



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 05:52 AM EST

PDB ID : 3AUP
Title : Crystal structure of Basic 7S globulin from soybean
Authors : Yoshizawa, T.; Shimizu, T.; Taichi, M.; Nishiuchi, Y.; Yamabe, M.; Shichijo, N.; Unzai, S.; Hirano, H.; Sato, M.; Hashimoto, H.
Deposited on : 2011-02-14
Resolution : 1.91 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

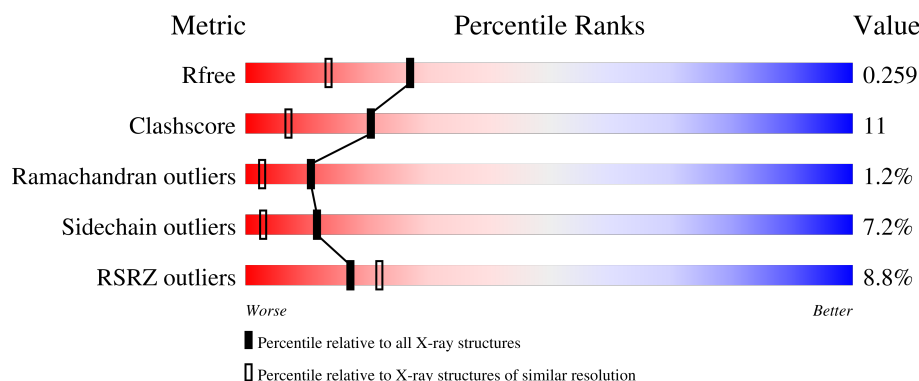
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	403	
1	B	403	
1	C	403	
1	D	403	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11918 atoms, of which 0 are hydrogens and 0 are deuteriums.

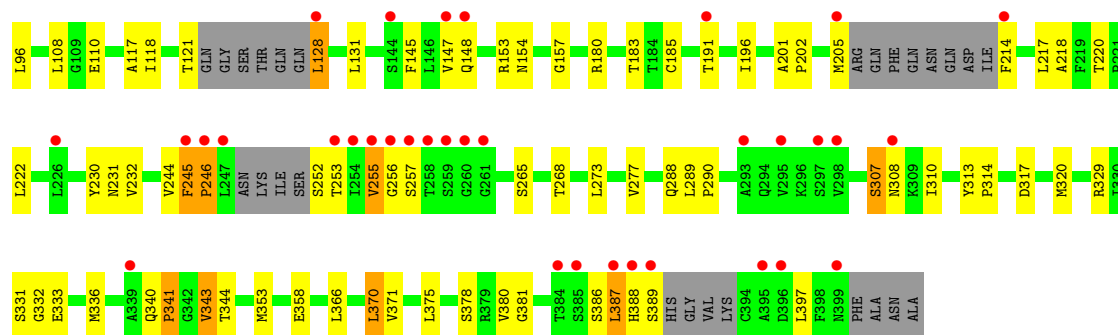
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Basic 7S globulin.

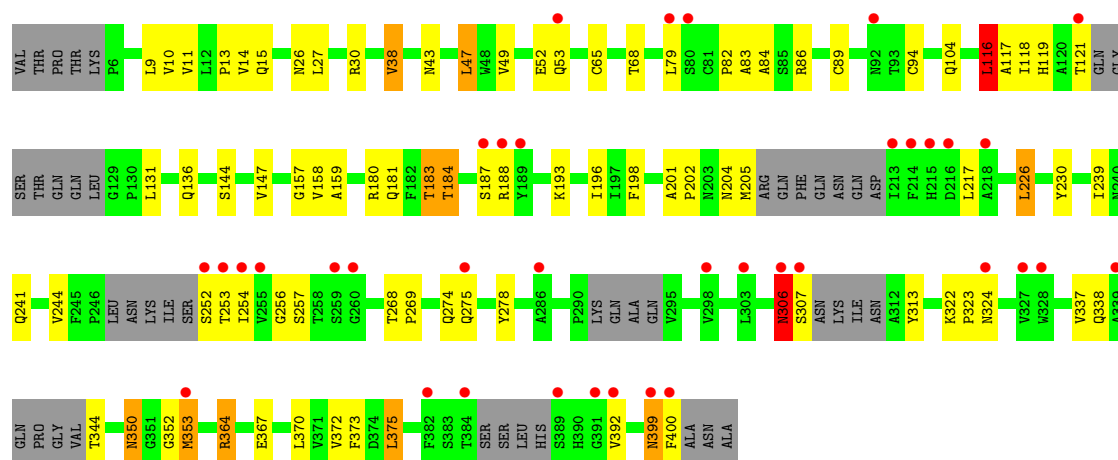
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	133	3	0
			2888	1824	512	531	21			
1	B	372	Total	C	N	O	S	126	2	0
			2842	1796	503	522	21			
1	C	372	Total	C	N	O	S	70	1	0
			2830	1781	503	525	21			
1	D	360	Total	C	N	O	S	96	1	0
			2737	1728	482	506	21			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	180	Total	O	0	0
			180	180		
2	B	163	Total	O	0	0
			163	163		
2	C	170	Total	O	0	0
			170	170		
2	D	108	Total	O	0	0
			108	108		



