



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:07 AM UTC

PDB ID : 4K2C / pdb_00004k2c
Title : HSA Ligand Free
Authors : Wang, Y.; Luo, Z.; Shi, X.; Huang, M.
Deposited on : 2013-04-08
Resolution : 3.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

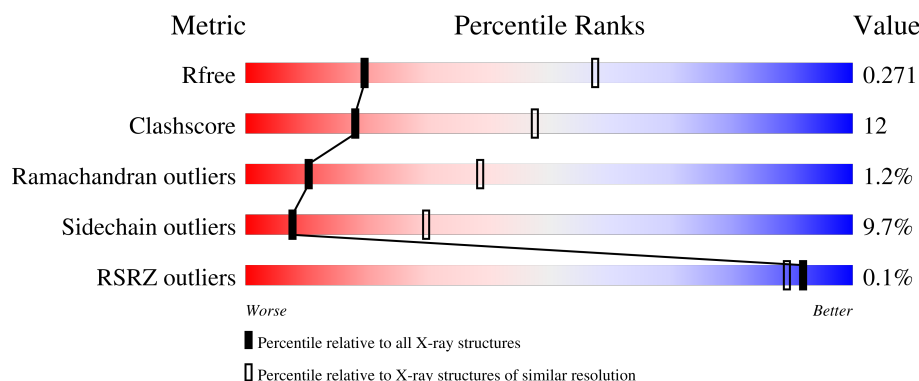
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	585	 65% 30% . .
1	B	585	 64% 32% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9182 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.

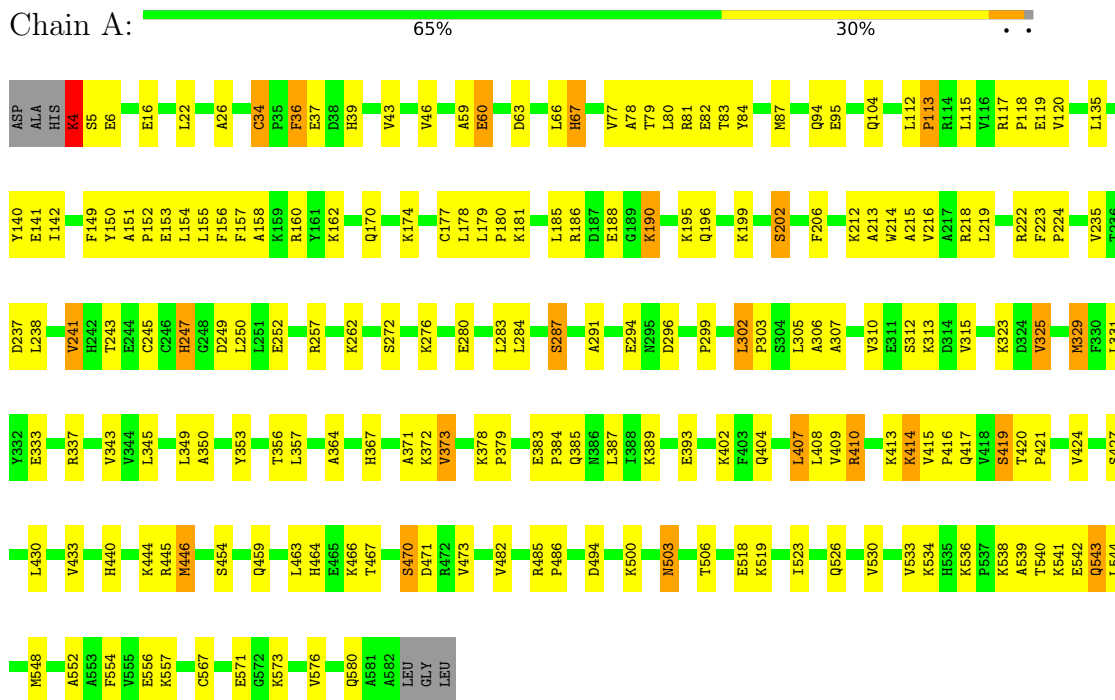
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4591	2898	775	877	41			
1	B	579	Total	C	N	O	S	0	0	0
			4591	2898	775	877	41			

