



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:54 PM GMT

PDB ID : 3S7G
Title : Aglycosylated human igg1 fc fragment
Authors : Borrok, M.J.; Georgiou, G.
Deposited on : 2011-05-26
Resolution : 3.13 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

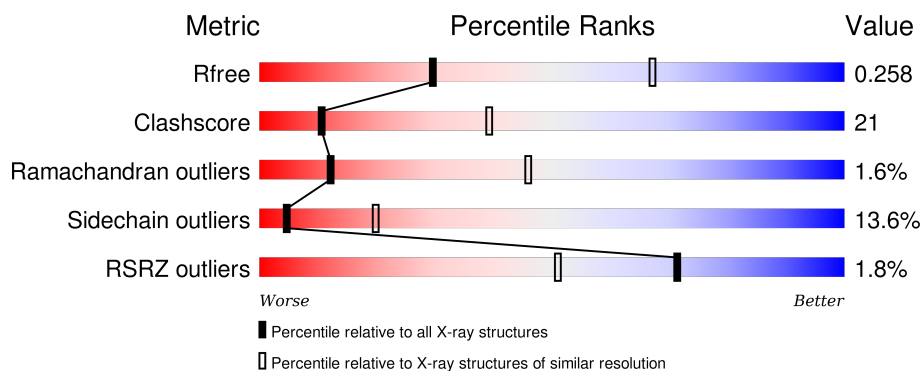
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	227	<div> <div></div> <div>55% 30% 6% 8%</div> </div>
1	B	227	<div> <div>3%</div> <div>59% 26% 6% 9%</div> </div>
1	C	227	<div> <div></div> <div>52% 33% 5% 8%</div> </div>
1	D	227	<div> <div>3%</div> <div>55% 30% 7% 9%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6662 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.

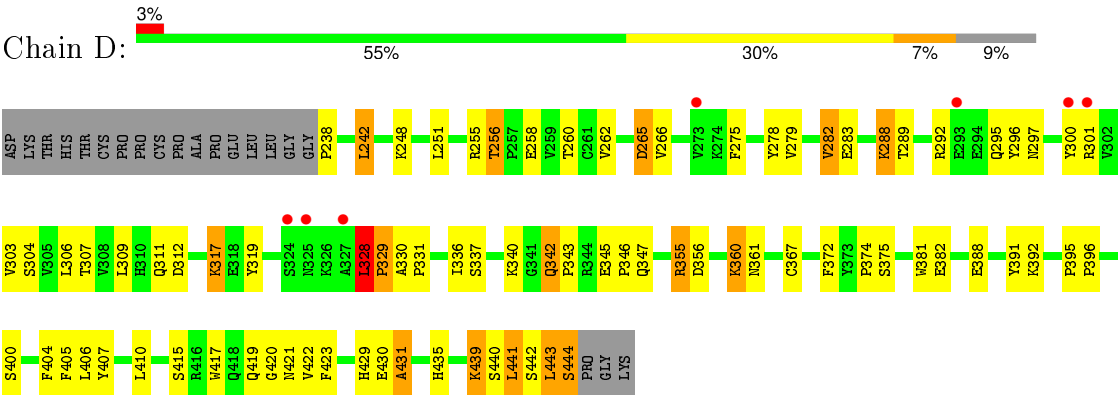
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1662	1058	280	318	6			
1	B	207	Total	C	N	O	S	0	0	0
			1654	1052	279	317	6			
1	C	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			
1	D	207	Total	C	N	O	S	0	0	0
			1660	1057	279	318	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	6	Total	O	0	0
			6	6		
2	C	8	Total	O	0	0
			8	8		
2	D	4	Total	O	0	0
			4	4		

● Molecule 1: Ig gamma-1 chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.69Å 65.77Å 77.81Å 98.18° 100.50° 116.92°	Depositor
Resolution (Å)	45.00 – 3.13 45.19 – 3.13	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.00-3.13) 82.9 (45.19-3.13)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.259 , 0.323 0.257 , 0.258	Depositor DCC
R_{free} test set	962 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	95.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.1	EDS
Estimated twinning fraction	0.237 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 18883 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6662	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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

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	0.79	0/1708	0.78	0/2327
1	B	0.78	0/1700	0.78	1/2316 (0.0%)
1	C	0.79	0/1710	0.75	1/2330 (0.0%)
1	D	0.77	0/1706	0.76	1/2324 (0.0%)
All	All	0.78	0/6824	0.77	3/9297 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	PRO	CA-N-CD	-7.93	100.40	111.50
1	D	328	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	328	LEU	CA-CB-CG	5.66	128.31	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1662	0	1629	76	0
1	B	1654	0	1618	50	0
1	C	1664	0	1631	89	0
1	D	1660	0	1629	81	0
2	A	4	0	0	2	0
2	B	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	0	2	0
2	D	4	0	0	0	0
All	All	6662	0	6507	280	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 21.

