



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:29 am GMT

PDB ID : 1H3V
Title : CRYSTAL STRUCTURE OF THE HUMAN IGG1 FC-FRAGMENT, GLYC
OFORM (G2F)2, SG P212121
Authors : Krapp, S.; Mimura, Y.; Jefferis, R.; Huber, R.; Sonderrmann, P.
Deposited on : 2002-09-19
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

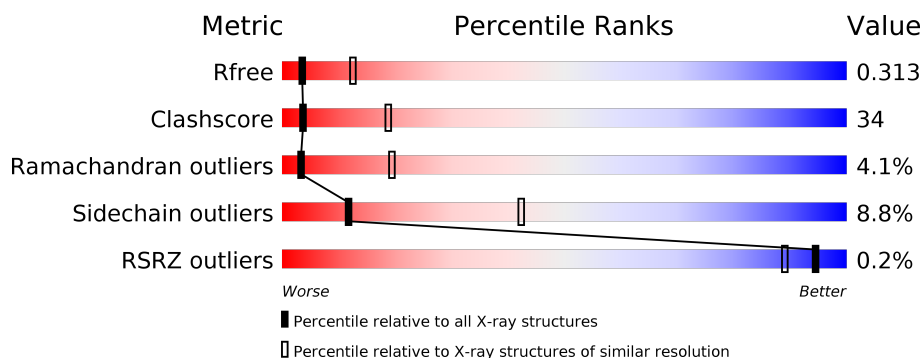
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	GAL	A	1451	-	-	X	X
3	NAG	B	1444	X	-	-	-
3	GAL	B	1450	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3600 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	208	Total	C	N	O	S	45	0	1
			1661	1057	283	314	7			
1	B	207	Total	C	N	O	S	131	0	1
			1656	1054	282	313	7			

- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	8	Total	C	N	O	0	0
			96	54	3	39		

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	8	Total	C	N	O	15	0
			96	54	3	39		

- Molecule 4 is water.

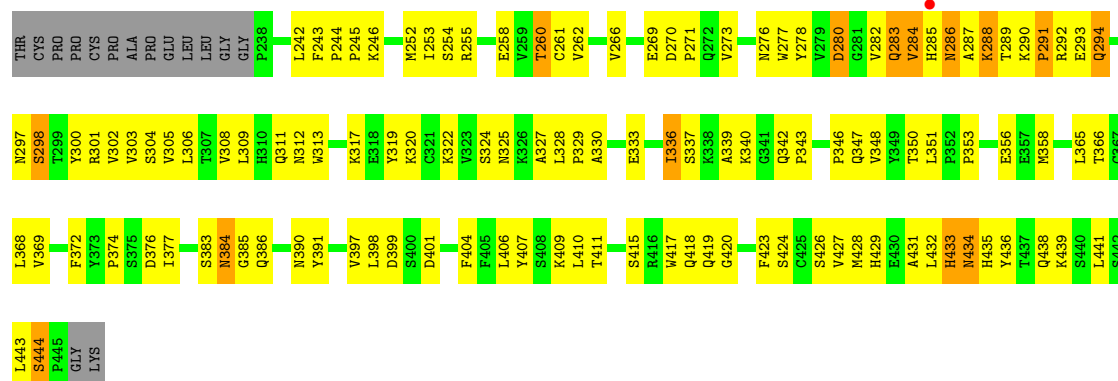
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	40	Total	O	0	0
			40	40		

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 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.

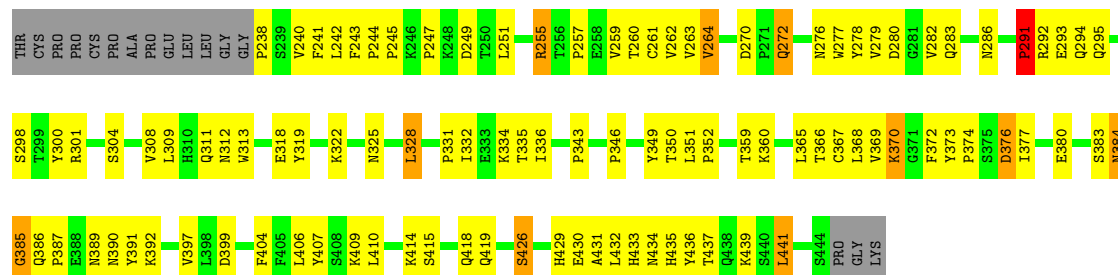
• Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain A: 



• Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.47Å 80.85Å 141.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 24.37 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.8 (50.00-3.10) 82.9 (24.37-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.17Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.314 0.233 , 0.313	Depositor DCC
R_{free} test set	445 reflections (5.75%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3600	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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: GAL, 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	0.46	0/1707	0.73	1/2325 (0.0%)
1	B	0.44	0/1702	0.67	0/2318
All	All	0.45	0/3409	0.70	1/4643 (0.0%)

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
3	B	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	383	SER	N-CA-C	-5.61	95.85	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1444	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	1661	0	1630	119	0
1	B	1656	0	1628	93	0
2	A	96	0	82	16	0
3	B	96	0	82	11	0
4	A	51	0	0	14	0
4	B	40	0	0	7	0
All	All	3600	0	3422	223	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 34.

All (223) 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)
3:B:1444:NAG:H62	3:B:1445:FUL:C6	1.82	1.10
1:A:351:LEU:HB2	1:A:366:THR:HB	1.33	1.10
1:A:433:HIS:O	1:A:435:HIS:N	1.85	1.07
1:B:433:HIS:O	1:B:435:HIS:N	1.88	1.07
3:B:1444:NAG:C6	3:B:1445:FUL:H63	1.89	1.01
1:B:238:PRO:HB2	4:B:2001:HOH:O	1.60	1.01
1:A:350:THR:HB	1:A:441:LEU:HG	1.46	0.97
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.44	0.96
3:B:1444:NAG:H61	3:B:1445:FUL:O3	1.65	0.96
1:A:253:ILE:H	1:A:253:ILE:HD12	1.29	0.94
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.55	0.88
3:B:1444:NAG:H62	3:B:1445:FUL:H63	0.92	0.86
1:A:292:ARG:HG2	1:A:293:GLU:H	1.41	0.85
1:B:351:LEU:HB2	1:B:366:THR:HB	1.59	0.84
1:B:260:THR:HG21	4:B:2040:HOH:O	1.79	0.82
1:A:309:LEU:HB2	1:A:312:ASN:HD22	1.43	0.82
1:A:320:LYS:HD3	1:A:333:GLU:HG2	1.61	0.82
1:B:350:THR:HB	1:B:441:LEU:HG	1.60	0.81
1:A:260:THR:HG23	1:A:305:VAL:HG22	1.65	0.77
1:B:312:ASN:HB3	1:B:319:TYR:OH	1.83	0.77
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.66	0.76
1:A:253:ILE:H	1:A:253:ILE:CD1	1.97	0.76
1:A:292:ARG:HG2	1:A:293:GLU:N	2.01	0.76
1:B:249:ASP:O	1:B:257:PRO:HG3	1.87	0.75
