



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 AM GMT

PDB ID : 2Y7Q
Title : THE HIGH-AFFINITY COMPLEX BETWEEN IGE AND ITS RECEPTOR
FC EPSILON RI
Authors : Davies, A.M.; Holdom, M.D.; Nettleship, J.E.; Beavil, A.J.; Owens, R.J.;
Sutton, B.J.
Deposited on : 2011-02-01
Resolution : 3.40 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

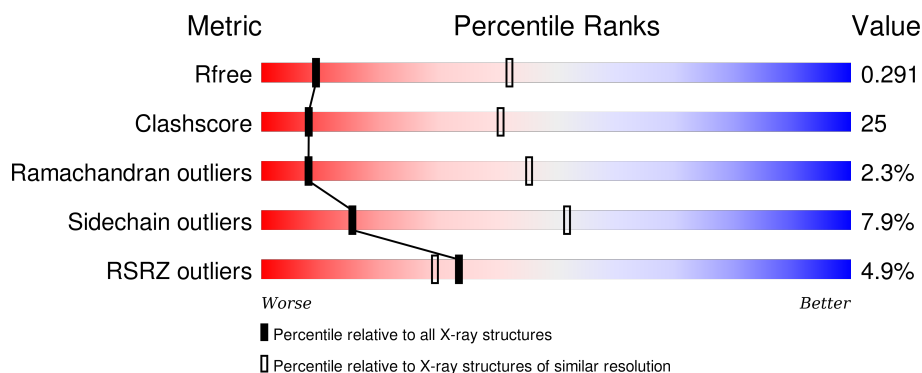
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	188	<div> <div>5%</div> <div>51% 27% 6% 16%</div> </div>
2	B	327	<div> <div>2%</div> <div>53% 32% • 12%</div> </div>
2	D	327	<div> <div>6%</div> <div>57% 26% 5% 11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5355 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 HIGH AFFINITY IMMUNOGLOBULIN EPSILON RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1188	773	189	222	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLU	-	CLONING ARTIFACT	UNP P12319
A	-1	THR	-	CLONING ARTIFACT	UNP P12319
A	0	GLY	-	CLONING ARTIFACT	UNP P12319
A	74	ALA	ASN	ENGINEERED MUTATION	UNP P12319
A	135	ALA	ASN	ENGINEERED MUTATION	UNP P12319
A	142	ALA	THR	ENGINEERED MUTATION	UNP P12319
A	143	ALA	VAL	CLONING ARTIFACT	UNP P12319
A	177	GLY	-	CLONING ARTIFACT	UNP P12319
A	178	THR	-	CLONING ARTIFACT	UNP P12319
A	179	LYS	-	CLONING ARTIFACT	UNP P12319
A	180	HIS	-	EXPRESSION TAG	UNP P12319
A	181	HIS	-	EXPRESSION TAG	UNP P12319
A	182	HIS	-	EXPRESSION TAG	UNP P12319
A	183	HIS	-	EXPRESSION TAG	UNP P12319
A	184	HIS	-	EXPRESSION TAG	UNP P12319
A	185	HIS	-	EXPRESSION TAG	UNP P12319

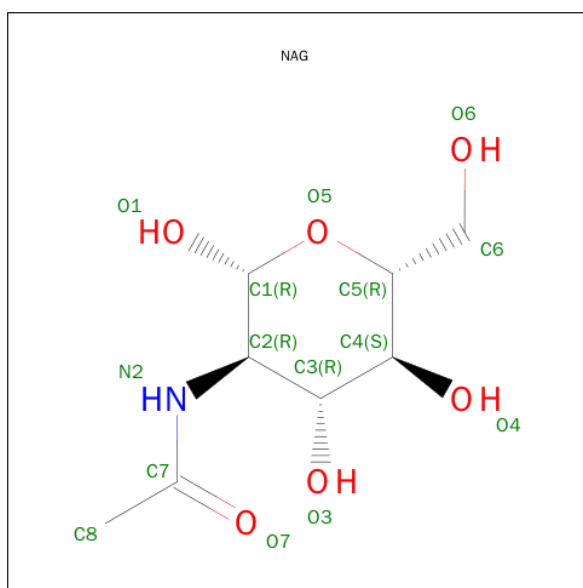
- Molecule 2 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	287	Total	C	N	O	S	0	0	0
			2043	1290	351	391	11			
2	D	290	Total	C	N	O	S	0	0	0
			2032	1287	350	385	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ASP	-	EXPRESSION TAG	UNP P01854
B	223	ILE	-	EXPRESSION TAG	UNP P01854
B	225	ALA	CYS	ENGINEERED MUTATION	UNP P01854
B	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
B	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	222	ASP	-	EXPRESSION TAG	UNP P01854
D	223	ILE	-	EXPRESSION TAG	UNP P01854
D	225	ALA	CYS	ENGINEERED MUTATION	UNP P01854
D	265	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854