All (280) 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:D:422:VAL:CA	1:D:442:SER:HB3	1.52	1.40
1:C:328:LEU:HD22	1:C:329:PRO:N	1.36	1.40
1:D:422:VAL:HA	1:D:442:SER:CB	1.59	1.32
1:A:328:LEU:HD22	1:A:329:PRO:N	1.63	1.13
1:D:443:LEU:HG	1:D:444:SER:H	1.04	1.09
1:A:328:LEU:HD22	1:A:329:PRO:CD	1.88	1.02
1:B:342:GLN:OE1	1:B:342:GLN:HA	1.59	1.01
1:D:422:VAL:HG22	1:D:442:SER:OG	1.62	0.99
1:A:237:GLY:HA3	1:B:236:GLY:N	1.76	0.99
1:A:355:ARG:HE	1:A:355:ARG:H	1.04	0.95
1:C:442:SER:HA	1:C:443:LEU:HB3	1.48	0.95
1:D:422:VAL:HG22	1:D:442:SER:CB	1.98	0.94
1:D:355:ARG:HE	1:D:355:ARG:H	1.13	0.94
1:C:355:ARG:HE	1:C:355:ARG:H	1.08	0.93
1:C:328:LEU:CD2	1:C:329:PRO:N	2.30	0.93
1:D:443:LEU:HG	1:D:444:SER:N	1.84	0.93
1:A:246:LYS:HB3	2:A:20:HOH:O	1.68	0.92
1:A:251:LEU:O	1:C:253:ILE:HD11	1.72	0.90
1:A:328:LEU:HD22	1:A:329:PRO:HD2	1.54	0.88
1:B:355:ARG:HE	1:B:355:ARG:H	1.18	0.86
1:A:355:ARG:H	1:A:355:ARG:NE	1.72	0.85
1:C:355:ARG:NE	1:C:355:ARG:H	1.75	0.84
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.59	0.83
1:A:328:LEU:CD2	1:A:329:PRO:HD2	2.09	0.83
1:D:422:VAL:CB	1:D:442:SER:HB3	2.08	0.82
1:A:355:ARG:HE	1:A:355:ARG:N	1.79	0.81
1:A:340:LYS:H	1:A:340:LYS:HD2	1.45	0.81
1:D:355:ARG:NE	1:D:355:ARG:H	1.79	0.80
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.64	0.80
1:C:442:SER:CA	1:C:443:LEU:HB3	2.12	0.80
1:D:311:GLN:OE1	1:D:311:GLN:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:O	1:A:328:LEU:HD13	1.83	0.79
1:C:346:PRO:HB3	1:C:372:PHE:HB3	1.66	0.78
1:B:311:GLN:N	1:B:311:GLN:OE1	2.15	0.78
1:A:328:LEU:HD13	1:A:328:LEU:C	2.05	0.77
1:D:423:PHE:N	1:D:441:LEU:O	2.17	0.77
1:D:346:PRO:HB3	1:D:372:PHE:HB3	1.67	0.76
1:C:443:LEU:O	1:C:444:SER:HB2	1.86	0.76
1:C:311:GLN:OE1	1:C:311:GLN:N	2.16	0.75
1:C:355:ARG:N	1:C:355:ARG:HE	1.83	0.75
1:D:355:ARG:HE	1:D:355:ARG:N	1.85	0.74
1:D:421:ASN:O	1:D:442:SER:CB	2.36	0.73
1:D:422:VAL:CG2	1:D:442:SER:CB	2.66	0.73
1:B:355:ARG:NE	1:B:355:ARG:H	1.84	0.73
1:D:420:GLY:HA2	1:D:443:LEU:HB2	1.70	0.73
1:A:311:GLN:OE1	1:A:311:GLN:N	2.19	0.73
1:A:417:TRP:CH2	1:A:442:SER:CB	2.71	0.73
1:D:417:TRP:CZ3	1:D:441:LEU:HD11	2.25	0.72
1:A:256:THR:HG23	1:C:311:GLN:HE21	1.53	0.72
1:C:328:LEU:HD13	1:C:328:LEU:C	2.09	0.72
1:D:422:VAL:HA	1:D:442:SER:HB3	0.75	0.72