1:A:244:PRO:HB3	1:A:336:ILE:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PRO:HA	2:A:1451:GAL:H61	1.69	0.74
1:A:253:ILE:N	1:A:253:ILE:HD12	2.03	0.73
1:A:297:ASN:O	1:A:298:SER:HB2	1.88	0.72
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.71	0.71
1:B:272:GLN:OE1	1:B:272:GLN:HA	1.90	0.71
1:B:238:PRO:HB2	1:B:328:LEU:HD11	1.71	0.70
1:A:245:PRO:HA	2:A:1451:GAL:C6	2.21	0.70
1:A:391:TYR:HB3	1:A:410:LEU:HD12	1.75	0.69
1:A:433:HIS:C	1:A:435:HIS:H	1.93	0.69
1:A:273:VAL:HG21	1:A:302:VAL:HG21	1.74	0.68
1:A:423:PHE:HB2	4:A:2047:HOH:O	1.92	0.67
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.77	0.67
1:A:309:LEU:HB2	1:A:312:ASN:ND2	2.08	0.66
1:B:359:THR:HG22	1:B:359:THR:O	1.94	0.66
2:A:1447:NAG:H81	2:A:1449:MAN:O4	1.96	0.65
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.31	0.65
2:A:1445:NAG:H82	4:A:2048:HOH:O	1.97	0.65
1:B:311:GLN:N	1:B:311:GLN:OE1	2.28	0.64
2:A:1450:NAG:H4	2:A:1451:GAL:O2	1.96	0.64
1:B:291:PRO:HB3	1:B:304:SER:HA	1.79	0.64
1:B:278:TYR:HA	1:B:282:VAL:O	1.97	0.64
1:A:284:VAL:HG13	1:A:285:HIS:ND1	2.13	0.64
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.34	0.62
1:B:241:PHE:HE1	3:B:1446:NAG:H4	1.64	0.62
1:A:441:LEU:CB	4:A:2047:HOH:O	2.47	0.62
1:B:360:LYS:HB3	4:B:2021:HOH:O	1.99	0.61
1:B:247:PRO:O	1:B:251:LEU:HG	2.01	0.60
1:B:241:PHE:CE1	3:B:1446:NAG:H4	2.36	0.60
1:A:398:LEU:HD12	1:A:399:ASP:N	2.16	0.60
2:A:1445:NAG:H61	2:A:1447:NAG:HN2	1.66	0.59
1:B:332:ILE:HG23	1:B:334:LYS:NZ	2.17	0.59
1:B:383:SER:O	1:B:385:GLY:N	2.35	0.59
1:A:242:LEU:HD13	1:A:336:ILE:HG22	1.83	0.59
1:B:247:PRO:HB3	1:B:376:ASP:HB3	1.84	0.59
1:A:289:THR:HG22	1:A:290:LYS:H	1.68	0.59
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.85	0.58
1:B:335:THR:HG22	1:B:336:ILE:N	2.18	0.58
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.84	0.58
1:B:432:LEU:C	1:B:433:HIS:O	2.38	0.58
1:A:301:ARG:HH12	1:A:303:VAL:HG21	1.69	0.58
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TYR:CE1	1:A:438:GLN:HG3	2.40	0.57
1:A:325:ASN:HD21	1:A:327:ALA:HB3	1.70	0.57
1:A:347:GLN:NE2	1:B:360:LYS:HE3	2.19	0.57
1:A:289:THR:HG22	1:A:290:LYS:N	2.20	0.57
1:A:391:TYR:HB3	1:A:410:LEU:CD1	2.35	0.56
3:B:1444:NAG:C6	3:B:1445:FUL:O3	2.48	0.56
1:B:346:PRO:HB3	1:B:372:PHE:CB	2.31	0.56
1:A:325:ASN:ND2	1:A:327:ALA:HB3	2.21	0.55
1:A:280:ASP:OD2	1:A:317:LYS:HD3	2.07	0.55
1:B:383:SER:O	1:B:384:ASN:C	2.46	0.55