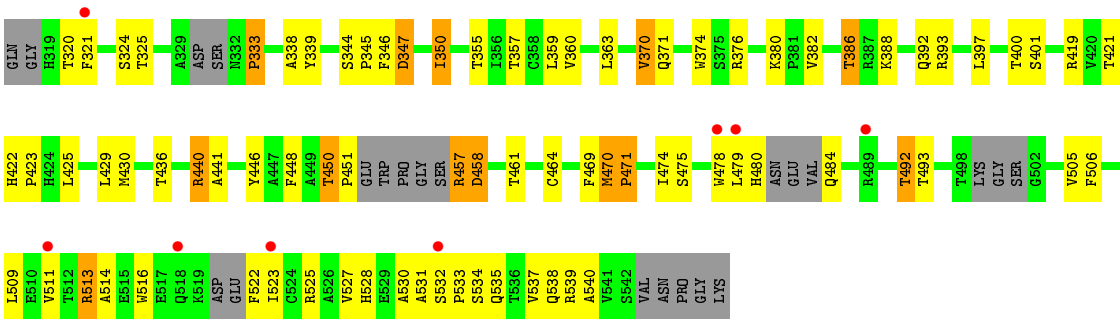
- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.49Å 103.34Å 110.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.68 – 3.40 37.68 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.68-3.40) 99.8 (37.68-3.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.245 , 0.292 0.243 , 0.291	Depositor DCC
R_{free} test set	812 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 103.9	EDS
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 16127 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: 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	0.32	0/1225	0.50	0/1679
2	B	0.30	0/2089	0.55	1/2847 (0.0%)
2	D	0.30	0/2077	0.53	1/2829 (0.0%)
All	All	0.31	0/5391	0.53	2/7355 (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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	SER	C-N-CA	6.14	147.79	122.00
2	D	532	SER	C-N-CA	6.03	147.32	122.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	470	MET	Peptide
2	D	470	MET	Peptide

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	1188	0	1015	52	0
2	B	2043	0	1789	111	0
2	D	2032	0	1769	96	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	D	14	0	13	0	0
4	A	50	0	43	2	0
All	All	5355	0	4655	247	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 25.