1:A:253:ILE:HD11	1:C:251:LEU:O	1.90	0.72
1:B:355:ARG:HE	1:B:355:ARG:N	1.88	0.71
1:A:341:GLY:O	1:A:343:PRO:HD3	1.91	0.70
1:D:421:ASN:O	1:D:442:SER:HB2	1.91	0.70
1:C:328:LEU:HD22	1:C:329:PRO:CD	2.21	0.70
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.74	0.70
1:B:317:LYS:HB3	1:B:319:TYR:CE1	2.27	0.69
1:C:328:LEU:HD11	1:C:330:ALA:C	2.12	0.69
1:D:421:ASN:O	1:D:442:SER:CA	2.41	0.69
1:B:248:LYS:HD2	1:B:255:ARG:HH12	1.57	0.69
1:B:417:TRP:CH2	1:B:442:SER:CB	2.78	0.67
1:C:238:PRO:HA	1:C:265:ASP:HB2	1.76	0.67
1:A:253:ILE:HG23	1:C:310:HIS:HB3	1.76	0.67
1:D:422:VAL:CG2	1:D:442:SER:HB3	2.23	0.67
1:C:328:LEU:HD11	1:C:330:ALA:O	1.95	0.67
1:A:311:GLN:HE21	1:C:256:THR:HG23	1.60	0.67
1:B:360:LYS:HD2	1:B:361:ASN:OD1	1.95	0.67
1:A:309:LEU:HD23	1:C:309:LEU:HD23	1.76	0.66
1:B:442:SER:OG	2:B:15:HOH:O	2.12	0.66
1:B:238:PRO:HA	1:B:265:ASP:HB2	1.77	0.66
1:B:391:TYR:HB3	1:B:410:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LYS:HB3	1:D:319:TYR:CE1	2.31	0.65
1:A:340:LYS:H	1:A:340:LYS:CD	2.09	0.65
1:D:238:PRO:HA	1:D:265:ASP:HB2	1.77	0.65
1:C:442:SER:OG	1:C:443:LEU:HB3	1.96	0.65
1:A:310:HIS:HB3	1:C:253:ILE:HG23	1.79	0.65
1:D:417:TRP:CH2	1:D:441:LEU:HD11	2.32	0.65
1:D:342:GLN:OE1	1:D:343:PRO:HD2	1.96	0.65
1:B:350:THR:HB	1:B:441:LEU:HG	1.79	0.63
1:A:309:LEU:HD23	1:C:309:LEU:CD2	2.28	0.63
1:D:328:LEU:HD11	1:D:331:PRO:HA	1.81	0.63
1:A:350:THR:HB	1:A:441:LEU:HG	1.81	0.63
1:C:441:LEU:HD22	1:C:442:SER:H	1.64	0.62
1:D:422:VAL:CA	1:D:442:SER:CB	2.42	0.62
1:A:309:LEU:CD2	1:C:309:LEU:HD23	2.28	0.62
1:C:443:LEU:N	1:C:443:LEU:HD13	2.15	0.62
1:A:360:LYS:HD2	1:A:361:ASN:OD1	1.98	0.61
1:D:242:LEU:HD13	1:D:336:ILE:HG12	1.82	0.61
1:C:328:LEU:HD22	1:C:329:PRO:CA	2.29	0.61
1:C:443:LEU:N	1:C:443:LEU:CD1	2.64	0.61
1:A:328:LEU:HD22	1:A:328:LEU:C	2.21	0.60
1:D:422:VAL:HA	1:D:442:SER:CA	2.29	0.60
1:A:429:HIS:CD2	1:A:431:ALA:H	2.20	0.59
1:A:342:GLN:HA	1:A:342:GLN:OE1	2.02	0.59
1:C:443:LEU:O	1:C:444:SER:CB	2.50	0.59
1:D:391:TYR:HB3	1:D:410:LEU:HD13	1.83	0.59
1:C:328:LEU:HD22	1:C:328:LEU:C	2.16	0.59
1:A:417:TRP:CH2	1:A:442:SER:HB3	2.38	0.59
1:C:360:LYS:HD2	1:C:361:ASN:OD1	2.03	0.59
1:C:391:TYR:HB3	1:C:410:LEU:HD13	1.84	0.59
1:C:442:SER:HA	1:C:443:LEU:CB	2.14	0.59
