Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:04 PM GMT

PDB ID	:	3SN2
Title	:	Crystal structure analysis of iron regulatory protein 1 in complex with transferrin receptor IRE B RNA
Authors	:	Volz, K.; Selezneva, A.I.; Walden, W.E.
Deposited on	:	2011-06-28
Resolution	:	2.99 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:

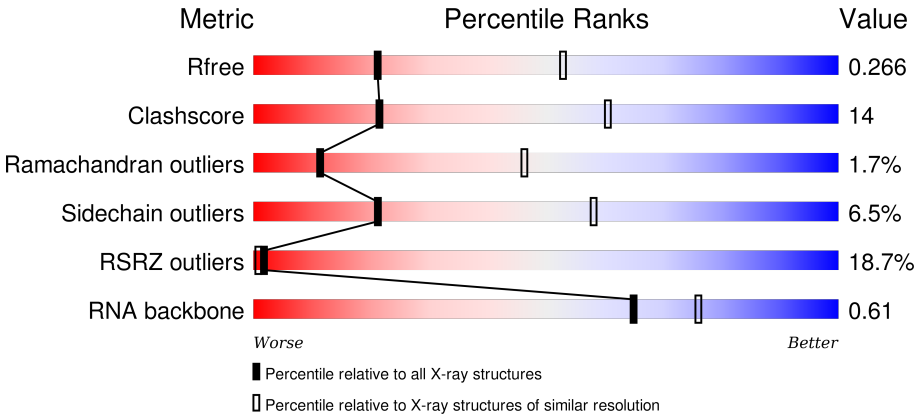
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	908	18% 61% 29% • 7%
2	B	29	10% 62% 34% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14323 atoms, of which 6934 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 Cytoplasmic aconitate hydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	848	13259	4241	6627	1138	1229	24	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP Q01059
A	-17	GLY	-	EXPRESSION TAG	UNP Q01059
A	-16	HIS	-	EXPRESSION TAG	UNP Q01059
A	-15	HIS	-	EXPRESSION TAG	UNP Q01059
A	-14	HIS	-	EXPRESSION TAG	UNP Q01059
A	-13	HIS	-	EXPRESSION TAG	UNP Q01059
A	-12	HIS	-	EXPRESSION TAG	UNP Q01059
A	-11	HIS	-	EXPRESSION TAG	UNP Q01059
A	-10	ALA	-	EXPRESSION TAG	UNP Q01059
A	-9	ASP	-	EXPRESSION TAG	UNP Q01059
A	-8	ASP	-	EXPRESSION TAG	UNP Q01059
A	-7	ASP	-	EXPRESSION TAG	UNP Q01059
A	-6	ASP	-	EXPRESSION TAG	UNP Q01059
A	-5	LYS	-	EXPRESSION TAG	UNP Q01059
A	-4	ASP	-	EXPRESSION TAG	UNP Q01059
A	-3	GLY	-	EXPRESSION TAG	UNP Q01059
A	-2	VAL	-	EXPRESSION TAG	UNP Q01059
A	-1	ASP	-	EXPRESSION TAG	UNP Q01059
A	0	LYS	-	EXPRESSION TAG	UNP Q01059
A	1	LEU	-	EXPRESSION TAG	UNP Q01059
A	283	PRO	LEU	SEE REMARK 999	UNP Q01059
A	437	SER	CYS	ENGINEERED MUTATION	UNP Q01059
A	503	SER	CYS	ENGINEERED MUTATION	UNP Q01059
A	874	PHE	LEU	SEE REMARK 999	UNP Q01059

- Molecule 2 is a RNA chain called transferrin receptor iron regulatory element B RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	29	Total	C	H	N	O	P	0	0	0
			918	275	307	107	201	28			

- Molecule 3 is water.