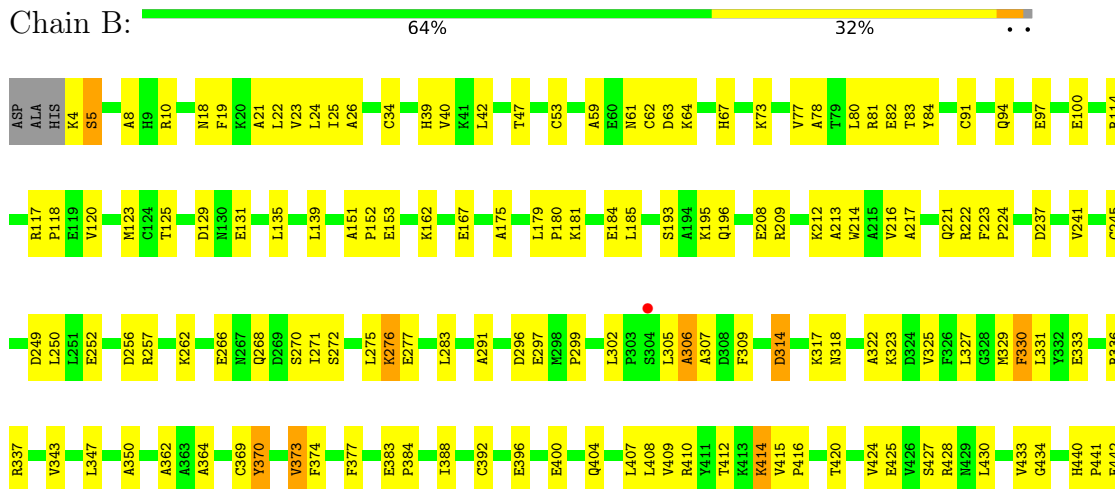
3 Residue-property plots

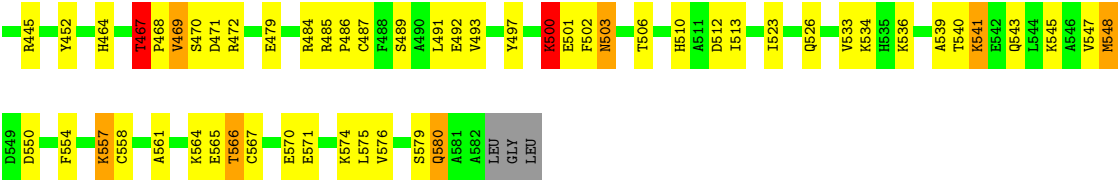
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serum albumin