1:D:360:LYS:HD2	1:D:361:ASN:H	1.68	0.59
1:D:421:ASN:O	1:D:442:SER:HA	2.03	0.58
1:B:417:TRP:CH2	1:B:442:SER:HB3	2.39	0.58
1:D:251:LEU:HD22	1:D:435:HIS:HB3	1.86	0.58
1:C:338:LYS:HE3	1:C:430:GLU:OE2	2.02	0.58
1:C:429:HIS:CD2	1:C:431:ALA:H	2.22	0.58
1:D:295:GLN:HB2	1:D:301:ARG:HB2	1.85	0.58
1:B:279:VAL:O	1:B:282:VAL:HG13	2.04	0.58
1:C:443:LEU:HD22	1:C:444:SER:N	2.19	0.57
1:B:328:LEU:HD11	1:B:331:PRO:HA	1.86	0.57
1:C:378:ALA:HA	2:C:12:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:VAL:HG22	1:D:442:SER:HB3	1.83	0.57
1:D:306:LEU:HG	1:D:307:THR:O	2.05	0.57
1:B:430:GLU:HG3	1:B:431:ALA:N	2.21	0.56
1:A:391:TYR:HB3	1:A:410:LEU:HD13	1.88	0.56
1:C:372:PHE:CE1	1:C:405:PHE:HA	2.42	0.55
1:C:443:LEU:HD13	1:C:444:SER:H	1.72	0.55
1:C:272:GLU:O	1:C:325:ASN:ND2	2.39	0.55
1:C:274:LYS:HB3	1:C:324:SER:HB2	1.88	0.55
1:C:361:ASN:HA	1:C:414:LYS:NZ	2.22	0.55
1:D:279:VAL:O	1:D:282:VAL:HG13	2.07	0.54
1:C:278:TYR:CE2	1:C:283:GLU:HB2	2.42	0.54
1:D:421:ASN:C	1:D:442:SER:HB2	2.28	0.54
1:C:392:LYS:NZ	1:D:400:SER:HB3	2.23	0.54
1:C:328:LEU:O	1:C:328:LEU:HD13	2.06	0.54
1:D:295:GLN:O	1:D:295:GLN:HG3	2.07	0.54
1:B:342:GLN:CA	1:B:342:GLN:OE1	2.42	0.54
1:D:443:LEU:CG	1:D:444:SER:H	1.88	0.54
1:A:248:LYS:HD2	1:A:255:ARG:HH12	1.73	0.53
1:C:360:LYS:HD2	1:C:361:ASN:H	1.73	0.53
1:A:317:LYS:HB3	1:A:319:TYR:CE1	2.43	0.53
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.43	0.53
1:D:443:LEU:O	1:D:444:SER:HB3	2.07	0.53
1:D:420:GLY:HA2	1:D:443:LEU:CB	2.38	0.53
1:A:392:LYS:NZ	1:B:400:SER:HB3	2.24	0.53
1:C:350:THR:HB	1:C:441:LEU:HG	1.91	0.53
1:A:360:LYS:HD2	1:A:361:ASN:H	1.74	0.52
1:A:279:VAL:O	1:A:282:VAL:HG13	2.10	0.52
1:D:375:SER:HB3	1:D:404:PHE:CE1	2.44	0.52
1:D:248:LYS:HD2	1:D:255:ARG:HH12	1.75	0.52
1:D:262:VAL:HG13	1:D:303:VAL:HG22	1.91	0.52
1:B:242:LEU:HD13	1:B:336:ILE:HG12	1.91	0.52
1:D:417:TRP:CZ3	1:D:441:LEU:CD1	2.93	0.51
1:B:405:PHE:CD1	1:B:405:PHE:C	2.84	0.51
1:D:375:SER:HB3	1:D:404:PHE:CD1	2.45	0.51
1:A:430:GLU:HG3	1:A:431:ALA:N	2.26	0.51
1:D:372:PHE:CE1	1:D:405:PHE:HA	2.46	0.51
1:C:442:SER:CB	1:C:443:LEU:HB3	2.41	0.51
1:A:272:GLU:O	1:A:325:ASN:ND2	2.43	0.51
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.93	0.51
1:B:248:LYS:HD2	1:B:255:ARG:NH1	2.23	0.50