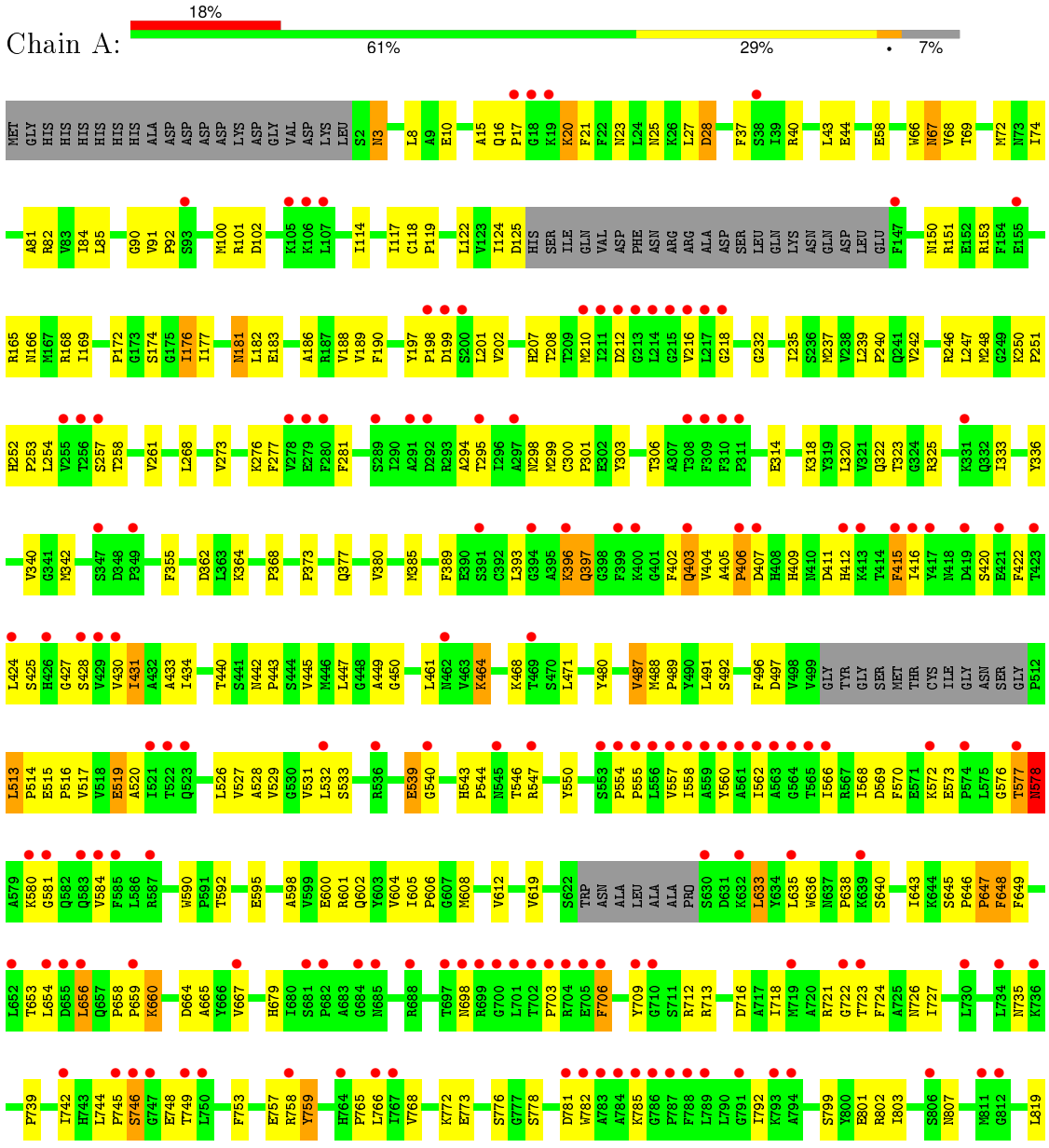
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	15	Total	O	0	0
			15	15		

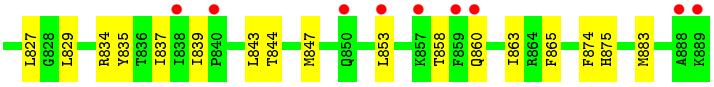
3 Residue-property plots (i)

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.

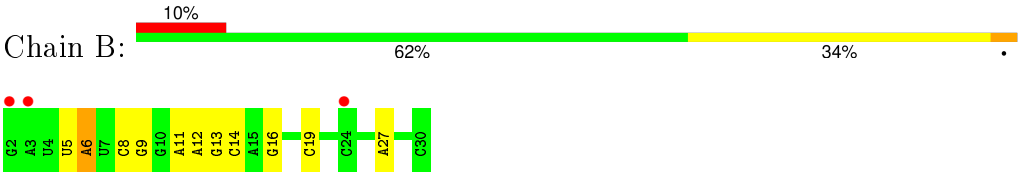
- Molecule 1: Cytoplasmic aconitate hydratase

Chain A:





• Molecule 2: transferrin receptor iron regulatory element B RNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.67Å 101.67Å 281.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.64 – 2.99 32.64 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.64-2.99) 99.8 (32.64-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.227 , 0.275 0.210 , 0.266	Depositor DCC
R_{free} test set	1991 reflections (6.50%)	DCC
Wilson B-factor (Å^2)	99.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 92.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 30703 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14323	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]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	0.29	0/6785	0.46	0/9210
2	B	0.31	0/682	0.76	0/1060
All	All	0.29	0/7467	0.50	0/10270

There are no bond length outliers.

