Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:58 PM GMT

PDB ID	:	4K2C
Title	:	HSA Ligand Free
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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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

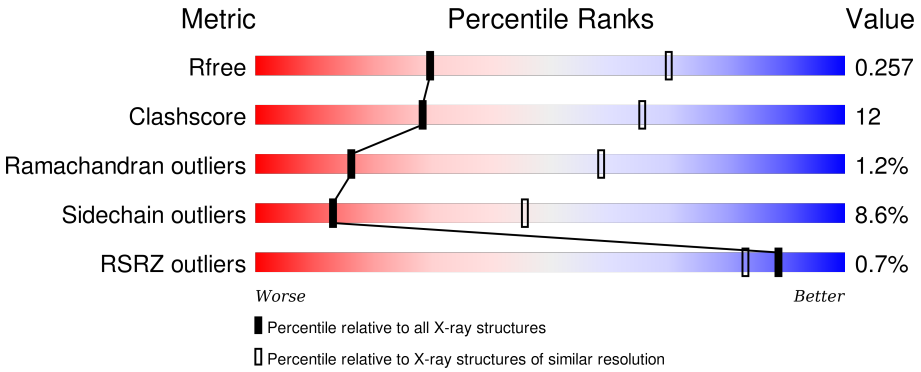
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (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 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 <=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	% 69% 26%
1	B	585	% 66% 30%

2 Entry composition (i)

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.

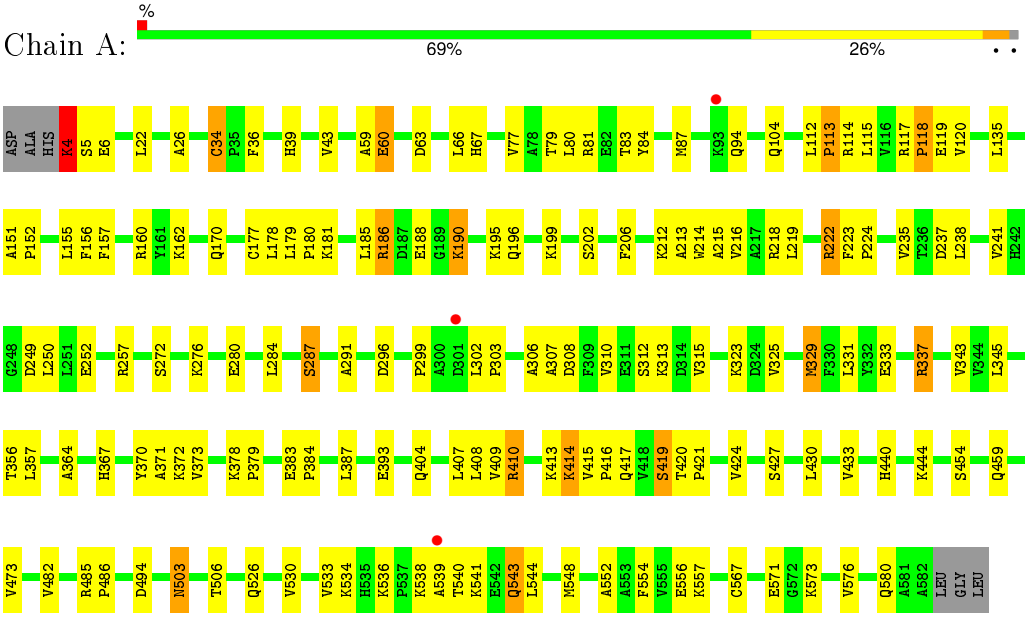
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4591	2898	775	877	41			
1	B	579	Total	C	N	O	S	0	0	0
			4591	2898	775	877	41			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