1:C:295:GLN:N	1:C:299:THR:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:PHE:O	1:D:441:LEU:N	2.45	0.50
1:B:375:SER:HB3	1:B:404:PHE:CD1	2.47	0.50
1:A:328:LEU:HD23	1:A:329:PRO:HD2	1.90	0.49
1:A:340:LYS:N	1:A:340:LYS:HD2	2.15	0.49
1:A:356:ASP:OD1	1:A:356:ASP:N	2.45	0.49
1:C:374:PRO:O	1:C:429:HIS:HE1	1.94	0.49
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.94	0.49
1:A:295:GLN:N	1:A:299:THR:O	2.45	0.49
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.47	0.49
1:B:360:LYS:HD2	1:B:361:ASN:H	1.77	0.49
1:A:328:LEU:CD2	1:A:329:PRO:CD	2.70	0.49
1:D:360:LYS:HD2	1:D:361:ASN:OD1	2.12	0.49
1:C:441:LEU:O	1:C:442:SER:O	2.31	0.48
1:C:341:GLY:HA3	1:C:373:TYR:CE1	2.48	0.48
1:C:238:PRO:HB3	1:C:265:ASP:O	2.13	0.48
1:D:356:ASP:OD1	1:D:356:ASP:N	2.46	0.48
1:C:430:GLU:HG3	1:C:431:ALA:N	2.28	0.48
1:B:375:SER:HB3	1:B:404:PHE:CE1	2.48	0.48
1:B:328:LEU:HA	1:B:329:PRO:HD2	1.73	0.48
1:C:317:LYS:HB3	1:C:319:TYR:CE1	2.48	0.48
1:A:328:LEU:C	1:A:328:LEU:CD1	2.76	0.48
1:A:372:PHE:CE1	1:A:405:PHE:HA	2.49	0.48
1:D:256:THR:O	1:D:258:GLU:HG3	2.14	0.47
1:C:443:LEU:C	1:C:443:LEU:HD22	2.34	0.47
1:D:278:TYR:CE2	1:D:283:GLU:HB2	2.49	0.47
1:B:256:THR:O	1:B:258:GLU:HG3	2.14	0.47
1:A:253:ILE:HG22	1:C:314:LEU:HD22	1.96	0.47
1:D:430:GLU:HG3	1:D:431:ALA:N	2.29	0.47
1:C:372:PHE:HE1	1:C:405:PHE:HA	1.79	0.47
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.96	0.47
1:C:279:VAL:O	1:C:282:VAL:HG13	2.15	0.47
1:C:309:LEU:HD22	2:C:22:HOH:O	2.15	0.47
1:C:368:LEU:HD13	1:C:407:TYR:CZ	2.49	0.47
1:B:429:HIS:CD2	1:B:431:ALA:H	2.33	0.47
1:A:278:TYR:CE2	1:A:283:GLU:HB2	2.49	0.47
1:D:430:GLU:HG3	1:D:431:ALA:H	1.79	0.46
1:B:295:GLN:HB2	1:B:301:ARG:HB2	1.98	0.46
1:B:317:LYS:HB3	1:B:319:TYR:HE1	1.76	0.46
1:B:374:PRO:O	1:B:429:HIS:HE1	1.98	0.46
1:C:400:SER:HB3	1:D:392:LYS:NZ	2.31	0.46
1:D:444:SER:OG	1:D:444:SER:O	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HG	1:B:307:THR:O	2.15	0.46
1:A:360:LYS:O	1:A:414:LYS:NZ	2.43	0.46
1:D:328:LEU:HA	1:D:329:PRO:HD2	1.74	0.45
1:C:306:LEU:HG	1:C:307:THR:O	2.15	0.45
1:C:278:TYR:HB2	1:C:320:LYS:HB3	1.99	0.45
1:B:309:LEU:HB2	1:B:312:ASP:CG	2.36	0.45
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.52	0.45
1:A:374:PRO:O	1:A:429:HIS:HE1	1.99	0.45
1:D:406:LEU:HD12	1:D:406:LEU:C	2.38	0.45