There are no bond angle outliers.

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	6632	6627	6643	196	0
2	B	611	307	313	4	0
3	A	131	0	0	1	0
3	B	15	0	0	0	0
All	All	7389	6934	6956	200	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 14.

All (200) 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:188:VAL:HG21	1:A:320:LEU:HD11	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LYS:HA	1:A:403:GLN:HB3	1.71	0.72
1:A:605:ILE:HB	1:A:606:PRO:HD3	1.72	0.70
1:A:744:LEU:HB2	1:A:745:PRO:HD3	1.73	0.70
1:A:252:HIS:ND1	1:A:253:PRO:HD2	2.07	0.69
1:A:210:MET:HG3	1:A:298:ASN:HB2	1.74	0.69
1:A:300:CYS:HA	1:A:303:TYR:CZ	2.29	0.68
1:A:528:ALA:HB3	1:A:546:THR:HA	1.77	0.67
1:A:514:PRO:HB2	1:A:517:VAL:HG23	1.76	0.66
1:A:450:GLY:HA3	1:A:487:VAL:HG11	1.79	0.65
1:A:404:VAL:HG23	1:A:409:HIS:CD2	2.32	0.64
1:A:124:ILE:HG21	1:A:172:PRO:HG3	1.81	0.63
1:A:299:MET:C	1:A:301:PRO:HD2	2.18	0.63
1:A:202:VAL:HG11	1:A:235:ILE:CD1	2.30	0.61
2:B:13:G:C6	2:B:14:C:N4	2.69	0.60
1:A:543:HIS:CG	1:A:544:PRO:HD2	2.37	0.60
1:A:703:PRO:HA	1:A:706:PHE:CD2	2.37	0.60
1:A:742:ILE:HG12	1:A:749:THR:HG22	1.84	0.59
1:A:647:PRO:O	1:A:649:PHE:N	2.35	0.59
1:A:819:LEU:HD11	1:A:860:GLN:HB2	1.83	0.59
1:A:721:ARG:HG2	1:A:753:PHE:CE2	2.39	0.58
1:A:430:VAL:HG11	1:A:513:LEU:HD22	1.85	0.57
1:A:415:PHE:CE2	1:A:422:PHE:HB2	2.39	0.57
1:A:515:GLU:HB2	1:A:516:PRO:HD3	1.86	0.57
1:A:91:VAL:HB	1:A:92:PRO:HD3	1.87	0.57
1:A:721:ARG:HG2	1:A:753:PHE:CZ	2.40	0.57
1:A:122:LEU:HB2	1:A:169:ILE:HG13	1.85	0.57
1:A:782:TRP:CE3	1:A:785:LYS:HB3	2.40	0.56
1:A:189:VAL:HB	1:A:333:ILE:HG12	1.86	0.56
1:A:449:ALA:HB2	1:A:554:PRO:HB2	1.89	0.55
1:A:827:LEU:HB2	1:A:829:LEU:CD1	2.37	0.55
1:A:464:LYS:HD2	1:A:464:LYS:H	1.71	0.55
1:A:212:ASP:HA	1:A:216:VAL:O	2.07	0.55
1:A:471:LEU:HB3	1:A:497:ASP:O	2.07	0.55
1:A:396:LYS:HG3	1:A:403:GLN:HB3	1.88	0.54
1:A:424:LEU:CD1	1:A:428:SER:HB2	2.38	0.54
1:A:27:LEU:O	1:A:28:ASP:HB2	2.08	0.54
1:A:254:LEU:HB2	1:A:368:PRO:HG2	1.90	0.54
1:A:10:GLU:C	1:A:20:LYS:HG2	2.28	0.54
1:A:69:THR:HA	1:A:72:MET:HG3	1.89	0.54
1:A:242:VAL:HG22	1:A:277:PHE:HB2	1.91	0.53
1:A:434:ILE:HD11	1:A:558:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:OG1	1:A:325:ARG:HG2	2.08	0.53