All (247) 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:B:342:ARG:HH11	2:B:342:ARG:HG3	1.12	1.06
2:B:471:PRO:HD2	2:B:528:HIS:CE1	1.99	0.97
2:D:471:PRO:HD2	2:D:528:HIS:CE1	1.99	0.97
2:D:344:SER:HB3	2:D:347:ASP:HB2	1.48	0.95
2:B:344:SER:HB3	2:B:347:ASP:HB2	1.50	0.93
2:D:363:LEU:HD13	2:D:370:VAL:HG21	1.55	0.89
1:A:65:GLU:HB2	1:A:80:TYR:CZ	2.11	0.86
2:B:333:PRO:HG2	2:B:429:LEU:HD11	1.57	0.85
2:B:342:ARG:NH1	2:B:342:ARG:HG3	1.90	0.85
2:B:251:ILE:HD13	2:B:304:TRP:CD1	2.12	0.85
1:A:156:TRP:CZ3	2:D:333:PRO:HG2	2.12	0.84
2:B:539:ARG:HG2	2:B:540:ALA:H	1.46	0.80
1:A:65:GLU:HB2	1:A:80:TYR:CE2	2.19	0.78
2:B:251:ILE:HD13	2:B:304:TRP:CG	2.20	0.77
1:A:156:TRP:HZ3	2:D:333:PRO:HG2	1.48	0.76
2:D:539:ARG:HG2	2:D:540:ALA:H	1.51	0.75
2:D:513:ARG:HA	2:D:516:TRP:CG	2.22	0.74
1:A:41:HIS:HE1	1:A:63:SER:O	1.70	0.74
2:D:471:PRO:HD2	2:D:528:HIS:NE2	2.02	0.74
2:B:528:HIS:CD2	2:B:530:ALA:H	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:GLN:HG2	2:B:298:THR:HG23	1.71	0.71
2:B:242:ASP:HB3	2:B:246:HIS:H	1.54	0.71
2:B:471:PRO:HD2	2:B:528:HIS:NE2	2.04	0.71
1:A:77:GLU:HB3	1:A:78:PRO:CD	2.20	0.70
2:D:528:HIS:CD2	2:D:530:ALA:H	2.09	0.70
2:B:365:PRO:HA	2:B:397:LEU:HD13	1.75	0.69
2:B:259:TYR:HE1	2:B:292:SER:HA	1.57	0.69
4:A:1175:NAG:H62	4:A:1176:NAG:H82	1.75	0.69
2:D:440:ARG:HD3	2:D:440:ARG:N	2.07	0.68
2:D:346:PHE:HA	2:D:527:VAL:HG11	1.76	0.67
1:A:105:LEU:HB2	1:A:136:ILE:HB	1.76	0.67
1:A:130:TRP:HB3	1:A:134:HIS:CD2	2.30	0.66
2:B:492:THR:HG23	2:B:505:VAL:CG1	2.25	0.66
2:D:457:ARG:O	2:D:458:ASP:HB2	1.95	0.65
2:D:492:THR:HG23	2:D:505:VAL:CG1	2.26	0.64
2:B:475:SER:HB2	2:B:527:VAL:HB	1.79	0.64
2:B:342:ARG:HH11	2:B:342:ARG:CG	2.00	0.63
2:D:269:LEU:HB2	2:D:311:THR:HB	1.81	0.63
2:D:363:LEU:CD1	2:D:370:VAL:HG21	2.26	0.63
2:B:422:HIS:CG	2:B:423:PRO:HD2	2.34	0.62
2:B:377:ALA:HB2	2:B:415:THR:HB	1.81	0.62
2:B:448:PHE:CD2	2:D:448:PHE:CD2	2.86	0.62
2:B:425:LEU:HD13	2:B:429:LEU:HD13	1.81	0.61
2:D:371:GLN:HB2	2:D:421:THR:OG1	2.01	0.61
2:B:448:PHE:HD2	2:D:448:PHE:HD2	1.49	0.61
2:D:513:ARG:HD2	2:D:514:ALA:N	2.15	0.60
1:A:155:VAL:HG12	1:A:156:TRP:CD1	2.36	0.60
2:D:523:ILE:HD13	2:D:540:ALA:HB2	1.81	0.60
2:D:475:SER:HB2	2:D:527:VAL:HB	1.83	0.60
2:B:315:THR:HG23	2:B:320:THR:HG22	1.82	0.60
2:B:441:ALA:O	2:B:469:PHE:HA	2.02	0.60
1:A:133:ASN:HD22	1:A:134:HIS:H	1.47	0.60
2:B:374:TRP:HZ2	2:B:401:SER:O	1.85	0.59
2:B:493:THR:HG21	2:D:493:THR:HG21	1.84	0.59
1:A:77:GLU:HB3	1:A:78:PRO:HD3	1.82	0.59
2:B:464:CYS:HB2	2:B:478:TRP:CH2	2.38	0.59
2:B:446:TYR:CE1	2:D:451:PRO:HD2	2.37	0.59
2:D:425:LEU:HD13	2:D:429:LEU:HD13	1.84	0.59
2:D:479:LEU:O	2:D:480:HIS:HB2	2.02	0.58
2:B:448:PHE:CD2	2:D:448:PHE:HD2	2.20	0.58
2:B:478:TRP:CG	2:B:509:LEU:HD22	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:VAL:HG22	2:B:422:HIS:CD2	2.38	0.58