1:B:346:PRO:CB	1:B:372:PHE:HB3	2.32	0.54
1:A:441:LEU:O	4:A:2047:HOH:O	2.18	0.54
1:B:238:PRO:CB	1:B:328:LEU:HD11	2.38	0.54
1:B:243:PHE:O	1:B:259:VAL:HG13	2.07	0.54
1:B:415:SER:O	1:B:419:GLN:N	2.40	0.54
1:A:353:PRO:HD3	1:A:365:LEU:CD2	2.37	0.53
1:B:373:TYR:CD1	1:B:374:PRO:HA	2.44	0.53
1:A:273:VAL:CG2	1:A:302:VAL:HG21	2.38	0.53
1:A:443:LEU:O	1:A:444:SER:CB	2.56	0.53
1:A:287:ALA:N	4:A:2008:HOH:O	2.39	0.53
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.38	0.53
1:B:368:LEU:HD11	1:B:370:LYS:HB3	1.91	0.53
1:A:311:GLN:NE2	1:A:311:GLN:HA	2.24	0.52
1:B:433:HIS:C	1:B:435:HIS:H	2.07	0.52
2:A:1445:NAG:H61	2:A:1447:NAG:N2	2.24	0.52
1:B:244:PRO:HD3	1:B:336:ILE:HD11	1.90	0.52
1:B:429:HIS:HB3	1:B:432:LEU:HG	1.91	0.52
1:A:258:GLU:O	2:A:1451:GAL:H61	2.10	0.52
1:B:309:LEU:O	1:B:312:ASN:HB2	2.09	0.51
1:A:293:GLU:HG3	1:A:294:GLN:H	1.75	0.51
1:B:279:VAL:O	1:B:282:VAL:HG22	2.10	0.51
1:A:271:PRO:O	1:A:273:VAL:HG23	2.10	0.51
1:B:322:LYS:NZ	1:B:331:PRO:HG3	2.26	0.51
1:A:258:GLU:O	2:A:1451:GAL:C6	2.59	0.51
1:A:308:VAL:HG12	1:A:319:TYR:CE2	2.46	0.51
2:A:1445:NAG:H2	4:A:2048:HOH:O	2.10	0.51
1:B:349:TYR:O	1:B:367:CYS:HA	2.10	0.51
1:A:427:VAL:O	1:A:436:TYR:HA	2.11	0.51
1:B:397:VAL:O	1:B:404:PHE:HA	2.10	0.50
1:A:252:MET:HB2	1:A:255:ARG:HD3	1.92	0.50
1:B:415:SER:O	1:B:419:GLN:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD22	1:A:336:ILE:HG21	1.93	0.50
1:B:308:VAL:HG12	1:B:309:LEU:N	2.25	0.50
1:A:293:GLU:HG3	1:A:294:GLN:N	2.27	0.50
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.77	0.49
1:A:278:TYR:HA	1:A:282:VAL:O	2.12	0.49
1:B:376:ASP:HB2	4:B:2031:HOH:O	2.13	0.49
1:A:432:LEU:C	1:A:433:HIS:O	2.50	0.49
1:A:415:SER:O	1:A:419:GLN:N	2.45	0.49
1:B:322:LYS:HZ1	1:B:331:PRO:HG3	1.77	0.49
1:A:432:LEU:O	1:A:433:HIS:O	2.30	0.49
1:A:429:HIS:CD2	1:A:431:ALA:H	2.31	0.49
1:A:434:ASN:O	1:A:435:HIS:HB2	2.12	0.49
1:A:283:GLN:NE2	4:A:2008:HOH:O	2.29	0.49
1:A:397:VAL:O	1:A:404:PHE:HA	2.13	0.49
1:B:414:LYS:O	1:B:418:GLN:CG	2.61	0.48
1:A:426:SER:HB3	1:A:436:TYR:CE2	2.48	0.48
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.13	0.48
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.94	0.48
1:A:340:LYS:HA	4:A:2025:HOH:O	2.14	0.48
1:A:266:VAL:O	1:A:300:TYR:HB2	2.14	0.48
1:A:336:ILE:HG13	1:A:337:SER:N	2.28	0.48
3:B:1449:NAG:H4	3:B:1450:GAL:O2	2.14	0.48
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.79	0.48