1:B:430:GLU:HG3	1:B:431:ALA:H	1.82	0.44
1:A:262:VAL:HG13	1:A:303:VAL:HG22	1.98	0.44
1:D:312:ASP:O	1:D:317:LYS:HB2	2.17	0.44
1:B:295:GLN:O	1:B:295:GLN:HG3	2.17	0.44
1:C:248:LYS:HD2	1:C:255:ARG:HH12	1.82	0.44
1:C:328:LEU:CD1	1:C:328:LEU:C	2.78	0.44
1:C:309:LEU:O	1:C:310:HIS:C	2.56	0.44
1:B:355:ARG:N	1:B:355:ARG:NE	2.57	0.44
1:B:372:PHE:CE1	1:B:405:PHE:HA	2.53	0.44
1:C:329:PRO:HB2	1:C:330:ALA:H	1.63	0.44
1:A:295:GLN:O	1:A:298:SER:N	2.51	0.44
1:C:406:LEU:HD12	1:C:406:LEU:C	2.37	0.44
1:D:329:PRO:HB2	1:D:330:ALA:H	1.64	0.44
1:B:356:ASP:N	1:B:356:ASP:OD1	2.50	0.44
1:C:356:ASP:OD1	1:C:356:ASP:N	2.51	0.44
1:A:328:LEU:HD11	1:A:330:ALA:C	2.39	0.43
1:D:248:LYS:HD2	1:D:255:ARG:NH1	2.32	0.43
1:A:256:THR:O	1:A:258:GLU:HG3	2.18	0.43
1:C:413:ASP:O	1:C:414:LYS:C	2.56	0.43
1:D:295:GLN:CG	1:D:295:GLN:O	2.66	0.43
1:D:417:TRP:HZ3	1:D:441:LEU:CD1	2.31	0.43
1:D:288:LYS:HB2	1:D:288:LYS:HE2	1.85	0.43
1:C:328:LEU:HD21	1:C:330:ALA:O	2.19	0.43
1:B:262:VAL:HG13	1:B:303:VAL:HG22	2.00	0.43
1:C:355:ARG:NE	1:C:355:ARG:N	2.52	0.43
1:A:417:TRP:CZ3	1:A:442:SER:HB3	2.54	0.43
1:B:278:TYR:CE2	1:B:283:GLU:HB2	2.54	0.43
1:A:372:PHE:HE1	1:A:405:PHE:HA	1.84	0.43
1:D:439:LYS:HA	1:D:439:LYS:HE3	2.00	0.43
1:C:340:LYS:HB2	1:C:340:LYS:HE3	1.41	0.43
1:A:248:LYS:HD2	1:A:255:ARG:NH1	2.33	0.43
1:C:256:THR:O	1:C:258:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:HA	1:A:414:LYS:NZ	2.34	0.43
1:C:242:LEU:HD13	1:C:336:ILE:HG23	2.00	0.43
1:C:297:ASN:O	1:C:297:ASN:OD1	2.36	0.42
1:C:351:LEU:HB2	1:C:366:THR:HB	2.00	0.42
1:C:375:SER:HB3	1:C:404:PHE:CD1	2.54	0.42
1:A:355:ARG:N	1:A:355:ARG:NE	2.50	0.42
1:A:351:LEU:HB2	1:A:366:THR:HB	2.00	0.42
1:D:421:ASN:C	1:D:442:SER:CB	2.85	0.42
1:B:439:LYS:HA	1:B:439:LYS:HE3	2.01	0.42
1:A:329:PRO:HB2	1:A:330:ALA:H	1.60	0.42
1:C:443:LEU:HD22	1:C:444:SER:C	2.40	0.42
1:B:417:TRP:CZ3	1:B:442:SER:HB3	2.55	0.42
1:A:413:ASP:O	1:A:414:LYS:C	2.58	0.42
1:C:277:TRP:O	1:C:283:GLU:HA	2.20	0.42
1:D:374:PRO:O	1:D:429:HIS:HE1	2.03	0.42
1:D:417:TRP:CH2	1:D:441:LEU:CD1	3.00	0.42
1:D:266:VAL:HB	1:D:300:TYR:HB2	2.01	0.42
1:B:295:GLN:O	1:B:296:TYR:HB2	2.20	0.42
1:D:422:VAL:HG22	1:D:442:SER:HG	1.75	0.41
1:D:443:LEU:CG	1:D:444:SER:N	2.59	0.41
1:D:360:LYS:HD2	1:D:361:ASN:N	2.35	0.41