1:A:393:LEU:HD22	1:A:404:VAL:HG21	1.90	0.53
1:A:415:PHE:HE1	1:A:517:VAL:HG22	1.74	0.52
1:A:442:ASN:HB3	1:A:443:PRO:HD3	1.90	0.52
1:A:844:THR:H	1:A:847:MET:HE3	1.75	0.52
1:A:257:SER:O	1:A:261:VAL:HG23	2.10	0.52
1:A:8:LEU:HD11	1:A:27:LEU:HD13	1.92	0.52
1:A:578:ASN:HB3	1:A:580:LYS:HG2	1.91	0.52
1:A:712:ARG:HD2	1:A:718:ILE:CD1	2.40	0.52
2:B:11:A:C2	2:B:12:A:C4	2.98	0.51
1:A:82:ARG:HD2	3:A:1004:HOH:O	2.10	0.51
1:A:424:LEU:HG	1:A:526:LEU:CD1	2.40	0.51
1:A:281:PHE:CD2	1:A:355:PHE:CE2	2.98	0.51
1:A:433:ALA:HB3	1:A:532:LEU:HD22	1.92	0.51
1:A:772:LYS:HA	1:A:799:SER:HB3	1.93	0.51
1:A:656:LEU:HD11	1:A:875:HIS:HB3	1.92	0.50
1:A:404:VAL:O	1:A:405:ALA:C	2.49	0.50
1:A:513:LEU:HD21	1:A:543:HIS:CD2	2.46	0.50
1:A:153:ARG:HG2	1:A:643:ILE:HD11	1.92	0.50
1:A:865:PHE:CZ	1:A:874:PHE:CD1	3.00	0.50
1:A:578:ASN:C	1:A:580:LYS:H	2.15	0.50
1:A:176:ILE:CG2	1:A:612:VAL:HG22	2.41	0.50
1:A:198:PRO:HG3	1:A:342:MET:CE	2.42	0.49
1:A:300:CYS:HA	1:A:303:TYR:CE2	2.47	0.49
1:A:177:ILE:H	1:A:177:ILE:HD12	1.77	0.49
1:A:281:PHE:CE2	1:A:355:PHE:CE2	3.01	0.49
1:A:431:ILE:HG12	1:A:468:LYS:HB3	1.93	0.49
1:A:246:ARG:HB2	1:A:281:PHE:CZ	2.47	0.49
1:A:273:VAL:O	1:A:276:LYS:HG2	2.12	0.49
1:A:322:GLN:HG3	1:A:601:ARG:HG2	1.94	0.49
1:A:647:PRO:HD3	1:A:716:ASP:OD1	2.12	0.48
1:A:415:PHE:CD2	1:A:415:PHE:N	2.80	0.48
1:A:84:ILE:HD13	1:A:182:LEU:HD22	1.95	0.48
1:A:15:ALA:O	1:A:17:PRO:HD3	2.14	0.48
1:A:527:VAL:O	1:A:527:VAL:HG13	2.12	0.48
1:A:665:ALA:HB2	1:A:765:PRO:HB2	1.94	0.48
1:A:442:ASN:N	1:A:443:PRO:CD	2.77	0.48
1:A:385:MET:HG3	1:A:560:TYR:OH	2.13	0.48
1:A:100:MET:HE1	1:A:883:MET:HB3	1.95	0.48
1:A:174:SER:C	1:A:176:ILE:H	2.17	0.48
1:A:527:VAL:HG23	1:A:547:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:TYR:CD2	1:A:766:LEU:HD21	2.50	0.47
1:A:81:ALA:O	1:A:119:PRO:HD2	2.15	0.47
1:A:37:PHE:O	1:A:40:ARG:HB2	2.14	0.47
1:A:827:LEU:HB2	1:A:829:LEU:HD11	1.96	0.47
1:A:424:LEU:HD12	1:A:425:SER:N	2.29	0.47
1:A:176:ILE:CG1	1:A:181:ASN:HD21	2.28	0.47
1:A:568:ILE:HG13	1:A:573:GLU:HB2	1.97	0.47
1:A:745:PRO:O	1:A:746:SER:CB	2.62	0.46
1:A:533:SER:HB2	1:A:557:VAL:HG21	1.96	0.46
1:A:300:CYS:N	1:A:301:PRO:CD	2.79	0.46
1:A:572:LYS:HG3	1:A:573:GLU:H	1.81	0.46
1:A:727:ILE:HA	1:A:739:PRO:HG3	1.97	0.46
1:A:396:LYS:O	1:A:397:GLN:C	2.54	0.46