• Molecule 1: Serum albumin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.41Å 179.89Å 57.46Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	47.70 – 3.23 47.70 – 3.23	Depositor EDS
% Data completeness (in resolution range)	80.0 (47.70-3.23) 79.9 (47.70-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.01Å)	Xtriage
Refinement program	CNS, REFMAC 5.7.0032	Depositor
R, R_{free}	0.213 , 0.265 0.231 , 0.271	Depositor DCC
R_{free} test set	975 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	90.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for l,k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9182	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.78	0/4680	1.06	6/6316 (0.1%)
1	B	0.73	0/4680	1.03	4/6316 (0.1%)
All	All	0.75	0/9360	1.05	10/12632 (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
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	THR	CA-C-N	8.25	130.15	119.84
1	B	467	THR	C-N-CA	8.25	130.15	119.84
1	A	36	PHE	N-CA-C	7.75	120.70	111.33
1	A	95	GLU	N-CA-C	6.67	117.27	109.60
1	A	500	LYS	N-CA-C	6.42	119.74	108.56
1	A	241	VAL	N-CA-C	-6.01	104.77	110.42
1	B	500	LYS	N-CA-C	5.84	118.27	108.23
1	B	373	VAL	N-CA-C	5.42	115.62	110.53
1	A	78	ALA	N-CA-C	-5.10	106.89	113.01
1	A	16	GLU	N-CA-C	5.09	117.21	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	LYS	Peptide
1	B	4	LYS	Peptide
1	B	500	LYS	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	4591	0	4494	104	0
1	B	4591	0	4494	118	0
All	All	9182	0	8988	222	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 12.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HB2	1:A:84:TYR:HE2	1.46	0.81
1:B:151:ALA:HB2	1:B:250:LEU:HD22	1.65	0.78
1:B:302:LEU:HD13	1:B:337:ARG:HG2	1.67	0.77
1:A:299:PRO:HB2	1:A:302:LEU:HD21	1.66	0.76
1:A:222:ARG:NH1	1:A:291:ALA:O	2.20	0.75
1:A:536:LYS:O	1:A:540:THR:HG21	1.86	0.74
1:B:424:VAL:O	1:B:428:ARG:HG3	1.86	0.74
1:B:305:LEU:HB2	1:B:374:PHE:HZ	1.51	0.74
1:A:503:ASN:HB3	1:A:506:THR:OG1	1.88	0.74
1:B:536:LYS:HE3	1:B:539:ALA:HB3	1.70	0.73
1:B:550:ASP:OD2	1:B:575:LEU:HD13	1.89	0.73
1:B:5:SER:HA	1:B:62:CYS:O	1.89	0.72
1:B:567:CYS:HB2	1:B:571:GLU:HG2	1.71	0.71
1:B:567:CYS:HA	1:B:570:GLU:HB2	1.73	0.69
1:B:333:GLU:O	1:B:336:ARG:HG2	1.92	0.69
1:B:8:ALA:HB2	1:B:53:CYS:HB2	1.76	0.67
1:B:196:GLN:NE2	1:B:196:GLN:HA	2.09	0.67
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.77	0.66
1:B:80:LEU:O	1:B:83:THR:N	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.77	0.65
1:B:392:CYS:O	1:B:396:GLU:HG2	1.98	0.63
1:A:80:LEU:HB2	1:A:84:TYR:CE2	2.30	0.63
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.80	0.63
1:A:410:ARG:O	1:A:414:LYS:HB2	1.99	0.63
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.81	0.62
1:A:303:PRO:O	1:A:337:ARG:NH1	2.33	0.62
1:A:567:CYS:HA	1:A:571:GLU:HG2	1.81	0.61
1:B:330:PHE:C	1:B:330:PHE:CD2	2.78	0.61
1:A:430:LEU:O	1:A:433:VAL:HG12	2.00	0.61
1:A:541:LYS:CB	1:A:543:GLN:HE21	2.14	0.61
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.84	0.60