● Molecule 1: Basic 7S globulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.24Å 161.17Å 84.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.91 20.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.1 (20.00-1.91) 95.4 (20.00-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.255 0.214 , 0.259	Depositor DCC
R_{free} test set	6904 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11918	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.80	2/2961 (0.1%)	0.81	2/4028 (0.0%)
1	B	0.73	0/2913	0.80	1/3965 (0.0%)
1	C	0.71	1/2895 (0.0%)	0.83	3/3939 (0.1%)
1	D	0.67	1/2799 (0.0%)	0.78	1/3805 (0.0%)
All	All	0.73	4/11568 (0.0%)	0.80	7/15737 (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
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	38	VAL	CB-CG1	-7.35	1.37	1.52
1	A	94	CYS	CB-SG	-6.72	1.70	1.82
1	A	110	GLU	CB-CG	-6.55	1.39	1.52
1	D	94	CYS	CB-SG	-6.34	1.71	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	GLN	N-CA-CB	-5.86	100.05	110.60
1	C	245	PHE	C-N-CD	-5.60	108.27	120.60
1	D	116	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	94	CYS	CA-CB-SG	-5.50	104.10	114.00
1	C	47	LEU	CB-CG-CD2	5.07	119.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	CYS	CA-CB-SG	-5.06	104.90	114.00
1	A	70	CYS	CA-CB-SG	-5.01	104.98	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	GLN	Peptide
1	B	52	GLU	Peptide
1	C	245	PHE	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	2888	0	2855	59	0
1	B	2842	0	2814	56	0
1	C	2830	0	2797	65	0
1	D	2737	0	2695	82	0
2	A	180	0	0	5	0
2	B	163	0	0	6	0
2	C	170	0	0	5	0
2	D	108	0	0	9	0
All	All	11918	0	11161	236	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 11.