2:A:1450:NAG:C4	2:A:1451:GAL:O2	2.62	0.47
1:B:359:THR:O	1:B:360:LYS:HD3	2.14	0.47
1:A:301:ARG:NH1	1:A:303:VAL:HG21	2.29	0.47
1:B:391:TYR:O	1:B:392:LYS:HD3	2.14	0.47
1:B:283:GLN:HG2	4:B:2007:HOH:O	2.13	0.47
1:B:380:GLU:HG2	4:B:2023:HOH:O	2.14	0.47
1:A:288:LYS:HD3	1:A:306:LEU:HD11	1.97	0.47
1:A:312:ASN:O	1:A:313:TRP:C	2.52	0.47
1:B:391:TYR:HA	1:B:409:LYS:O	2.15	0.47
1:B:439:LYS:HD2	1:B:439:LYS:HA	1.72	0.47
1:A:245:PRO:HA	2:A:1451:GAL:O6	2.15	0.46
1:A:328:LEU:HG	1:A:330:ALA:O	2.15	0.46
1:B:245:PRO:HD3	1:B:259:VAL:HG22	1.97	0.46
1:A:311:GLN:CA	1:A:311:GLN:NE2	2.77	0.46
1:A:365:LEU:HD21	1:A:417:TRP:CE3	2.51	0.46
1:A:406:LEU:C	1:A:406:LEU:HD12	2.36	0.45
1:B:368:LEU:C	1:B:368:LEU:HD12	2.36	0.45
1:A:399:ASP:OD2	1:B:409:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.51	0.45
1:B:247:PRO:HG2	1:B:377:ILE:H	1.81	0.45
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.80	0.45
1:A:391:TYR:HA	1:A:409:LYS:O	2.17	0.45
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.52	0.45
1:A:293:GLU:OE2	4:A:2013:HOH:O	2.21	0.45
1:A:353:PRO:HG2	1:A:358:MET:HE1	1.98	0.45
1:A:409:LYS:HB2	1:B:407:TYR:OH	2.16	0.45
1:A:246:LYS:HE2	2:A:1451:GAL:H3	1.99	0.45
1:B:426:SER:HB3	1:B:436:TYR:CE2	2.52	0.45
1:A:384:ASN:C	1:A:386:GLN:H	2.20	0.45
1:A:368:LEU:HD13	1:A:407:TYR:CE1	2.52	0.45
1:A:285:HIS:O	1:A:286:ASN:O	2.35	0.45
1:B:335:THR:CG2	1:B:336:ILE:N	2.80	0.45
1:A:243:PHE:CD2	2:A:1450:NAG:H5	2.52	0.44
1:B:292:ARG:HH11	1:B:293:GLU:H	1.65	0.44
1:A:423:PHE:CB	4:A:2047:HOH:O	2.57	0.44
1:A:441:LEU:HB2	4:A:2047:HOH:O	2.15	0.44
1:B:264:VAL:HG11	3:B:1444:NAG:O4	2.17	0.44
1:B:368:LEU:HD12	1:B:369:VAL:N	2.31	0.44
1:B:429:HIS:O	1:B:435:HIS:HA	2.17	0.44
1:A:246:LYS:HE2	2:A:1451:GAL:H5	1.98	0.44
1:B:260:THR:OG1	3:B:1449:NAG:H61	2.18	0.44
1:B:332:ILE:HG23	1:B:334:LYS:HZ2	1.83	0.44
1:B:365:LEU:HB2	1:B:410:LEU:HB3	1.99	0.44
1:A:423:PHE:CD1	1:A:423:PHE:N	2.85	0.44
1:B:441:LEU:HD23	4:B:2020:HOH:O	2.17	0.44
1:A:288:LYS:CD	1:A:306:LEU:HD11	2.48	0.44
1:A:384:ASN:O	1:A:386:GLN:N	2.50	0.44
1:B:263:VAL:O	1:B:301:ARG:HA	2.18	0.44
1:A:369:VAL:HG12	1:A:372:PHE:CD2	2.53	0.44
1:B:430:GLU:CG	1:B:431:ALA:N	2.81	0.44
1:A:286:ASN:HA	4:A:2008:HOH:O	2.18	0.43
1:B:312:ASN:HB3	1:B:319:TYR:HH	1.81	0.43
1:A:376:ASP:O	1:A:377:ILE:HB	2.18	0.43
1:B:308:VAL:HG11	1:B:313:TRP:HB2	2.00	0.43