1:B:576:VAL:O	1:B:580:GLN:HB2	2.02	0.60
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.35	0.59
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.84	0.59
1:A:196:GLN:NE2	1:A:199:LYS:HD2	2.17	0.59
1:B:213:ALA:HB1	1:B:347:LEU:CD2	2.32	0.59
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.18	0.58
1:B:217:ALA:HB3	1:B:343:VAL:HG13	1.84	0.58
1:A:34:CYS:HB3	1:A:39:HIS:NE2	2.18	0.58
1:B:430:LEU:O	1:B:433:VAL:HG12	2.02	0.58
1:A:39:HIS:O	1:A:43:VAL:HG23	2.04	0.58
1:B:566:THR:HG22	1:B:570:GLU:HG3	1.84	0.58
1:B:503:ASN:HD22	1:B:506:THR:CB	2.15	0.58
1:B:554:PHE:CB	1:B:575:LEU:HD11	2.34	0.57
1:A:5:SER:HA	1:A:63:ASP:HA	1.85	0.57
1:B:262:LYS:HG2	1:B:266:GLU:OE2	2.05	0.57
1:A:413:LYS:HG3	1:A:533:VAL:HG11	1.87	0.57
1:A:503:ASN:HD22	1:A:506:THR:CB	2.18	0.57
1:B:305:LEU:HB2	1:B:374:PHE:CZ	2.36	0.57
1:A:367:HIS:O	1:A:371:ALA:HB2	2.05	0.56
1:B:433:VAL:HG23	1:B:452:TYR:HD2	1.71	0.56
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.88	0.55
1:B:547:VAL:HG11	1:B:579:SER:HA	1.88	0.55
1:B:503:ASN:HD22	1:B:506:THR:HB	1.71	0.55
1:A:115:LEU:HD22	1:A:141:GLU:HB3	1.89	0.55
1:A:243:THR:O	1:A:247:HIS:HB2	2.06	0.54
1:A:413:LYS:HG3	1:A:533:VAL:CG1	2.36	0.54
1:A:177:CYS:O	1:A:181:LYS:HG3	2.07	0.54
1:B:305:LEU:O	1:B:306:ALA:C	2.51	0.54
1:A:120:VAL:HG13	1:A:178:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ALA:HB1	1:B:347:LEU:HD22	1.89	0.54
1:A:212:LYS:O	1:A:216:VAL:HG23	2.07	0.54
1:B:222:ARG:NH1	1:B:291:ALA:O	2.40	0.53
1:B:117:ARG:HB2	1:B:123:MET:CE	2.38	0.53
1:B:510:HIS:HB2	1:B:512:ASP:OD1	2.09	0.53
1:A:552:ALA:O	1:A:556:GLU:HG2	2.08	0.53
1:A:120:VAL:HG13	1:A:178:LEU:CD2	2.38	0.53
1:B:80:LEU:O	1:B:82:GLU:N	2.42	0.53
1:A:503:ASN:HD22	1:A:506:THR:HG21	1.74	0.53
1:A:67:HIS:NE2	1:A:249:ASP:OD1	2.41	0.53
1:A:4:LYS:O	1:A:5:SER:HB3	2.10	0.52
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.90	0.52
1:B:416:PRO:O	1:B:534:LYS:HE2	2.09	0.52
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.90	0.52
1:A:503:ASN:HB2	1:A:506:THR:HB	1.90	0.52
1:A:353:TYR:HD1	1:A:373:VAL:HG11	1.75	0.52
1:A:503:ASN:CB	1:A:506:THR:OG1	2.56	0.52
1:A:312:SER:O	1:A:315:VAL:HG23	2.10	0.52
1:B:94:GLN:O	1:B:97:GLU:HB2	2.10	0.52
1:B:117:ARG:HB2	1:B:123:MET:HE3	1.92	0.52
1:B:558:CYS:HA	1:B:561:ALA:HB2	1.91	0.51
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.92	0.51
1:A:329:MET:O	1:A:333:GLU:HG2	2.11	0.51
1:A:385:GLN:HG3	1:A:446:MET:HE2	1.92	0.51
1:B:67:HIS:CE1	1:B:249:ASP:OD1	2.63	0.51
1:B:217:ALA:CB	1:B:343:VAL:HG13	2.41	0.51
1:B:468:PRO:O	1:B:469:VAL:HG23	2.09	0.50
1:B:302:LEU:HD13	1:B:337:ARG:CG	2.39	0.50
1:A:257:ARG:CZ	1:A:287:SER:HB3	2.42	0.50
1:B:125:THR:O	1:B:129:ASP:HB2	2.12	0.50
1:A:345:LEU:O	1:A:349:LEU:HG	2.11	0.50
1:B:118:PRO:HD2	1:B:123:MET:HE3	1.94	0.50
1:B:314:ASP:O	1:B:318:ASN:HB2	2.12	0.50
1:A:223:PHE:HD1	1:A:272:SER:HB2	1.77	0.49
1:B:322:ALA:HB1	1:B:325:VAL:HB	1.93	0.49
1:B:325:VAL:O	1:B:329:MET:HB2	2.12	0.49
1:A:218:ARG:HD3	1:A:343:VAL:CG2	2.43	0.49
1:B:213:ALA:O	1:B:214:TRP:C	2.54	0.49