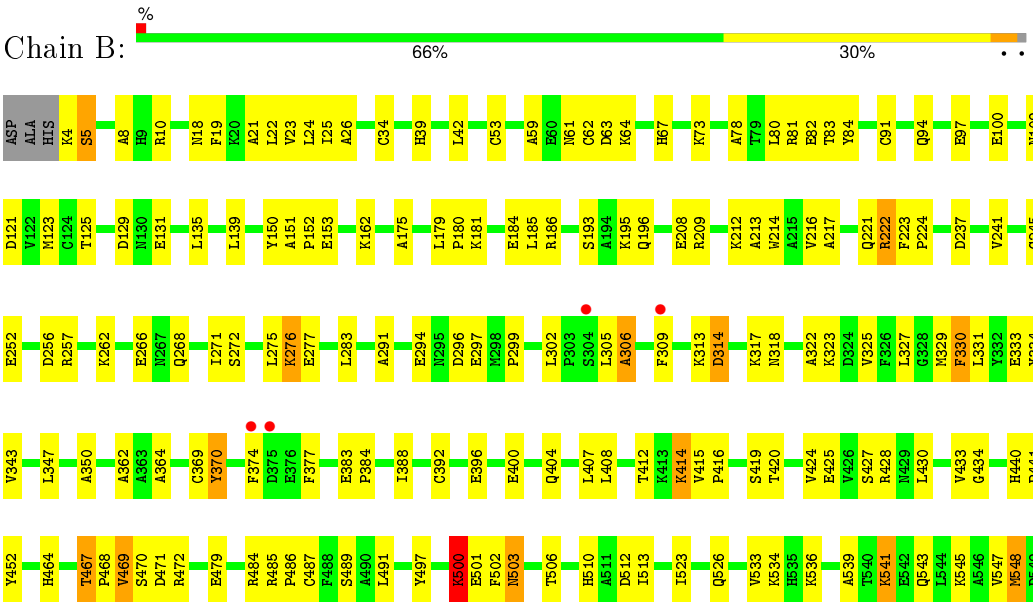
- Molecule 1: Serum albumin

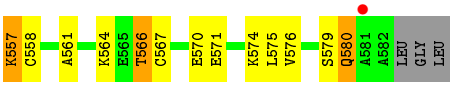
Chain A:



- Molecule 1: Serum albumin

Chain B:




K557
C558
A561
K564
E565
T566
C567
E570
E571
K574
L575
V576
S579
Q580
A581
A582
LEU
GLY
LEU

4 Data and refinement statistics (i)

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 47.65 – 2.99	Depositor EDS
% Data completeness (in resolution range)	80.0 (47.70-3.23) 82.4 (47.65-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.213 , 0.265 0.213 , 0.257	Depositor DCC
R_{free} test set	753 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 18953 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.57	0/4680	0.76	0/6316
1	B	0.53	0/4680	0.72	0/6316
All	All	0.55	0/9360	0.74	0/12632

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.

There are no bond angle outliers.