All (236) 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:B:261:GLY:HA2	2:B:434:HOH:O	1.62	0.99
1:B:183:THR:HG22	1:B:372:VAL:HG22	1.47	0.97
1:D:201:ALA:HB1	1:D:205:MET:HE1	1.47	0.94
1:D:184:THR:HG23	2:D:432:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ASN:C	1:D:399:ASN:HD22	1.77	0.87
1:B:183:THR:CG2	1:B:372:VAL:HG22	2.08	0.83
1:D:201:ALA:HB1	1:D:205:MET:CE	2.08	0.83
1:B:370:LEU:HD22	1:B:387:LEU:HD13	1.62	0.81
1:A:79:LEU:HD13	1:D:252:SER:HB2	1.61	0.81
1:D:79:LEU:CD1	2:D:466:HOH:O	2.28	0.80
1:C:310:ILE:HD12	1:C:310:ILE:O	1.81	0.80
1:B:225:THR:HB	1:D:254:ILE:HD13	1.62	0.78
1:C:255:VAL:HG22	2:C:503:HOH:O	1.82	0.78
1:C:353:MET:HE3	1:D:52:GLU:HG2	1.66	0.78
1:D:10:VAL:HG12	1:D:198:PHE:HB2	1.67	0.77
1:C:313:TYR:OH	1:C:344:THR:HG21	1.88	0.73
1:B:310:ILE:HG21	1:B:313:TYR:CZ	2.23	0.73
1:B:138:LEU:H	1:B:171:GLN:HE22	1.36	0.72
1:C:43:ASN:ND2	1:C:230:TYR:H	1.86	0.72
1:B:10[A]:VAL:CG1	1:B:118:ILE:HD13	2.20	0.71
1:B:27:LEU:HD22	1:B:38:VAL:HG21	1.73	0.71
1:C:10:VAL:CG1	1:C:118:ILE:HD13	2.20	0.70
1:B:183:THR:HG23	2:B:494:HOH:O	1.92	0.69
1:D:350:ASN:ND2	1:D:352:GLY:H	1.91	0.69
1:C:222:LEU:HD13	1:C:380:VAL:CG2	2.23	0.68
1:A:79:LEU:HD13	1:D:252:SER:CB	2.24	0.68
1:A:244:VAL:HG21	1:A:281:PHE:HA	1.77	0.67
1:D:350:ASN:HD22	1:D:352:GLY:H	1.44	0.66
1:C:93:THR:HG22	2:C:715:HOH:O	1.96	0.66
1:D:375:LEU:H	1:D:375:LEU:HD12	1.61	0.66
1:C:54:GLN:H	1:C:54:GLN:NE2	1.94	0.65
1:D:275:GLN:NE2	1:D:353:MET:HG3	2.11	0.65
1:A:226:LEU:HD12	1:B:77:GLN:HB2	1.78	0.65
1:C:222:LEU:HD13	1:C:380:VAL:HG23	1.79	0.64
1:D:10:VAL:HG21	1:D:118:ILE:HG23	1.78	0.64
1:B:362:GLY:O	1:B:366[A]:LEU:HD13	1.97	0.64
1:A:104:GLN:HG2	2:A:652:HOH:O	1.99	0.63
1:D:239:ILE:CD1	1:D:244:VAL:HG21	2.30	0.62
1:D:399:ASN:C	1:D:399:ASN:ND2	2.52	0.62
1:A:38[A]:VAL:HG13	1:A:158:VAL:CA	2.30	0.61
1:A:77:GLN:HE21	1:D:254:ILE:HG12	1.66	0.61
1:A:43:ASN:ND2	1:A:230:TYR:H	1.98	0.61
1:D:375:LEU:HD12	1:D:375:LEU:N	2.16	0.61
1:C:232:VAL:HG21	1:C:320:MET:HE1	1.83	0.61
1:C:307:SER:O	1:C:308:ASN:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLN:HG2	2:D:419:HOH:O	1.99	0.60
1:A:242:HIS:HB2	2:A:658:HOH:O	2.00	0.60
1:B:27:LEU:HD22	1:B:38:VAL:CG2	2.32	0.60
1:B:10[A]:VAL:HG11	1:B:118:ILE:HG21	1.84	0.59
1:C:51:CYS:O	1:C:53:GLN:N	2.33	0.59
1:C:353:MET:HE2	1:D:86:ARG:HD2	1.85	0.59
1:D:183:THR:HG23	2:D:436:HOH:O	2.02	0.59
1:C:65:CYS:HA	1:C:94:CYS:SG	2.43	0.58
1:C:66:HIS:CD2	1:D:256:GLY:HA3	2.39	0.58
1:B:83:ALA:HB3	1:B:89:CYS:SG	2.43	0.58
1:C:90:HIS:HB2	1:C:93:THR:HG21	1.84	0.58
1:C:52:GLU:O	1:C:54:GLN:NE2	2.37	0.57
1:D:183:THR:CG2	2:D:436:HOH:O	2.53	0.57
1:C:332:GLY:O	1:C:336:MET:HG2	2.04	0.57
1:A:38[A]:VAL:HG13	1:A:158:VAL:HA	1.87	0.56
1:D:10:VAL:HG22	1:D:118:ILE:HG12	1.86	0.56
1:B:222:LEU:HD13	1:B:380:VAL:HG23	1.87	0.56
1:D:239:ILE:HD12	1:D:244:VAL:HG21	1.88	0.56
1:D:201:ALA:HB3	1:D:202:PRO:HD3	1.86	0.56
1:D:275:GLN:HE22	1:D:353:MET:HG3	1.70	0.56
1:D:10:VAL:HG21	1:D:118:ILE:CG2	2.36	0.56
1:A:86:ARG:HD2	1:B:353:MET:HE2	1.89	0.55
1:D:322:LYS:HB2	1:D:323:PRO:HD2	1.87	0.55
1:A:38[A]:VAL:CG1	1:A:159:ALA:N	2.70	0.55
1:B:104:GLN:HG2	2:B:596:HOH:O	2.06	0.55
2:A:657:HOH:O	1:C:253:THR:HG21	2.06	0.55
1:C:340:GLN:HB2	1:C:343:VAL:HG13	1.89	0.54
1:D:9:LEU:HD13	1:D:204:ASN:HB2	1.90	0.54
1:C:386:SER:O	1:C:387:LEU:C	2.45	0.54
1:A:128:LEU:HD13	2:A:411:HOH:O	2.06	0.54
1:D:181:GLN:HA	1:D:375:LEU:CD1	2.38	0.54
1:B:233:ARG:HG2	2:B:434:HOH:O	2.07	0.54
1:D:13:PRO:HB2	1:D:193:LYS:HD3	1.88	0.54
1:C:121:THR:HG23	1:C:128:LEU:HD22	1.90	0.54
1:D:226:LEU:O	1:D:226:LEU:HD13	2.07	0.54