1:B:384:PRO:O	1:B:388:ILE:HG12	2.12	0.49
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.48	0.49
1:A:419:SER:OG	1:A:421:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLN:O	1:B:224:PRO:HD3	2.13	0.48
1:B:272:SER:HB3	1:B:275:LEU:HD11	1.94	0.48
1:A:59:ALA:O	1:A:60:GLU:C	2.57	0.48
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.95	0.48
1:B:333:GLU:HA	1:B:336:ARG:CD	2.43	0.48
1:B:414:LYS:HG3	1:B:491:LEU:HB3	1.95	0.48
1:B:135:LEU:HD11	1:B:162:LYS:HG3	1.94	0.48
1:A:356:THR:HG21	1:A:373:VAL:CG2	2.44	0.48
1:B:212:LYS:O	1:B:216:VAL:HG23	2.14	0.48
1:A:416:PRO:O	1:A:534:LYS:HE3	2.13	0.48
1:B:309:PHE:CZ	1:B:330:PHE:HA	2.49	0.47
1:B:10:ARG:CZ	1:B:252:GLU:HB3	2.44	0.47
1:A:218:ARG:HD3	1:A:343:VAL:HG21	1.96	0.47
1:A:215:ALA:HB3	1:A:235:VAL:HG13	1.96	0.47
1:A:356:THR:HG21	1:A:373:VAL:HG22	1.97	0.47
1:B:467:THR:HA	1:B:468:PRO:HD2	1.67	0.47
1:B:554:PHE:HB3	1:B:575:LEU:HD11	1.96	0.47
1:B:327:LEU:O	1:B:330:PHE:HB3	2.14	0.47
1:A:440:HIS:HB3	1:A:444:LYS:HB2	1.96	0.46
1:A:573:LYS:HA	1:A:576:VAL:HG22	1.97	0.46
1:B:412:THR:HG21	1:B:533:VAL:HB	1.96	0.46
1:B:296:ASP:OD1	1:B:297:GLU:N	2.43	0.46
1:A:306:ALA:O	1:A:307:ALA:C	2.58	0.46
1:B:181:LYS:O	1:B:185:LEU:N	2.46	0.46
1:A:36:PHE:HB2	1:A:140:TYR:CE2	2.51	0.46
1:B:557:LYS:O	1:B:561:ALA:HB2	2.15	0.46
1:A:213:ALA:O	1:A:214:TRP:C	2.58	0.46
1:B:374:PHE:HA	1:B:377:PHE:CD2	2.50	0.46
1:A:536:LYS:O	1:A:540:THR:CG2	2.62	0.46
1:A:160:ARG:NH1	1:A:185:LEU:HD23	2.30	0.46
1:A:409:VAL:O	1:A:410:ARG:C	2.59	0.46
1:A:544:LEU:O	1:A:548:MET:N	2.46	0.46
1:B:404:GLN:HA	1:B:407:LEU:HD12	1.99	0.45
1:B:545:LYS:HA	1:B:548:MET:HB3	1.96	0.45
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.41	0.45
1:A:539:ALA:C	1:A:540:THR:HG23	2.42	0.45
1:B:433:VAL:HG13	1:B:434:GLY:N	2.31	0.45
1:A:408:LEU:HD23	1:A:427:SER:HB2	1.98	0.45
1:A:408:LEU:HD23	1:A:427:SER:CB	2.45	0.45
1:B:484:ARG:O	1:B:487:CYS:HB3	2.17	0.45
1:B:427:SER:O	1:B:430:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:O	1:A:190:LYS:HG3	2.16	0.45
1:B:442:GLU:HA	1:B:445:ARG:HB2	1.97	0.45
1:B:272:SER:HB3	1:B:275:LEU:CD1	2.47	0.45
1:B:369:CYS:SG	1:B:370:TYR:N	2.90	0.45
1:B:18:ASN:O	1:B:19:PHE:C	2.59	0.45
1:B:196:GLN:HA	1:B:196:GLN:HE21	1.81	0.44
1:B:256:ASP:O	1:B:257:ARG:C	2.58	0.44
1:A:276:LYS:O	1:A:280:GLU:HG3	2.17	0.44
1:A:135:LEU:HD11	1:A:162:LYS:HD2	1.98	0.44
1:A:156:PHE:HA	1:A:284:LEU:HD13	2.00	0.44
1:A:179:LEU:N	1:A:180:PRO:HD2	2.33	0.44
1:A:325:VAL:HG12	1:A:329:MET:CE	2.48	0.44
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.99	0.44
1:B:503:ASN:OD1	1:B:503:ASN:N	2.51	0.44
1:B:153:GLU:HG2	1:B:257:ARG:NH2	2.33	0.44
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.99	0.44
1:A:305:LEU:O	1:A:306:ALA:C	2.61	0.44
1:B:21:ALA:O	1:B:24:LEU:HB3	2.18	0.44
1:A:503:ASN:HD22	1:A:506:THR:CG2	2.30	0.43
1:B:19:PHE:O	1:B:23:VAL:HG23	2.18	0.43
1:A:404:GLN:O	1:A:407:LEU:N	2.48	0.43
1:B:80:LEU:HD12	1:B:84:TYR:HE2	1.83	0.43
1:B:78:ALA:HB3	1:B:91:CYS:SG	2.59	0.43
