	A	1450	GLA	3	0
2	A	1451	MAN	6	0
2	A	1452	NAG	9	0
3	B	1445	FUL	3	0
3	B	1446	NAG	2	0
3	B	1447	BMA	1	0
3	B	1449	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1450	GLA	2	0
3	B	1451	MAN	4	0
3	B	1452	NAG	4	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	207/223 (92%)	-0.51	0 100 100	28, 32, 47, 47	0
1	B	206/223 (92%)	-0.76	0 100 100	14, 17, 22, 23	0
All	All	413/446 (92%)	-0.63	0 100 100	14, 23, 46, 47	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLA	A	1450	11/12	0.91	0.26	-0.03	71,72,76,76	0
2	NAG	A	1452	14/15	0.88	0.25	-	71,73,75,76	0
2	NAG	A	1446	14/15	0.89	0.28	-	71,74,75,76	0
3	MAN	B	1451	11/12	0.89	0.26	-	33,35,38,38	0
3	NAG	B	1446	14/15	0.96	0.15	-	33,35,38,39	0
3	FUL	B	1445	10/11	0.95	0.19	-	33,36,38,39	0
2	NAG	A	1444	14/15	0.88	0.24	-	71,73,76,76	0
2	NAG	A	1449	14/15	0.90	0.24	-	71,74,76,76	0
2	MAN	A	1448	11/12	0.89	0.23	-	71,73,76,76	0
3	GLA	B	1450	11/12	0.89	0.23	-	33,34,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	1444	14/15	0.91	0.19	-	33,35,39,39	0
3	BMA	B	1447	11/12	0.95	0.12	-	33,36,38,39	0
2	FUL	A	1445	10/11	0.92	0.20	-	70,73,75,76	0
2	MAN	A	1447	11/12	0.84	0.19	-	71,73,76,76	0
3	NAG	B	1449	14/15	0.91	0.17	-	33,35,38,38	0
2	MAN	A	1451	11/12	0.85	0.23	-	73,75,76,76	0
3	MAN	B	1448	11/12	0.89	0.23	-	33,35,38,38	0
3	NAG	B	1452	14/15	0.90	0.20	-	33,36,39,39	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.