1:B:10[A]:VAL:HG13	1:B:118:ILE:HG12	1.90	0.54
1:C:93:THR:HB	2:C:714:HOH:O	2.08	0.54
1:D:38[A]:VAL:HG22	1:D:158:VAL:CA	2.38	0.53
1:A:82:PRO:O	1:A:83:ALA:HB2	2.09	0.53
1:C:340:GLN:HB3	1:C:341:PRO:HD2	1.91	0.53
1:C:340:GLN:HB2	1:C:343:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ASN:O	1:D:307:SER:CB	2.57	0.53
1:C:255:VAL:O	1:C:257:SER:N	2.41	0.53
1:B:10[A]:VAL:HG12	1:B:118:ILE:HD13	1.89	0.52
1:A:216:ASP:HB3	1:A:384:THR:HG22	1.91	0.52
1:D:47:LEU:HD23	1:D:159:ALA:HA	1.90	0.52
1:D:184:THR:CG2	2:D:432:HOH:O	2.46	0.52
1:D:201:ALA:CB	1:D:205:MET:HE1	2.30	0.52
1:D:14:VAL:HG21	1:D:196:ILE:CD1	2.39	0.52
1:B:400:PHE:O	1:B:401:ALA:HB2	2.10	0.52
1:B:10[A]:VAL:CG1	1:B:118:ILE:CD1	2.88	0.51
1:C:45:ASN:HB3	2:C:450:HOH:O	2.10	0.51
1:B:117:ALA:HB1	1:B:131:LEU:HG	1.93	0.51
1:C:205:MET:CE	1:C:397:LEU:HD22	2.40	0.51
1:D:79:LEU:HD11	2:D:466:HOH:O	2.03	0.51
1:B:43:ASN:ND2	1:B:230:TYR:H	2.09	0.51
1:A:104:GLN:HE21	1:A:356:ARG:HH21	1.59	0.51
1:D:322:LYS:HB2	1:D:323:PRO:CD	2.41	0.51
1:D:337:VAL:HG12	1:D:338:GLN:N	2.26	0.51
1:D:252:SER:N	2:D:409:HOH:O	2.43	0.51
1:C:340:GLN:HB3	1:C:341:PRO:CD	2.41	0.50
1:A:86:ARG:HD2	1:B:353:MET:CE	2.41	0.50
1:A:240:ASN:HD21	1:A:314:PRO:HA	1.77	0.50
1:A:29:LYS:HB2	1:A:30:ARG:HG3	1.92	0.50
1:A:224:ILE:HD11	1:D:68:THR:HG22	1.92	0.50
1:A:54:GLN:CG	1:A:54:GLN:O	2.60	0.50
1:C:90:HIS:HB2	1:C:93:THR:CG2	2.42	0.50
1:A:82:PRO:HG3	1:B:358:GLU:CB	2.41	0.50
1:A:246:PRO:O	1:A:247:LEU:HB2	2.12	0.50
1:C:38:VAL:HG22	1:C:157:GLY:C	2.32	0.50
1:C:10:VAL:HG11	1:C:118:ILE:HD13	1.91	0.49
1:A:14[A]:VAL:HG21	1:A:196:ILE:HG13	1.95	0.49
1:D:10:VAL:CG1	1:D:198:PHE:HB2	2.41	0.49
1:A:119:HIS:CE1	1:A:131:LEU:HD13	2.48	0.49
1:B:65:CYS:HA	1:B:94:CYS:SG	2.53	0.49
1:B:313:TYR:OH	1:B:344:THR:HG21	2.12	0.49
1:D:181:GLN:HA	1:D:375:LEU:HD13	1.93	0.49
1:A:313:TYR:OH	1:A:344:THR:HG21	2.13	0.49
1:D:116:LEU:HD13	1:D:117:ALA:N	2.28	0.49
1:C:14:VAL:HG21	1:C:196:ILE:HG13	1.95	0.49
1:C:66:HIS:NE2	1:D:256:GLY:CA	2.76	0.48
1:C:273:LEU:HD13	1:C:277:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ALA:HB1	1:C:131:LEU:HG	1.95	0.48
1:A:102:ILE:HD13	1:A:267:SER:HB2	1.96	0.48
1:C:81:CYS:N	1:C:90:HIS:O	2.47	0.48
1:A:260:GLY:N	1:C:255:VAL:CG1	2.77	0.48
1:C:205:MET:HE1	1:C:397:LEU:HD22	1.94	0.48
1:D:43:ASN:ND2	1:D:230:TYR:H	2.11	0.48
1:C:28:GLN:HE22	1:C:35:GLN:HG2	1.79	0.48
1:D:373:PHE:O	1:D:375:LEU:HD12	2.14	0.48
1:D:83:ALA:HB3	1:D:89:CYS:SG	2.54	0.47
1:A:226:LEU:HD12	1:B:77:GLN:CB	2.41	0.47
1:A:244:VAL:O	1:A:244:VAL:HG22	2.13	0.47
1:D:10:VAL:CG2	1:D:118:ILE:HG23	2.44	0.47
1:A:82:PRO:HG3	1:B:358:GLU:HB2	1.95	0.47
1:A:65:CYS:HA	1:A:94:CYS:SG	2.54	0.47
1:C:10:VAL:CG1	1:C:118:ILE:CD1	2.91	0.47
1:B:275:GLN:O	1:B:279:GLN:NE2	2.48	0.47
1:C:185:CYS:SG	1:C:370:LEU:CD1	3.02	0.47
1:C:358:GLU:OE1	1:D:82:PRO:HB3	2.14	0.47
1:A:244:VAL:HG21	1:A:281:PHE:CA	2.45	0.46
1:C:201:ALA:HB3	1:C:202:PRO:HD3	1.96	0.46
1:D:38[A]:VAL:HG22	1:D:158:VAL:N	2.29	0.46
1:A:311:ASN:O	1:A:312:ALA:HB2	2.14	0.46
1:B:74:ASN:ND2	2:B:573:HOH:O	2.41	0.46
1:C:66:HIS:NE2	1:D:256:GLY:HA3	2.30	0.46
1:D:313:TYR:OH	1:D:344:THR:HG21	2.16	0.46
1:D:38[A]:VAL:CG2	1:D:157:GLY:C	2.84	0.46
1:C:96:LEU:HD12	1:C:96:LEU:HA	1.40	0.46
1:A:192:SER:OG	1:A:395:ALA:CB	2.63	0.46
1:C:79:LEU:HD23	1:C:108:LEU:HD21	1.98	0.46
1:B:10[A]:VAL:HG11	1:B:118:ILE:HD13	1.97	0.45
1:A:77:GLN:HE21	1:D:254:ILE:CG1	2.28	0.45
2:B:694:HOH:O	1:D:254:ILE:HG21	2.16	0.45
1:A:38[A]:VAL:HG11	1:A:159:ALA:N	2.31	0.45
1:C:317:ASP:OD1	1:C:329:ARG:HG3	2.16	0.45