2:D:464:CYS:HB2	2:D:478:TRP:CH2	2.39	0.58
2:D:425:LEU:HD13	2:D:429:LEU:CD1	2.34	0.57
2:B:446:TYR:HB3	2:B:448:PHE:CE1	2.40	0.57
1:A:37:THR:O	1:A:49:THR:HA	2.04	0.57
2:D:229:PHE:CD2	2:D:230:THR:N	2.72	0.57
2:D:450:THR:HG21	2:D:461:THR:HB	1.86	0.56
2:D:315:THR:CG2	2:D:320:THR:HG22	2.34	0.56
2:D:531:ALA:O	2:D:535:GLN:HA	2.06	0.56
1:A:11:PRO:HB2	1:A:13:TRP:CD1	2.41	0.56
2:D:363:LEU:HB2	2:D:397:LEU:HB3	1.87	0.55
1:A:40:PHE:CE1	1:A:45:LEU:HD12	2.41	0.55
2:D:478:TRP:CG	2:D:509:LEU:HD22	2.42	0.55
2:D:266:ILE:HD12	2:D:295:SER:HB2	1.88	0.55
2:B:444:GLU:O	2:B:466:ILE:HA	2.06	0.55
2:D:422:HIS:CG	2:D:423:PRO:HD2	2.41	0.55
2:D:492:THR:HG23	2:D:505:VAL:HG11	1.88	0.55
2:B:531:ALA:O	2:B:535:GLN:HA	2.06	0.55
1:A:110:TRP:O	1:A:113:TRP:HB2	2.07	0.55
2:B:333:PRO:HG2	2:B:429:LEU:CD1	2.32	0.55
2:B:250:THR:CG2	2:B:298:THR:HG22	2.36	0.55
1:A:77:GLU:CB	1:A:78:PRO:HD3	2.38	0.55
2:B:448:PHE:HD2	2:D:448:PHE:CD2	2.25	0.55
1:A:104:PHE:O	1:A:105:LEU:HD23	2.07	0.54
1:A:156:TRP:O	1:A:157:GLN:HB2	2.07	0.54
2:D:513:ARG:O	2:D:516:TRP:HB2	2.07	0.54
2:D:311:THR:HG23	2:D:324:SER:OG	2.07	0.54
2:B:492:THR:HG23	2:B:505:VAL:HG11	1.88	0.54
2:B:338:ALA:HA	2:B:359:LEU:O	2.07	0.54
2:B:387:ARG:HG3	2:B:387:ARG:O	2.07	0.54
2:B:539:ARG:HG2	2:B:540:ALA:N	2.21	0.54
2:B:269:LEU:HB2	2:B:311:THR:HB	1.90	0.54
2:B:425:LEU:HD13	2:B:429:LEU:CD1	2.38	0.54
2:D:446:TYR:HB3	2:D:448:PHE:CE1	2.43	0.53
1:A:133:ASN:ND2	1:A:134:HIS:H	2.06	0.53
2:D:359:LEU:HD12	2:D:360:VAL:N	2.23	0.53
2:B:446:TYR:CD1	2:D:451:PRO:HD2	2.43	0.53
2:B:434:THR:HG22	2:B:435:LYS:N	2.22	0.53
2:B:331:SER:C	2:B:333:PRO:HD3	2.30	0.52
2:D:339:TYR:N	2:D:339:TYR:CD1	2.77	0.52
1:A:119:ILE:HD12	1:A:152:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:THR:HG23	2:B:324:SER:OG	2.10	0.51
2:D:251:ILE:HD13	2:D:304:TRP:CD1	2.45	0.51
2:B:301:GLN:O	2:B:305:LEU:HG	2.11	0.51
2:B:465:LEU:HG	2:B:465:LEU:O	2.09	0.51
2:B:304:TRP:CZ2	2:B:327:LYS:HA	2.46	0.51
2:B:251:ILE:CD1	2:B:304:TRP:CD1	2.90	0.50
2:D:229:PHE:HD2	2:D:230:THR:H	1.59	0.50
2:D:376:ARG:HD3	2:D:380:LYS:O	2.12	0.50
2:B:434:THR:CG2	2:B:435:LYS:N	2.74	0.50
2:D:299:LEU:HD21	2:D:310:TYR:CE2	2.46	0.50
2:B:250:THR:HG22	2:B:298:THR:HG22	1.94	0.49
2:B:445:VAL:CG1	2:B:464:CYS:SG	3.00	0.49
2:D:479:LEU:HA	2:D:484:GLN:HA	1.94	0.49
1:A:41:HIS:NE2	4:A:1175:NAG:H82	2.28	0.49
2:B:342:ARG:NH1	2:B:342:ARG:CG	2.67	0.49
2:D:422:HIS:HB3	2:D:425:LEU:HG	1.95	0.49
2:B:344:SER:HB3	2:B:347:ASP:CB	2.31	0.49
2:B:371:GLN:HB2	2:B:421:THR:OG1	2.13	0.49
2:B:331:SER:O	2:B:333:PRO:HD3	2.13	0.48
1:A:15:ARG:HB3	1:A:84:PHE:HE1	1.78	0.48
2:B:236:ILE:HA	2:B:253(A):LEU:O	2.13	0.48
2:D:345:PRO:HB2	2:D:527:VAL:O	2.13	0.48
2:D:338:ALA:HA	2:D:359:LEU:O	2.13	0.48
2:D:256:VAL:HG11	2:D:264:ILE:CD1	2.43	0.48
1:A:101:GLN:O	1:A:141:ALA:HB2	2.13	0.48
2:B:377:ALA:CB	2:B:415:THR:HB	2.44	0.48