1:C:395:PRO:HA	1:C:396:PRO:HD3	1.91	0.41
1:A:259:VAL:CG1	1:A:260:THR:N	2.82	0.41
1:C:292:ARG:HB3	1:C:302:VAL:HG22	2.02	0.41
1:A:251:LEU:C	1:C:253:ILE:HD11	2.38	0.41
1:C:368:LEU:HD13	1:C:407:TYR:CE1	2.56	0.41
1:C:367:CYS:HB2	1:C:381:TRP:CZ2	2.56	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.56	0.41
1:A:340:LYS:N	1:A:340:LYS:CD	2.77	0.41
1:D:309:LEU:HB2	1:D:312:ASP:CG	2.40	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.91	0.41
1:D:395:PRO:HA	1:D:396:PRO:HD3	1.91	0.41
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.98	0.41
1:C:443:LEU:HD13	1:C:444:SER:N	2.36	0.41
1:D:275:PHE:CE1	1:D:304:SER:HB2	2.56	0.41
1:A:306:LEU:HG	1:A:307:THR:O	2.21	0.41
1:A:248:LYS:N	2:A:20:HOH:O	2.38	0.41
1:D:372:PHE:HE1	1:D:405:PHE:HA	1.84	0.41
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.56	0.41
1:C:409:LYS:HB2	1:D:407:TYR:OH	2.21	0.40
1:A:406:LEU:C	1:A:406:LEU:HD12	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PRO:HG3	1:B:406:LEU:HD23	2.03	0.40
1:B:338:LYS:HE3	1:B:430:GLU:OE2	2.21	0.40
1:D:355:ARG:NE	1:D:355:ARG:N	2.55	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	206/227 (91%)	181 (88%)	24 (12%)	1 (0%)	34	74
1	B	205/227 (90%)	182 (89%)	20 (10%)	3 (2%)	13	48
1	C	206/227 (91%)	181 (88%)	22 (11%)	3 (2%)	13	48
1	D	205/227 (90%)	182 (89%)	17 (8%)	6 (3%)	6	30
All	All	822/908 (90%)	726 (88%)	83 (10%)	13 (2%)	12	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
1	B	297	ASN
1	B	329	PRO
1	C	329	PRO
1	C	442	SER
1	D	297	ASN
1	D	329	PRO
1	C	443	LEU
1	D	296	TYR
1	D	443	LEU
1	B	296	TYR
1	D	431	ALA

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Mol	Chain	Res	Type
1	D	441	LEU

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	193/210 (92%)	165 (86%)	28 (14%)	4	17
1	B	192/210 (91%)	167 (87%)	25 (13%)	5	21
1	C	194/210 (92%)	166 (86%)	28 (14%)	4	17
1	D	194/210 (92%)	170 (88%)	24 (12%)	6	23
All	All	773/840 (92%)	668 (86%)	105 (14%)	5	20

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	256	THR
1	A	260	THR
1	A	261	CYS
1	A	282	VAL
1	A	284	VAL
1	A	288	LYS
1	A	289	THR
1	A	292	ARG
1	A	298	SER
1	A	317	LYS
1	A	328	LEU
1	A	337	SER
1	A	340	LYS
1	A	342	GLN
1	A	345	GLU
1	A	347	GLN
1	A	355	ARG
1	A	360	LYS
1	A	382	GLU