1:B:27:LEU:CD2	1:B:38:VAL:HG21	2.46	0.45
1:B:98:SER:O	1:B:106:THR:HA	2.17	0.45
1:B:188:ARG:HB2	1:B:368:GLU:HG2	1.99	0.45
1:A:233:ARG:HG3	1:A:260:GLY:O	2.17	0.44
1:A:335:LEU:HD13	1:A:346:LEU:HD11	1.98	0.44
1:A:260:GLY:N	1:C:255:VAL:HG11	2.32	0.44
1:D:79:LEU:HD13	2:D:466:HOH:O	2.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HB2	1:B:30:ARG:HG3	1.99	0.44
1:C:80:SER:HA	1:C:90:HIS:O	2.17	0.44
1:C:244:VAL:O	1:C:246:PRO:HA	2.17	0.44
1:D:10:VAL:HG23	1:D:119:HIS:O	2.17	0.44
1:D:350:ASN:HD22	1:D:350:ASN:C	2.20	0.44
1:C:183:THR:HA	1:C:371:VAL:O	2.17	0.44
1:C:222:LEU:O	1:C:378:SER:OG	2.35	0.44
1:D:306:ASN:O	1:D:307:SER:HB3	2.18	0.44
1:C:145:PHE:HA	1:C:148:GLN:HG2	1.99	0.44
1:B:183:THR:HG22	1:B:372:VAL:CG2	2.33	0.43
1:B:144:SER:O	1:B:147:VAL:HG22	2.17	0.43
1:B:222:LEU:HD13	1:B:380:VAL:CG2	2.48	0.43
1:D:399:ASN:HD22	1:D:400:PHE:N	2.15	0.43
1:B:327:VAL:HG12	1:B:329:ARG:HG3	1.99	0.43
1:A:77:GLN:NE2	1:D:254:ILE:HD11	2.34	0.43
1:A:377:ARG:HG3	1:D:136:GLN:HE22	1.83	0.43
1:B:310:ILE:HG21	1:B:313:TYR:CE1	2.52	0.43
1:D:117:ALA:HB1	1:D:131:LEU:HG	2.00	0.43
1:A:289:LEU:HD12	1:A:305:PHE:CZ	2.53	0.43
1:D:188:ARG:HG3	1:D:367:GLU:HB3	1.99	0.43
1:A:29:LYS:HD2	1:A:116:LEU:HD12	2.00	0.43
1:A:29:LYS:HE2	1:A:29:LYS:HB3	1.92	0.43
1:A:201:ALA:N	1:A:202:PRO:CD	2.82	0.43
1:D:183:THR:CG2	1:D:372:VAL:HG22	2.48	0.43
1:B:104:GLN:HE21	1:B:356:ARG:HH21	1.65	0.43
1:C:153:ARG:O	1:C:154:ASN:HB2	2.18	0.43
1:A:43:ASN:HD21	1:A:230:TYR:H	1.65	0.43
1:B:29:LYS:O	1:B:30:ARG:HB2	2.19	0.42
1:A:192:SER:OG	1:A:395:ALA:HB2	2.20	0.42
1:C:387:LEU:O	1:C:388:HIS:CD2	2.73	0.42
1:D:239:ILE:HD12	1:D:244:VAL:CG2	2.48	0.42
1:A:38[A]:VAL:CG1	1:A:159:ALA:H	2.33	0.42
1:B:269:PRO:HA	1:B:363:ALA:HB3	2.02	0.42
1:A:402:ASN:O	1:A:403:ALA:C	2.58	0.42
1:C:289:LEU:HB3	1:C:290:PRO:CD	2.49	0.42
1:D:274:GLN:NE2	1:D:275:GLN:HG2	2.34	0.42
1:A:26:ASN:HB3	1:A:35:GLN:HE21	1.85	0.42
1:C:307:SER:O	1:C:308:ASN:CB	2.67	0.42
1:D:275:GLN:O	1:D:278:TYR:HB3	2.20	0.42
1:B:10[A]:VAL:HG12	1:B:118:ILE:CD1	2.49	0.42
1:D:144:SER:O	1:D:147:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:CD1	1:B:77:GLN:HB2	2.49	0.41
1:A:237:ILE:HG13	1:A:245:PHE:HB3	2.01	0.41
1:C:218:ALA:O	1:C:381:GLY:HA2	2.20	0.41
1:D:38[A]:VAL:HG11	1:D:159:ALA:HB2	2.02	0.41
1:D:217:LEU:HD21	1:D:372:VAL:HG21	2.02	0.41
1:C:93:THR:CG2	2:C:715:HOH:O	2.61	0.41
1:A:48:TRP:CD1	1:A:98:SER:HB3	2.55	0.41
1:A:86:ARG:CD	1:B:353:MET:HE1	2.50	0.41
1:B:183:THR:HG21	1:B:372:VAL:HG22	1.98	0.41
1:B:356:ARG:O	1:D:252:SER:O	2.38	0.41
1:D:375:LEU:H	1:D:375:LEU:CD1	2.29	0.41
1:A:7:ILE:HD12	1:A:120:ALA:HB1	2.03	0.41
1:C:288:GLN:HB2	1:C:314:PRO:HG3	2.03	0.41
1:C:340:GLN:CB	1:C:343:VAL:CG1	2.99	0.41
1:A:104:GLN:NE2	1:A:356:ARG:HH21	2.19	0.41
1:B:371:VAL:HG12	1:B:373:PHE:CE2	2.56	0.41
1:C:220:THR:HG21	1:C:320:MET:HE2	2.03	0.41
1:D:38[A]:VAL:HG23	1:D:157:GLY:C	2.41	0.41
1:A:86:ARG:CD	1:B:353:MET:CE	2.99	0.41
1:B:286:ALA:HB2	1:B:303:LEU:HD21	2.03	0.40
1:D:269:PRO:O	1:D:364:ARG:HB3	2.21	0.40
2:A:510:HOH:O	1:D:226:LEU:HD21	2.20	0.40
1:B:238:ARG:HA	1:B:242:HIS:O	2.21	0.40
1:B:260:GLY:HA2	1:B:358:GLU:OE1	2.21	0.40
1:D:9:LEU:HD11	1:D:201:ALA:HA	2.04	0.40
1:A:38[A]:VAL:HG12	1:A:39:LEU:O	2.21	0.40
1:C:310:ILE:O	1:C:310:ILE:CD1	2.61	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	370/403 (92%)	355 (96%)	12 (3%)	3 (1%)	16	6
1	B	366/403 (91%)	354 (97%)	10 (3%)	2 (0%)	25	13
1	C	363/403 (90%)	340 (94%)	15 (4%)	8 (2%)	5	0
1	D	345/403 (86%)	325 (94%)	16 (5%)	4 (1%)	11	3
All	All	1444/1612 (90%)	1374 (95%)	53 (4%)	17 (1%)	11	3