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	95	0
1	B	4591	0	4494	115	0
All	All	9182	0	8988	210	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 (210) 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:HA	1:B:196:GLN:NE2	2.09	0.67
1:B:80:LEU:O	1:B:83:THR:N	2.19	0.66
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.77	0.66
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.77	0.65
1:B:117:ARG:HB2	1:B:123:MET:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:503:ASN:HD22	1:A:506:THR:CB	2.18	0.57
1:A:413:LYS:HG3	1:A:533:VAL:HG11	1.87	0.57
1:B:305:LEU:HB2	1:B:374:PHE:CZ	2.36	0.57
1:B:330:PHE:C	1:B:330:PHE:CD2	2.78	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:547:VAL:HG11	1:B:579:SER:HA	1.88	0.55
1:B:383:GLU:HB3	1:B:384:PRO:HD3	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:A:120:VAL:HG13	1:A:178:LEU:HD23	1.89	0.54
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:B:80:LEU:O	1:B:82:GLU:N	2.42	0.53
1:A:120:VAL:HG13	1:A:178:LEU:CD2	2.38	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:416:PRO:O	1:B:534:LYS:HE2	2.09	0.52
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ASN:HB2	1:A:506:THR:HB	1.90	0.52
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.90	0.52
1:A:503:ASN:CB	1:A:506:THR:OG1	2.56	0.52
1:A:353:TYR:HD1	1:A:373:VAL:HG11	1.75	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: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: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:314:ASP:O	1:B:318:ASN:HB2	2.12	0.50
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:223:PHE:HD1	1:A:272:SER:HB2	1.77	0.49
1:B:305:LEU:O	1:B:306:ALA:C	2.51	0.49
1:A:218:ARG:HD3	1:A:343:VAL:CG2	2.43	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
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: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: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:A:215:ALA:HB3	1:A:235:VAL:HG13	1.96	0.47
1:B:554:PHE:HB3	1:B:575:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:O	1:B:330:PHE:HB3	2.14	0.47
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:A:440:HIS:HB3	1:A:444:LYS:HB2	1.96	0.46
1:B:296:ASP:OD1	1:B:297:GLU:N	2.43	0.46
1:B:181:LYS:O	1:B:185:LEU:N	2.46	0.46
1:B:557:LYS:O	1:B:561:ALA:HB2	2.15	0.46
1:A:36:PHE:HB2	1:A:140:TYR:CE2	2.51	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:544:LEU:O	1:A:548:MET:N	2.46	0.46
1:A:160:ARG:NH1	1:A:185:LEU:HD23	2.30	0.46
1:B:545:LYS:HA	1:B:548:MET:HB3	1.96	0.45
1:B:404:GLN:HA	1:B:407:LEU:HD12	1.99	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
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:213:ALA:O	1:B:214:TRP:C	2.54	0.45
1:B:196:GLN:HA	1:B:196:GLN:HE21	1.81	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:B:503:ASN:OD1	1:B:503:ASN:N	2.51	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: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:B:179:LEU:HB2	1:B:180:PRO:HD3	1.99	0.44
1:B:153:GLU:HG2	1:B:257:ARG:NH2	2.33	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:A:59:ALA:O	1:A:60:GLU:C	2.57	0.43
1:B:19:PHE:O	1:B:23:VAL:HG23	2.18	0.43
1:B:80:LEU:HD12	1:B:84:TYR:HE2	1.83	0.43
1:A:404:GLN:O	1:A:407:LEU:N	2.48	0.43
1:B:78:ALA:HB3	1:B:91:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HB3	1:A:66:LEU:HD21	2.00	0.43
1:A:357:LEU:HA	1:A:357:LEU:HD23	1.76	0.43
1:A:420:THR:O	1:A:424:VAL:HG23	2.18	0.43
1:B:433:VAL:CG1	1:B:434:GLY:N	2.81	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:80:LEU:HB2	1:B:84:TYR:CD2	2.54	0.43
1:A:196:GLN:NE2	1:A:196:GLN:HA	2.34	0.43
1:B:276:LYS:HB3	1:B:276:LYS:HE2	1.84	0.43
1:B:501:GLU:HB3	1:B:502:PHE:H	1.51	0.43
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.01	0.42
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.75	0.42
1:B:428:ARG:HD2	1:B:523:ILE:HG12	2.01	0.42
1:A:152:PRO:O	1:A:155:LEU:HB2	2.19	0.42
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.71	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
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:B:541:LYS:H	1:B:543:GLN:HG2	1.84	0.42
1:B:503:ASN:HD22	1:B:506:THR:CG2	2.32	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: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:149:PHE:HD1	1:A:150:TYR:N	2.17	0.42
1:A:470:SER:OG	1:A:473:VAL:HG23	2.20	0.41
1:B:61:ASN:HB3	1:B:64:LYS:HE3	2.01	0.41
1:A:306:ALA:O	1:A:307:ALA:C	2.58	0.41
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.91	0.41
1:A:345:LEU:HD12	1:A:349:LEU:HD21	2.01	0.41
1:A:157:PHE:HE2	1:A:188:GLU:HG2	1.86	0.41
1:A:202:SER:HA	1:A:206:PHE:HD2	1.86	0.41
1:A:213:ALA:O	1:A:214:TRP:C	2.58	0.41
1:B:268:GLN:HA	1:B:271:ILE:HD12	2.03	0.41
1:A:503:ASN:N	1:A:503:ASN:OD1	2.53	0.41
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.61	0.41
1:A:409:VAL:O	1:A:410:ARG:C	2.59	0.41
1:B:408:LEU:HD11	1:B:526:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:VAL:HG22	1:B:256:ASP:HB3	2.02	0.41
1:B:256:ASP:O	1:B:257:ARG:C	2.58	0.41
1:B:18:ASN:O	1:B:19:PHE:C	2.59	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:539:ALA:C	1:A:540:THR:HG23	2.42	0.40
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.41	0.40
1:B:42:LEU:HD22	1:B:73:LYS:HG3	2.03	0.40
1:A:237:ASP:O	1:A:241:VAL:HG23	2.20	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:299:PRO:O	1:B:302:LEU:HG	2.22	0.40
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.88	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%)	19	62
1	B	577/585 (99%)	516 (89%)	53 (9%)	8 (1%)	14	55
All	All	1154/1170 (99%)	1032 (89%)	108 (9%)	14 (1%)	16	58