1:B:311:GLN:CD	1:B:311:GLN:H	2.17	0.43
1:B:292:ARG:HG3	1:B:292:ARG:NH1	2.34	0.43
1:A:417:TRP:CZ2	1:A:443:LEU:HB2	2.53	0.43
1:A:429:HIS:O	1:A:435:HIS:HA	2.19	0.43
1:B:309:LEU:HG	1:B:311:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG23	1:B:332:ILE:HD12	2.01	0.43
1:A:277:TRP:NE1	1:A:289:THR:HG21	2.34	0.42
1:A:435:HIS:O	1:A:436:TYR:HB2	2.19	0.42
1:B:262:VAL:HG21	3:B:1449:NAG:H62	2.00	0.42
1:A:339:ALA:HB3	1:A:374:PRO:HB3	2.00	0.42
1:A:242:LEU:HD13	1:A:336:ILE:CG2	2.48	0.42
1:A:291:PRO:HB3	1:A:304:SER:HA	2.00	0.42
1:A:348:VAL:HG22	1:A:427:VAL:HG21	2.01	0.42
1:B:406:LEU:C	1:B:406:LEU:HD12	2.40	0.42
1:A:284:VAL:HG13	1:A:285:HIS:CE1	2.55	0.42
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.93	0.42
1:A:297:ASN:O	1:A:298:SER:CB	2.62	0.41
1:B:383:SER:O	1:B:386:GLN:N	2.51	0.41
1:A:428:MET:HG2	1:A:436:TYR:HD2	1.86	0.41
1:B:255:ARG:CZ	1:B:255:ARG:HB3	2.50	0.41
1:B:332:ILE:HG23	1:B:334:LYS:HZ3	1.86	0.41
1:A:276:ASN:HB3	1:A:278:TYR:HE1	1.86	0.41
1:A:301:ARG:NH1	1:A:301:ARG:HG2	2.35	0.41
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.89	0.41
1:B:352:PRO:HG3	1:B:441:LEU:HD21	2.03	0.41
2:A:1449:MAN:O2	2:A:1450:NAG:H82	2.21	0.41
1:B:251:LEU:HD13	1:B:429:HIS:C	2.41	0.41
1:B:244:PRO:CD	1:B:336:ILE:HD11	2.51	0.41
1:A:297:ASN:HB3	4:A:2049:HOH:O	2.21	0.41
1:B:308:VAL:CG1	1:B:309:LEU:N	2.84	0.41
1:B:332:ILE:CG2	1:B:334:LYS:HZ3	2.33	0.41
1:A:424:SER:HA	1:A:439:LYS:O	2.21	0.41
1:A:292:ARG:CG	1:A:293:GLU:N	2.80	0.40
1:A:418:GLN:C	1:A:420:GLY:H	2.25	0.40
1:B:343:PRO:HA	1:B:373:TYR:O	2.22	0.40
1:A:266:VAL:HB	1:A:300:TYR:CB	2.49	0.40
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.76	0.40
1:A:441:LEU:HB3	4:A:2047:HOH:O	2.18	0.40
1:A:243:PHE:HE2	1:A:262:VAL:HG21	1.86	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	206/223 (92%)	171 (83%)	26 (13%)	9 (4%)	3	18
1	B	205/223 (92%)	176 (86%)	21 (10%)	8 (4%)	3	21
All	All	411/446 (92%)	347 (84%)	47 (11%)	17 (4%)	3	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	298	SER
1	A	384	ASN
1	A	433	HIS
1	A	434	ASN
1	B	286	ASN
1	B	298	SER
1	B	384	ASN
1	B	434	ASN
1	A	385	GLY
1	A	444	SER
1	A	291	PRO
1	B	291	PRO
1	B	270	ASP
1	A	356	GLU
1	B	387	PRO
1	B	385	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	193/206 (94%)	179 (93%)	14 (7%)	16	50
1	B	193/206 (94%)	173 (90%)	20 (10%)	8	31
All	All	386/412 (94%)	352 (91%)	34 (9%)	12	42