2:B:355:THR:HG22	2:B:404:PRO:HA	1.96	0.48
2:B:240:SER:HB2	2:D:325:THR:CB	2.44	0.48
2:B:303:HIS:HD2	2:B:310:TYR:OH	1.96	0.48
1:A:133:ASN:HD22	1:A:134:HIS:N	2.12	0.47
2:B:386:THR:CG2	2:B:387:ARG:N	2.77	0.47
2:B:478:TRP:CB	2:B:509:LEU:HD22	2.45	0.47
2:B:446:TYR:O	2:B:464:CYS:HA	2.14	0.47
2:D:231:PRO:HB3	2:D:321:PHE:CZ	2.49	0.47
1:A:19:GLY:O	1:A:57:ASN:HA	2.14	0.47
2:B:471:PRO:HD2	2:B:528:HIS:HE1	1.68	0.47
2:D:478:TRP:CB	2:D:509:LEU:HD22	2.45	0.47
2:B:339:TYR:CD1	2:B:339:TYR:N	2.82	0.47
2:D:345:PRO:HD2	2:D:475:SER:OG	2.14	0.47
1:A:37:THR:HG22	1:A:38:LYS:N	2.30	0.47
2:D:370:VAL:HG22	2:D:422:HIS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:TYR:CB	2:B:448:PHE:HE1	2.29	0.46
1:A:128:LYS:HG2	1:A:129:TYR:N	2.29	0.46
2:B:300:SER:HB2	2:B:303:HIS:H	1.80	0.46
1:A:86:ASP:OD1	1:A:87:TRP:N	2.44	0.46
2:D:474:ILE:HG12	2:D:475:SER:N	2.31	0.46
1:A:146:SER:HB3	1:A:168:THR:HG22	1.97	0.46
2:B:370:VAL:HG22	2:B:422:HIS:HD2	1.79	0.45
2:D:346:PHE:CE1	2:D:350:ILE:HG21	2.51	0.45
2:B:367:LYS:C	2:B:369:THR:H	2.19	0.45
2:D:231:PRO:HB3	2:D:321:PHE:CE2	2.51	0.45
1:A:155:VAL:HB	1:A:160:TYR:CE2	2.52	0.45
2:D:374:TRP:HZ2	2:D:401:SER:O	1.98	0.45
1:A:93:SER:CB	1:A:104:PHE:H	2.29	0.45
2:D:419:ARG:HD2	2:D:430:MET:SD	2.57	0.45
2:B:422:HIS:HB3	2:B:425:LEU:HG	1.99	0.45
2:B:336:VAL:HG12	2:B:337:SER:N	2.32	0.45
1:A:133:ASN:ND2	1:A:134:HIS:N	2.65	0.45
2:B:388:LYS:HB2	2:B:400:THR:HB	1.98	0.45
2:B:472:GLU:HG3	2:B:503:PHE:CE2	2.51	0.45
2:B:259:TYR:HE1	2:B:292:SER:CA	2.28	0.44
2:B:259:TYR:CE1	2:B:292:SER:HA	2.43	0.44
2:B:333:PRO:C	2:B:335:GLY:H	2.19	0.44
1:A:113:TRP:CD1	1:A:156:TRP:HZ2	2.35	0.44
2:B:346:PHE:CE1	2:B:350:ILE:HG21	2.52	0.44
2:B:405:VAL:HG13	2:B:416:TYR:OH	2.16	0.44
2:B:448:PHE:HB3	2:D:448:PHE:CE2	2.52	0.44
2:D:471:PRO:HD2	2:D:528:HIS:HE1	1.71	0.44
2:D:363:LEU:CB	2:D:397:LEU:HB3	2.47	0.44
2:B:270:GLU:HB3	2:B:275:MET:HG2	2.00	0.44
2:B:359:LEU:HD12	2:B:360:VAL:H	1.82	0.44
1:A:103:LEU:HD23	1:A:138:ILE:HD13	1.99	0.44
2:D:370:VAL:HG22	2:D:422:HIS:CD2	2.52	0.44
2:B:299:LEU:HD21	2:B:310:TYR:CE2	2.53	0.44
1:A:59:LYS:O	1:A:62:ASP:HB2	2.18	0.44
2:D:251:ILE:CD1	2:D:304:TRP:CD1	3.01	0.44
2:B:506:PHE:CD1	2:D:506:PHE:CD1	3.05	0.44
2:B:345:PRO:HB2	2:B:475:SER:OG	2.18	0.44
2:D:315:THR:HG23	2:D:320:THR:HG22	1.98	0.44
2:D:469:PHE:HB2	2:D:528:HIS:CE1	2.53	0.43
2:D:474:ILE:HG12	2:D:475:SER:H	1.83	0.43
2:D:441:ALA:O	2:D:469:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:TRP:HA	2:B:523:ILE:O	2.18	0.43
2:D:359:LEU:HD12	2:D:360:VAL:H	1.83	0.43
2:B:440:ARG:HD2	2:B:471:PRO:HG3	2.00	0.43
1:A:77:GLU:CB	1:A:78:PRO:CD	2.91	0.43
2:D:249:PRO:O	2:D:301:GLN:HB2	2.18	0.43
2:D:446:TYR:CB	2:D:448:PHE:HE1	2.32	0.43
1:A:169:VAL:HG12	1:A:170:ILE:N	2.33	0.43
1:A:93:SER:HB2	1:A:104:PHE:H	1.83	0.43
2:D:534:SER:O	2:D:535:GLN:HB2	2.19	0.43