1:A:6:GLU:HB3	1:A:66:LEU:HD21	2.00	0.43
1:A:80:LEU:C	1:A:82:GLU:N	2.76	0.43
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.76	0.43
1:A:420:THR:O	1:A:424:VAL:HG23	2.18	0.43
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.54	0.43
1:A:526:GLN:O	1:A:530:VAL:HG23	2.18	0.43
1:B:433:VAL:CG1	1:B:434:GLY:N	2.81	0.43
1:A:196:GLN:NE2	1:A:196:GLN:HA	2.34	0.43
1:B:80:LEU:HB2	1:B:84:TYR:CD2	2.54	0.43
1:B:276:LYS:HE2	1:B:276:LYS:HB3	1.84	0.43
1:A:157:PHE:O	1:A:158:ALA:C	2.62	0.43
1:B:501:GLU:HB3	1:B:502:PHE:H	1.51	0.43
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.75	0.42
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.01	0.42
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.71	0.42
1:A:152:PRO:O	1:A:155:LEU:HB2	2.19	0.42
1:A:331:LEU:HD13	1:A:350:ALA:HB2	2.01	0.42
1:B:22:LEU:HA	1:B:25:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:VAL:O	1:B:410:ARG:C	2.62	0.42
1:B:428:ARG:HD2	1:B:523:ILE:HG12	2.01	0.42
1:B:333:GLU:HA	1:B:336:ARG:HD2	2.02	0.42
1:B:181:LYS:O	1:B:184:GLU:HB3	2.20	0.42
1:B:503:ASN:HD22	1:B:506:THR:HG21	1.85	0.42
1:A:306:ALA:O	1:A:310:VAL:N	2.44	0.42
1:A:464:HIS:C	1:A:466:LYS:N	2.74	0.42
1:B:541:LYS:H	1:B:543:GLN:HG2	1.84	0.42
1:A:219:LEU:HD12	1:A:235:VAL:HG22	2.01	0.42
1:B:497:TYR:OH	1:B:500:LYS:HG3	2.20	0.42
1:B:503:ASN:HD22	1:B:506:THR:CG2	2.32	0.42
1:A:149:PHE:HD1	1:A:150:TYR:N	2.17	0.42
1:A:179:LEU:HB2	1:A:180:PRO:CD	2.50	0.42
1:A:238:LEU:HD12	1:A:238:LEU:O	2.19	0.42
1:A:470:SER:OG	1:A:473:VAL:HG23	2.20	0.41
1:A:542:GLU:C	1:A:544:LEU:N	2.78	0.41
1:B:61:ASN:HB3	1:B:64:LYS:HE3	2.01	0.41
1:B:306:ALA:O	1:B:307:ALA:C	2.62	0.41
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.91	0.41
1:A:112:LEU:O	1:A:113:PRO:C	2.62	0.41
1:A:153:GLU:O	1:A:154:LEU:C	2.62	0.41
1:A:157:PHE:HE2	1:A:188:GLU:HG2	1.86	0.41
1:A:345:LEU:HD12	1:A:349:LEU:HD21	2.01	0.41
1:A:202:SER:HA	1:A:206:PHE:HD2	1.86	0.41
1:B:268:GLN:HA	1:B:271:ILE:HD12	2.03	0.41
1:A:503:ASN:OD1	1:A:503:ASN:N	2.53	0.41
1:A:518:GLU:O	1:A:519:LYS:C	2.63	0.41
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.61	0.41
1:B:241:VAL:HG22	1:B:256:ASP:HB3	2.02	0.41
1:B:408:LEU:HD11	1:B:526:GLN:HB3	2.03	0.41
1:B:464:HIS:HE1	1:B:470:SER:H	1.69	0.41
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.92	0.41
1:A:237:ASP:O	1:A:241:VAL:HG23	2.20	0.40
1:B:42:LEU:HD22	1:B:73:LYS:HG3	2.03	0.40
1:B:440:HIS:HB3	1:B:441:PRO:HD2	2.03	0.40
1:B:420:THR:O	1:B:424:VAL:HG23	2.21	0.40
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.88	0.40
1:B:299:PRO:O	1:B:302:LEU:HG	2.22	0.40
1:B:472:ARG:H	1:B:472:ARG:HG3	1.74	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	577/585 (99%)	516 (89%)	55 (10%)	6 (1%)	12	42
1	B	577/585 (99%)	516 (89%)	53 (9%)	8 (1%)	9	35
All	All	1154/1170 (99%)	1032 (89%)	108 (9%)	14 (1%)	10	38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	364	ALA
1	A	60	GLU
1	B	81	ARG
1	B	362	ALA
1	B	364	ALA
1	B	469	VAL
1	A	113	PRO
1	A	543	GLN
1	B	5	SER
1	B	400	GLU
1	B	541	LYS
1	A	538	LYS
1	B	306	ALA