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	ALA
1	C	52	GLU
1	C	246	PRO
1	C	387	LEU
1	B	55	TYR
1	D	306	ASN
1	D	392	VAL
1	A	30	ARG
1	C	255	VAL
1	D	30	ARG
1	C	55	TYR
1	A	54	GLN
1	C	30	ARG
1	C	256	GLY
1	D	84	ALA
1	B	341	PRO
1	C	341	PRO

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	325/346 (94%)	311 (96%)	14 (4%)	25	10
1	B	320/346 (92%)	302 (94%)	18 (6%)	17	5
1	C	320/346 (92%)	289 (90%)	31 (10%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	309/346 (89%)	280 (91%)	29 (9%)	7	1
All	All	1274/1384 (92%)	1182 (93%)	92 (7%)	12	3

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	27	LEU
1	A	29	LYS
1	A	33	LEU
1	A	75	THR
1	A	192	SER
1	A	231	ASN
1	A	233	ARG
1	A	238	ARG
1	A	268	THR
1	A	366	LEU
1	A	370	LEU
1	A	375	LEU
1	A	386	SER
1	B	11	VAL
1	B	26	ASN
1	B	27	LEU
1	B	29	LYS
1	B	47	LEU
1	B	49	VAL
1	B	52	GLU
1	B	55	TYR
1	B	180	ARG
1	B	188	ARG
1	B	217	LEU
1	B	231	ASN
1	B	233	ARG
1	B	292	GLN
1	B	296	LYS
1	B	369	ASN
1	B	370	LEU
1	B	375	LEU
1	C	11	VAL
1	C	12	LEU
1	C	27	LEU
1	C	29	LYS