2:B:534:SER:O	2:B:535:GLN:HB2	2.19	0.43
2:B:525:ARG:HA	2:B:538:GLN:HB2	2.00	0.43
2:B:346:PHE:N	2:B:475:SER:OG	2.51	0.43
2:D:256:VAL:HG11	2:D:264:ILE:HD13	2.00	0.43
2:B:539:ARG:CG	2:B:540:ALA:H	2.24	0.43
1:A:41:HIS:CE1	1:A:63:SER:O	2.60	0.43
2:D:269:LEU:HA	2:D:273:GLN:O	2.19	0.43
2:D:344:SER:HB3	2:D:347:ASP:CB	2.33	0.42
2:D:400:THR:HG22	2:D:401:SER:N	2.33	0.42
2:B:333:PRO:C	2:B:335:GLY:N	2.72	0.42
2:B:333:PRO:CG	2:B:429:LEU:HD11	2.39	0.42
1:A:136:ILE:N	1:A:136:ILE:HD12	2.34	0.42
2:B:422:HIS:CE1	2:B:423:PRO:HG2	2.54	0.42
2:D:523:ILE:CD1	2:D:540:ALA:HB2	2.48	0.42
2:B:242:ASP:CB	2:B:246:HIS:HB2	2.48	0.42
2:B:303:HIS:CE1	2:B:308:ARG:NH1	2.87	0.42
2:D:386:THR:HG22	2:D:386:THR:O	2.19	0.42
1:A:17:PHE:O	1:A:20:GLU:HB2	2.19	0.42
1:A:88:LEU:HD21	1:A:153:GLY:HA3	2.00	0.42
1:A:119:ILE:HD12	1:A:152:THR:HG21	2.01	0.42
1:A:118:VAL:HA	1:A:152:THR:O	2.20	0.42
2:B:469:PHE:HB2	2:B:528:HIS:CE1	2.55	0.42
2:D:229:PHE:CE2	2:D:231:PRO:HD3	2.55	0.42
1:A:165:LEU:HD12	1:A:166:ASN:N	2.35	0.42
2:B:359:LEU:HD12	2:B:360:VAL:N	2.35	0.42
2:B:241:CYS:O	2:D:325:THR:HA	2.19	0.42
2:D:392:GLN:HE21	2:D:393:ARG:H	1.67	0.42
2:B:446:TYR:CB	2:B:448:PHE:CE1	3.02	0.41
2:D:450:THR:CG2	2:D:461:THR:HB	2.50	0.41
2:B:269:LEU:HD11	2:B:313:GLN:NE2	2.35	0.41
1:A:119:ILE:HA	1:A:128:LYS:O	2.20	0.41
1:A:9:LEU:HD23	1:A:22:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HG23	1:A:169:VAL:HG22	2.02	0.41
2:D:479:LEU:HD21	2:D:525:ARG:NH2	2.35	0.41
2:B:370:VAL:HG11	2:B:399:VAL:HG21	2.02	0.41
2:B:400:THR:HG22	2:B:401:SER:N	2.35	0.41
2:D:251:ILE:HD13	2:D:304:TRP:CG	2.56	0.41
2:D:511:VAL:HG21	2:D:522:PHE:CE2	2.55	0.41
2:D:478:TRP:HA	2:D:523:ILE:O	2.21	0.41
2:D:388:LYS:O	2:D:400:THR:HB	2.21	0.41
2:B:537:VAL:O	2:B:538:GLN:HB3	2.21	0.41
1:A:9:LEU:HD23	1:A:22:VAL:CG2	2.51	0.41
2:B:260:THR:HB	2:B:316:TYR:OH	2.20	0.41
2:D:539:ARG:HG2	2:D:540:ALA:N	2.27	0.40
2:B:242:ASP:HB3	2:B:246:HIS:HB2	2.03	0.40
2:B:464:CYS:HB2	2:B:478:TRP:CZ2	2.56	0.40
2:B:300:SER:HB2	2:B:303:HIS:HB2	2.03	0.40
1:A:90:LEU:HD23	1:A:165:LEU:HB3	2.03	0.40
1:A:98:MET:O	1:A:99:GLU:C	2.60	0.40
2:D:537:VAL:HG12	2:D:538:GLN:N	2.35	0.40
2:D:528:HIS:HD2	2:D:530:ALA:H	1.64	0.40
1:A:15:ARG:HB3	1:A:84:PHE:CE1	2.55	0.40
2:B:367:LYS:O	2:B:369:THR:N	2.53	0.40
2:D:303:HIS:O	2:D:306:SER:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	152/188 (81%)	135 (89%)	13 (9%)	4 (3%)	7 42
2	B	275/327 (84%)	246 (90%)	24 (9%)	5 (2%)	11 50
2	D	274/327 (84%)	244 (89%)	23 (8%)	7 (3%)	7 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	701/842 (83%)	625 (89%)	60 (9%)	16 (2%)	8	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	533	PRO
1	A	57	ASN
1	A	99	GLU
2	B	350	ILE
2	D	458	ASP
2	B	242	ASP
2	D	350	ILE
1	A	77	GLU
2	D	230	THR
2	D	333	PRO
1	A	141	ALA
2	B	471	PRO
2	D	471	PRO
2	B	533	PRO
2	B	470	MET
2	D	470	MET