5.3.2 Protein sidechains [i](#)

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	503/511 (98%)	449 (89%)	54 (11%)	6	25
1	B	503/511 (98%)	459 (91%)	44 (9%)	9	33
All	All	1006/1022 (98%)	908 (90%)	98 (10%)	8	30

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	34	CYS
1	A	37	GLU
1	A	46	VAL
1	A	67	HIS
1	A	77	VAL
1	A	81	ARG
1	A	83	THR
1	A	87	MET
1	A	94	GLN
1	A	104	GLN
1	A	119	GLU
1	A	142	ILE
1	A	170	GLN
1	A	174	LYS
1	A	190	LYS
1	A	195	LYS
1	A	202	SER
1	A	245	CYS
1	A	247	HIS
1	A	262	LYS
1	A	283	LEU
1	A	287	SER
1	A	294	GLU
1	A	302	LEU
1	A	313	LYS
1	A	323	LYS
1	A	325	VAL
1	A	329	MET
1	A	372	LYS
1	A	373	VAL
1	A	387	LEU
1	A	389	LYS
1	A	393	GLU
1	A	402	LYS

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Mol	Chain	Res	Type
1	A	407	LEU
1	A	410	ARG
1	A	414	LYS
1	A	415	VAL
1	A	419	SER
1	A	445	ARG
1	A	446	MET
1	A	454	SER
1	A	459	GLN
1	A	463	LEU
1	A	467	THR
1	A	470	SER
1	A	471	ASP
1	A	482	VAL
1	A	503	ASN
1	A	523	ILE
1	A	554	PHE
1	A	557	LYS
1	A	580	GLN
1	B	40	VAL
1	B	47	THR
1	B	63	ASP
1	B	77	VAL
1	B	100	GLU
1	B	114	ARG
1	B	131	GLU
1	B	167	GLU
1	B	193	SER
1	B	195	LYS
1	B	208	GLU
1	B	209	ARG
1	B	237	ASP
1	B	245	CYS
1	B	270	SER
1	B	276	LYS
1	B	277	GLU
1	B	283	LEU
1	B	314	ASP
1	B	317	LYS
1	B	323	LYS
1	B	330	PHE
1	B	370	TYR

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Mol	Chain	Res	Type
1	B	373	VAL
1	B	414	LYS
1	B	415	VAL
1	B	425	GLU
1	B	467	THR
1	B	471	ASP
1	B	479	GLU
1	B	489	SER
1	B	492	GLU
1	B	493	VAL
1	B	500	LYS
1	B	503	ASN
1	B	513	ILE
1	B	540	THR
1	B	548	MET
1	B	557	LYS
1	B	564	LYS
1	B	565	GLU
1	B	566	THR
1	B	574	LYS
1	B	580	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	104	GLN
1	A	109	ASN
1	A	130	ASN
1	A	170	GLN
1	A	196	GLN
1	A	247	HIS
1	A	385	GLN
1	A	397	GLN
1	A	503	ASN
1	A	543	GLN
1	B	33	GLN
1	B	67	HIS
1	B	94	GLN
1	B	109	ASN
1	B	128	HIS
1	B	196	GLN

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Mol	Chain	Res	Type
1	B	247	HIS
1	B	367	HIS
1	B	386	ASN
1	B	440	HIS
1	B	503	ASN
1	B	543	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	579/585 (98%)	-0.70	0	100 100	51, 95, 147, 202	0
1	B	579/585 (98%)	-0.61	1 (0%)	91 85	63, 106, 164, 221	0
All	All	1158/1170 (98%)	-0.66	1 (0%)	92 89	51, 100, 159, 221	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.