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	260	THR
1	A	269	GLU
1	A	270	ASP
1	A	280	ASP
1	A	283	GLN
1	A	284	VAL
1	A	288	LYS
1	A	294	GLN
1	A	324	SER
1	A	336	ILE
1	A	390	ASN
1	A	401	ASP
1	A	411	THR
1	B	242	LEU
1	B	255	ARG
1	B	264	VAL
1	B	272	GLN
1	B	280	ASP
1	B	291	PRO
1	B	294	GLN
1	B	295	GLN
1	B	300	TYR
1	B	318	GLU
1	B	325	ASN
1	B	328	LEU
1	B	370	LYS
1	B	376	ASP
1	B	389	ASN
1	B	390	ASN
1	B	399	ASP
1	B	426	SER
1	B	437	THR
1	B	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	311	GLN
1	A	312	ASN
1	A	325	ASN
1	A	347	GLN
1	A	361	ASN
1	A	390	ASN
1	A	418	GLN
1	A	419	GLN
1	A	429	HIS
1	A	438	GLN
1	B	347	GLN
1	B	390	ASN
1	B	419	GLN
1	B	429	HIS

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 ⓘ

16 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	1445	1,2	14,14,15	0.61	0	15,19,21	0.75	0
2	FUL	A	1446	2	9,10,11	0.87	1 (11%)	13,14,16	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1447	2	14,14,15	0.62	0	15,19,21	0.77	1 (6%)
2	BMA	A	1448	2	11,11,12	0.49	0	13,15,17	0.56	0
2	MAN	A	1449	2	11,11,12	0.36	0	13,15,17	0.97	1 (7%)
2	NAG	A	1450	2	14,14,15	0.61	0	15,19,21	0.91	1 (6%)
2	GAL	A	1451	2	11,11,12	0.43	0	13,15,17	0.52	0
2	MAN	A	1452	2	11,11,12	0.50	0	13,15,17	0.46	0
3	NAG	B	1444	1,3	14,14,15	0.85	0	15,19,21	0.87	1 (6%)
3	FUL	B	1445	3	9,10,11	0.59	0	13,14,16	1.66	4 (30%)
3	NAG	B	1446	3	14,14,15	0.66	0	15,19,21	0.80	0
3	BMA	B	1447	3	11,11,12	0.79	0	13,15,17	1.09	1 (7%)
3	BMA	B	1448	3	11,11,12	0.63	0	13,15,17	0.98	1 (7%)
3	NAG	B	1449	3	14,14,15	0.51	0	15,19,21	0.72	0
3	GAL	B	1450	3	11,11,12	0.53	0	13,15,17	0.60	0
3	MAN	B	1451	3	11,11,12	0.55	0	13,15,17	0.83	1 (7%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1446	FUL	C2-C3	2.12	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1444	NAG	C2-N2-C7	-2.40	119.45	122.94
3	B	1448	BMA	C1-C2-C3	-2.36	106.66	109.65
2	A	1450	NAG	C2-N2-C7	-2.19	119.74	122.94
2	A	1447	NAG	C1-C2-N2	-2.14	106.83	110.49
3	B	1445	FUL	C1-C2-C3	2.09	112.31	109.65
3	B	1445	FUL	C1-O5-C5	2.38	117.66	112.39
3	B	1451	MAN	C1-O5-C5	2.40	115.47	112.17
2	A	1449	MAN	C1-O5-C5	2.41	115.49	112.17
3	B	1445	FUL	O5-C5-C4	2.43	113.62	109.62
3	B	1447	BMA	C1-C2-C3	3.29	113.83	109.65
3	B	1445	FUL	C3-C4-C5	3.59	115.32	109.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1444	NAG	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1445	NAG	4	0
2	A	1447	NAG	3	0
2	A	1449	MAN	2	0
2	A	1450	NAG	4	0
2	A	1451	GAL	9	0
3	B	1444	NAG	6	0
3	B	1445	FUL	5	0
3	B	1446	NAG	2	0
3	B	1449	NAG	3	0
3	B	1450	GAL	1	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	208/223 (93%)	-0.62	1 (0%) 90 80	2, 21, 54, 65	15 (7%)
1	B	205/223 (91%)	-0.47	0 100 100	2, 30, 81, 90	37 (18%)
All	All	413/446 (92%)	-0.55	1 (0%) 94 89	2, 26, 70, 90	52 (12%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	HIS	2.2

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
3	GAL	B	1450	11/12	0.88	0.23	3.16	66,68,69,71	2
2	GAL	A	1451	11/12	0.92	0.24	2.07	52,53,56,59	0
2	NAG	A	1450	14/15	0.91	0.17	-0.04	42,47,52,55	0
3	NAG	B	1449	14/15	0.93	0.17	-0.26	63,64,65,66	3
3	NAG	B	1446	14/15	0.92	0.16	-1.70	78,82,84,85	1
3	NAG	B	1444	14/15	0.67	0.21	-	88,93,98,102	6
2	MAN	A	1449	11/12	0.93	0.14	-	37,38,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1445	14/15	0.88	0.14	-	42,44,50,56	0
2	FUL	A	1446	10/11	0.88	0.26	-	58,61,61,63	0
3	MAN	B	1451	11/12	0.82	0.25	-	71,73,75,76	0
2	NAG	A	1447	14/15	0.94	0.16	-	39,41,42,42	0
3	BMA	B	1447	11/12	0.96	0.19	-	72,75,76,76	1
2	MAN	A	1452	11/12	0.92	0.24	-	54,58,60,63	0
3	BMA	B	1448	11/12	0.91	0.14	-	65,68,69,69	2
2	BMA	A	1448	11/12	0.94	0.15	-	37,42,45,48	0
3	FUL	B	1445	10/11	0.84	0.49	-	106,109,110,110	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.