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	109/167 (65%)	98 (90%)	11 (10%)	9	38
2	B	188/289 (65%)	177 (94%)	11 (6%)	24	64
2	D	182/289 (63%)	166 (91%)	16 (9%)	12	46
All	All	479/745 (64%)	441 (92%)	38 (8%)	15	52

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	9	LEU
1	A	26	CYS
1	A	49	THR
1	A	51	SER
1	A	97	VAL
1	A	119	ILE
1	A	129	TYR
1	A	133	ASN
1	A	138	ILE
1	A	152	THR
2	B	263	THR
2	B	271	ASP
2	B	298	THR
2	B	300	SER
2	B	315	THR
2	B	342	ARG
2	B	351	ARG
2	B	357	THR
2	B	390	GLU
2	B	436	THR
2	B	491	SER
2	D	233	THR
2	D	298	THR
2	D	303	HIS
2	D	315	THR
2	D	347	ASP
2	D	355	THR
2	D	357	THR
2	D	370	VAL
2	D	382	VAL
2	D	386	THR
2	D	436	THR
2	D	440	ARG
2	D	450	THR
2	D	457	ARG
2	D	492	THR
2	D	513	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

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Mol	Chain	Res	Type
1	A	41	HIS
1	A	133	ASN
2	B	303	HIS
2	B	313	GLN
2	B	384	HIS
2	B	490	HIS
2	B	528	HIS
2	D	392	GLN
2	D	417	GLN
2	D	477	GLN
2	D	528	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 ⓘ