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

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Mol	Chain	Res	Type
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%)	459 (91%)	44 (9%)	13 45
1	B	503/511 (98%)	460 (92%)	43 (8%)	13 46
All	All	1006/1022 (98%)	919 (91%)	87 (9%)	13 46

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	34	CYS
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	114	ARG
1	A	118	PRO
1	A	119	GLU
1	A	140	TYR
1	A	149	PHE

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	186	ARG
1	A	190	LYS
1	A	195	LYS
1	A	222	ARG
1	A	245	CYS
1	A	247	HIS
1	A	287	SER
1	A	308	ASP
1	A	313	LYS
1	A	323	LYS
1	A	329	MET
1	A	337	ARG
1	A	370	TYR
1	A	372	LYS
1	A	387	LEU
1	A	393	GLU
1	A	410	ARG
1	A	414	LYS
1	A	415	VAL
1	A	419	SER
1	A	454	SER
1	A	459	GLN
1	A	467	THR
1	A	470	SER
1	A	471	ASP
1	A	482	VAL
1	A	503	ASN
1	A	554	PHE
1	A	557	LYS
1	A	580	GLN
1	B	63	ASP
1	B	100	GLU
1	B	109	ASN
1	B	121	ASP
1	B	131	GLU
1	B	150	TYR
1	B	186	ARG
1	B	193	SER
1	B	195	LYS
1	B	208	GLU
1	B	209	ARG

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Mol	Chain	Res	Type
1	B	222	ARG
1	B	237	ASP
1	B	245	CYS
1	B	276	LYS
1	B	277	GLU
1	B	283	LEU
1	B	294	GLU
1	B	313	LYS
1	B	314	ASP
1	B	317	LYS
1	B	323	LYS
1	B	330	PHE
1	B	334	TYR
1	B	370	TYR
1	B	414	LYS
1	B	415	VAL
1	B	419	SER
1	B	425	GLU
1	B	467	THR
1	B	471	ASP
1	B	479	GLU
1	B	489	SER
1	B	500	LYS
1	B	503	ASN
1	B	513	ILE
1	B	548	MET
1	B	554	PHE
1	B	557	LYS
1	B	564	LYS
1	B	566	THR
1	B	574	LYS
1	B	580	GLN

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	94	GLN
1	A	104	GLN
1	A	109	ASN
1	A	130	ASN
1	A	196	GLN
1	A	385	GLN

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Mol	Chain	Res	Type
1	A	543	GLN
1	B	67	HIS
1	B	94	GLN
1	B	109	ASN
1	B	128	HIS
1	B	130	ASN
1	B	196	GLN
1	B	221	GLN
1	B	503	ASN
1	B	543	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	-0.69	3 (0%)	91	88	51, 95, 147, 202	0
1	B	579/585 (98%)	-0.58	5 (0%)	85	79	63, 106, 164, 221	0
All	All	1158/1170 (98%)	-0.63	8 (0%)	89	83	51, 100, 159, 221	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	3.8
1	B	309	PHE	3.2
1	B	304	SER	3.2
1	A	93	LYS	2.9
1	B	374	PHE	2.6
1	B	375	ASP	2.4
1	A	301	ASP	2.2
1	B	581	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.