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Mol	Chain	Res	Type
1	C	38	VAL
1	C	47	LEU
1	C	54	GLN
1	C	56	SER
1	C	61	GLN
1	C	79	LEU
1	C	85	SER
1	C	91	LYS
1	C	110	GLU
1	C	128	LEU
1	C	147	VAL
1	C	180	ARG
1	C	191	THR
1	C	214	PHE
1	C	217	LEU
1	C	231	ASN
1	C	252	SER
1	C	265	SER
1	C	268	THR
1	C	307	SER
1	C	331	SER
1	C	333	GLU
1	C	343	VAL
1	C	366	LEU
1	C	370	LEU
1	C	375	LEU
1	C	389	SER
1	D	11	VAL
1	D	15	GLN
1	D	26	ASN
1	D	27	LEU
1	D	38[A]	VAL
1	D	38[B]	VAL
1	D	47	LEU
1	D	49	VAL
1	D	53	GLN
1	D	65	CYS
1	D	116	LEU
1	D	121	THR
1	D	180	ARG
1	D	183	THR
1	D	184	THR

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Mol	Chain	Res	Type
1	D	187	SER
1	D	226	LEU
1	D	241	GLN
1	D	253	THR
1	D	257	SER
1	D	268	THR
1	D	306	ASN
1	D	324	ASN
1	D	350	ASN
1	D	353	MET
1	D	364	ARG
1	D	370	LEU
1	D	375	LEU
1	D	399	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	35	GLN
1	A	43	ASN
1	A	77	GLN
1	A	104	GLN
1	A	119	HIS
1	A	235	ASN
1	A	240	ASN
1	A	287	GLN
1	A	308	ASN
1	B	26	ASN
1	B	43	ASN
1	B	74	ASN
1	B	104	GLN
1	B	119	HIS
1	B	170	ASN
1	B	171	GLN
1	B	227	GLN
1	B	240	ASN
1	B	294	GLN
1	C	26	ASN
1	C	43	ASN
1	C	54	GLN
1	C	61	GLN

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Mol	Chain	Res	Type
1	C	74	ASN
1	C	90	HIS
1	C	104	GLN
1	C	119	HIS
1	C	235	ASN
1	C	240	ASN
1	C	241	GLN
1	C	338	GLN
1	D	26	ASN
1	D	28	GLN
1	D	43	ASN
1	D	74	ASN
1	D	104	GLN
1	D	136	GLN
1	D	204	ASN
1	D	235	ASN
1	D	275	GLN
1	D	324	ASN
1	D	350	ASN
1	D	369	ASN
1	D	399	ASN