4 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	$\# Z > 2$
4	NAG	A	1175	1,4	14,14,15	0.59	0	15,19,21	1.00	1 (6%)
4	NAG	A	1176	4	14,14,15	0.53	0	15,19,21	1.45	1 (6%)
4	BMA	A	1177	4	11,11,12	0.86	0	14,15,17	0.89	0
4	MAN	A	1178	4	11,11,12	0.73	0	14,15,17	1.11	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
4	NAG	A	1175	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1176	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1177	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1178	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1176	NAG	C2-N2-C7	-4.28	117.54	123.04
4	A	1175	NAG	C2-N2-C7	-2.68	119.59	123.04
4	A	1178	MAN	C1-C2-C3	2.65	112.68	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1175	NAG	2	0
4	A	1176	NAG	1	0

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	A	1174	1	14,14,15	0.46	0	15,19,21	1.67	2 (13%)
3	NAG	B	1543	2	14,14,15	0.60	0	15,19,21	0.77	0
3	NAG	D	1543	2	14,14,15	0.41	0	15,19,21	1.90	3 (20%)

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	A	1174	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1543	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1543	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1543	NAG	C4-C3-C2	-3.61	105.61	111.23
3	D	1543	NAG	C2-N2-C7	-2.39	119.97	123.04
3	A	1174	NAG	C3-C4-C5	2.84	115.15	110.20
3	A	1174	NAG	C1-O5-C5	5.08	118.69	112.25
3	D	1543	NAG	C1-O5-C5	5.42	119.12	112.25

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	158/188 (84%)	0.19	9 (5%)	27 25	28, 64, 114, 146	0
2	B	287/327 (87%)	0.10	8 (2%)	56 52	33, 76, 120, 159	0
2	D	290/327 (88%)	0.38	19 (6%)	22 20	32, 81, 127, 154	0
All	All	735/842 (87%)	0.23	36 (4%)	33 29	28, 76, 124, 159	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	SER	4.4
2	D	479	LEU	4.1
1	A	70	HIS	3.9
2	D	261	PRO	3.8
2	D	518	GLN	3.6
2	D	263	THR	3.4
2	D	478	TRP	3.2
2	D	264	ILE	3.2
2	B	486	PRO	3.1
1	A	74	ALA	3.1
2	D	228	ASP	3.1
2	D	290	LEU	2.9
2	B	509	LEU	2.9
2	D	262	GLY	2.8
1	A	4	LYS	2.8
1	A	37	THR	2.7
1	A	69	GLN	2.6
2	D	315	THR	2.5
2	D	532	SER	2.4
2	B	278	ASP	2.4
2	D	511	VAL	2.4
2	B	489	ARG	2.4
2	D	281	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	307	ASP	2.3
2	D	489	ARG	2.3
2	D	230	THR	2.3
2	B	259	TYR	2.3
2	D	260	THR	2.3
1	A	5	PRO	2.3
2	B	479	LEU	2.2
2	B	488	ALA	2.2
1	A	75	GLU	2.1
2	D	523	ILE	2.1
2	D	321	PHE	2.1
2	D	280	SER	2.0
1	A	173	PRO	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](#)

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
4	MAN	A	1178	11/12	0.86	0.26	-0.69	101,101,101,101	0
4	NAG	A	1175	14/15	0.97	0.17	-0.69	44,44,44,44	0
4	NAG	A	1176	14/15	0.93	0.17	-0.84	56,56,56,56	0
4	BMA	A	1177	11/12	0.90	0.22	-	104,104,104,104	0

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. 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(\AA^2)	Q<0.9
3	NAG	D	1543	14/15	0.91	0.28	0.40	90,90,90,90	0
3	NAG	A	1174	14/15	0.92	0.14	-0.61	83,83,83,83	0
3	NAG	B	1543	14/15	0.89	0.23	-1.11	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.