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Mol	Chain	Res	Type
1	A	415	SER
1	A	419	GLN
1	A	421	ASN
1	A	439	LYS
1	A	440	SER
1	A	441	LEU
1	A	442	SER
1	A	443	LEU
1	B	242	LEU
1	B	256	THR
1	B	260	THR
1	B	282	VAL
1	B	284	VAL
1	B	288	LYS
1	B	289	THR
1	B	292	ARG
1	B	317	LYS
1	B	328	LEU
1	B	337	SER
1	B	340	LYS
1	B	342	GLN
1	B	345	GLU
1	B	347	GLN
1	B	355	ARG
1	B	360	LYS
1	B	361	ASN
1	B	382	GLU
1	B	415	SER
1	B	419	GLN
1	B	439	LYS
1	B	440	SER
1	B	441	LEU
1	B	442	SER
1	C	242	LEU
1	C	256	THR
1	C	260	THR
1	C	261	CYS
1	C	265	ASP
1	C	282	VAL
1	C	284	VAL
1	C	288	LYS
1	C	292	ARG

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Mol	Chain	Res	Type
1	C	298	SER
1	C	317	LYS
1	C	328	LEU
1	C	337	SER
1	C	340	LYS
1	C	342	GLN
1	C	345	GLU
1	C	347	GLN
1	C	355	ARG
1	C	360	LYS
1	C	361	ASN
1	C	382	GLU
1	C	415	SER
1	C	419	GLN
1	C	421	ASN
1	C	439	LYS
1	C	441	LEU
1	C	442	SER
1	C	443	LEU
1	D	242	LEU
1	D	256	THR
1	D	260	THR
1	D	265	ASP
1	D	282	VAL
1	D	288	LYS
1	D	289	THR
1	D	292	ARG
1	D	317	LYS
1	D	328	LEU
1	D	337	SER
1	D	340	LYS
1	D	342	GLN
1	D	345	GLU
1	D	347	GLN
1	D	355	ARG
1	D	360	LYS
1	D	382	GLU
1	D	388	GLU
1	D	415	SER
1	D	419	GLN
1	D	439	LYS
1	D	440	SER

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Mol	Chain	Res	Type
1	D	444	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	315	ASN
1	A	429	HIS
1	A	434	ASN
1	B	276	ASN
1	B	315	ASN
1	B	429	HIS
1	B	434	ASN
1	C	276	ASN
1	C	315	ASN
1	C	419	GLN
1	C	429	HIS
1	C	434	ASN
1	D	276	ASN
1	D	315	ASN
1	D	429	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

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	208/227 (91%)	0.04	1 (0%) 91 84	67, 87, 111, 124	6 (2%)
1	B	207/227 (91%)	0.04	7 (3%) 49 25	67, 88, 113, 125	5 (2%)
1	C	208/227 (91%)	0.00	0 100 100	67, 87, 111, 124	6 (2%)
1	D	207/227 (91%)	0.08	7 (3%) 49 25	67, 88, 113, 125	5 (2%)
All	All	830/908 (91%)	0.04	15 (1%) 71 51	67, 88, 113, 125	22 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	TYR	3.4
1	D	273	VAL	3.2
1	B	293	GLU	3.1
1	B	298	SER	2.9
1	D	300	TYR	2.7
1	D	293	GLU	2.6
1	D	324	SER	2.6
1	B	294	GLU	2.5
1	D	301	ARG	2.5
1	A	274	LYS	2.4
1	D	327	ALA	2.4
1	B	273	VAL	2.2
1	B	272	GLU	2.2
1	D	325	ASN	2.1
1	B	275	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.