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

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	377/403 (93%)	0.24	23 (6%)	28 33	17, 38, 64, 81	41 (10%)
1	B	372/403 (92%)	0.44	25 (6%)	25 30	18, 41, 71, 89	35 (9%)
1	C	372/403 (92%)	0.55	46 (12%)	9 12	20, 43, 76, 108	18 (4%)
1	D	360/403 (89%)	0.69	37 (10%)	13 18	22, 51, 77, 104	26 (7%)
All	All	1481/1612 (91%)	0.48	131 (8%)	17 22	17, 43, 74, 108	120 (8%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	387	LEU	6.1
1	D	252	SER	5.7
1	D	392	VAL	5.4
1	C	254	ILE	4.9
1	D	303	LEU	4.7
1	C	389	SER	4.4
1	A	310	ILE	4.4
1	D	189	TYR	4.4
1	D	254	ILE	4.4
1	C	255	VAL	4.3
1	C	214	PHE	4.0
1	B	128	LEU	4.0
1	C	339	ALA	3.9
1	C	89	CYS	3.8
1	C	147	VAL	3.8
1	B	189	TYR	3.8
1	D	328	TRP	3.7
1	C	395	ALA	3.7
1	D	255	VAL	3.6
1	A	384	THR	3.6
1	D	391	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	214	PHE	3.5
1	C	260	GLY	3.5
1	C	298	VAL	3.4
1	D	298	VAL	3.3
1	D	400	PHE	3.3
1	C	258	THR	3.3
1	A	6	PRO	3.3
1	C	388	HIS	3.3
1	D	121	THR	3.3
1	A	247	LEU	3.1
1	B	121	THR	3.1
1	C	88	GLY	3.1
1	C	259	SER	3.1
1	D	353	MET	3.1
1	D	384	THR	3.1
1	B	400	PHE	3.0
1	D	215	HIS	3.0
1	D	339	ALA	3.0
1	A	82	PRO	3.0
1	A	325	GLY	3.0
1	D	188	ARG	3.0
1	A	295	VAL	3.0
1	D	218	ALA	2.9
1	B	387	LEU	2.9
1	A	343	VAL	2.9
1	C	94	CYS	2.9
1	C	76	HIS	2.9
1	D	306	ASN	2.9
1	C	245	PHE	2.8
1	D	213	ILE	2.8
1	C	396	ASP	2.8
1	B	213	ILE	2.8
1	C	253	THR	2.7
1	D	259	SER	2.7
1	A	339	ALA	2.7
1	D	187	SER	2.7
1	B	247	LEU	2.7
1	C	84	ALA	2.6
1	C	385	SER	2.6
1	D	253	THR	2.6
1	B	52	GLU	2.6
1	C	257	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	256	GLY	2.6
1	C	384	THR	2.6
1	D	382	PHE	2.5
1	B	217	LEU	2.5
1	C	128	LEU	2.5
1	C	293	ALA	2.5
1	B	386	SER	2.5
1	D	260	GLY	2.5
1	A	54	GLN	2.5
1	A	313	TYR	2.5
1	B	6	PRO	2.5
1	C	297	SER	2.5
1	A	260	GLY	2.5
1	A	128	LEU	2.5
1	C	83	ALA	2.5
1	A	298	VAL	2.5
1	C	79	LEU	2.4
1	A	208	PHE	2.4
1	D	286	ALA	2.4
1	D	80	SER	2.4
1	C	191	THR	2.4
1	A	289	LEU	2.3
1	C	87	PRO	2.3
1	C	246	PRO	2.3
1	C	261	GLY	2.3
1	D	307	SER	2.3
1	B	328	TRP	2.3
1	C	82	PRO	2.3
1	A	402	ASN	2.3
1	A	312	ALA	2.3
1	B	342	GLY	2.2
1	C	399	ASN	2.2
1	B	83	ALA	2.2
1	D	327	VAL	2.2
1	D	92	ASN	2.2
1	B	279	GLN	2.2
1	D	216	ASP	2.2
1	A	328	TRP	2.2
1	C	226	LEU	2.2
1	C	6	PRO	2.2
1	B	26	ASN	2.1
1	B	385	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLN	2.1
1	C	92	ASN	2.1
1	D	53	GLN	2.1
1	B	343	VAL	2.1
1	B	312	ALA	2.1
1	D	399	ASN	2.1
1	A	388	HIS	2.1
1	A	353	MET	2.1
1	B	205	MET	2.1
1	C	7	ILE	2.1
1	C	308	ASN	2.1
1	B	401	ALA	2.0
1	D	79	LEU	2.0
1	A	243	SER	2.0
1	C	144	SER	2.0
1	C	205	MET	2.0
1	D	389	SER	2.0
1	B	306	ASN	2.0
1	B	302	GLY	2.0
1	B	339	ALA	2.0
1	C	148	GLN	2.0
1	C	295	VAL	2.0
1	D	275	GLN	2.0
1	C	247	LEU	2.0
1	A	305	PHE	2.0
1	D	324	ASN	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 monosaccharides 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.