1:A:560:TYR:CE2	1:A:570:PHE:CE1	3.03	0.46
1:A:835:TYR:CE2	1:A:853:LEU:HD21	2.50	0.46
1:A:69:THR:HB	1:A:74:ILE:HD11	1.97	0.46
1:A:85:LEU:HD13	1:A:90:GLY:HA2	1.96	0.46
1:A:480:TYR:CD2	1:A:608:MET:HG3	2.51	0.46
1:A:554:PRO:N	1:A:555:PRO:CD	2.79	0.46
1:A:709:TYR:CE1	1:A:722:GLY:HA3	2.49	0.46
1:A:396:LYS:CG	1:A:403:GLN:HB3	2.46	0.46
1:A:177:ILE:HD12	1:A:177:ILE:N	2.31	0.46
1:A:336:TYR:CZ	1:A:340:VAL:HG11	2.50	0.46
1:A:250:LYS:HG2	1:A:251:PRO:HD2	1.97	0.46
1:A:863:ILE:O	1:A:863:ILE:HG23	2.16	0.46
1:A:768:VAL:HG21	1:A:792:ILE:HD13	1.98	0.45
1:A:415:PHE:HD2	1:A:415:PHE:N	2.13	0.45
1:A:207:HIS:O	1:A:208:THR:C	2.53	0.45
1:A:592:THR:OG1	1:A:595:GLU:HG3	2.17	0.45
1:A:461:LEU:HD21	1:A:584:VAL:CG1	2.46	0.45
1:A:389:PHE:CE2	1:A:427:GLY:HA3	2.51	0.45
1:A:210:MET:HG2	1:A:294:ALA:HB1	1.98	0.45
1:A:539:GLU:HG3	1:A:540:GLY:N	2.32	0.45
1:A:176:ILE:HG22	1:A:612:VAL:HG22	1.98	0.45
1:A:863:ILE:O	1:A:863:ILE:CG2	2.63	0.45
1:A:529:VAL:HG11	1:A:566:ILE:HG21	1.98	0.45
1:A:519:GLU:O	1:A:520:ALA:C	2.55	0.45
1:A:746:SER:OG	1:A:748:GLU:HB2	2.17	0.45
1:A:119:PRO:HG2	1:A:190:PHE:CE2	2.52	0.45
1:A:759:TYR:HB3	1:A:766:LEU:HD11	1.98	0.44
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:PRO:C	1:A:640:SER:H	2.21	0.44
1:A:659:PRO:HB3	1:A:839:ILE:CG2	2.47	0.44
1:A:268:LEU:HD13	1:A:303:TYR:CE1	2.52	0.44
1:A:636:TRP:CE2	1:A:645:SER:HB2	2.53	0.44
1:A:646:PRO:HB2	1:A:648:PHE:CD1	2.53	0.44
1:A:716:ASP:HA	1:A:782:TRP:CH2	2.53	0.44
1:A:569:ASP:HB3	1:A:572:LYS:HG2	2.00	0.44
1:A:531:VAL:HG12	1:A:557:VAL:HG13	1.99	0.44
1:A:314:GLU:HG3	1:A:318:LYS:HE2	2.00	0.44
1:A:248:MET:O	1:A:362:ASP:HA	2.17	0.44
1:A:576:GLY:O	1:A:584:VAL:HG12	2.18	0.43
2:B:5:U:H2'	2:B:6:A:O4'	2.18	0.43
1:A:406:PRO:HA	1:A:409:HIS:CD2	2.53	0.43
2:B:12:A:O2'	2:B:13:G:H5'	2.19	0.43
1:A:81:ALA:O	1:A:118:CYS:HB2	2.18	0.43
1:A:15:ALA:O	1:A:17:PRO:CD	2.66	0.43
1:A:300:CYS:N	1:A:301:PRO:HD2	2.33	0.43
1:A:835:TYR:CE2	1:A:853:LEU:CD2	3.01	0.43
1:A:558:ILE:O	1:A:562:ILE:HG13	2.19	0.43
1:A:723:THR:HG22	1:A:724:PHE:CD2	2.54	0.43
1:A:202:VAL:HG11	1:A:235:ILE:HD12	2.01	0.42
1:A:803:ILE:HG22	1:A:807:ASN:OD1	2.19	0.42
1:A:759:TYR:CG	1:A:766:LEU:HD21	2.54	0.42
1:A:66:TRP:O	1:A:68:VAL:N	2.52	0.42
1:A:776:SER:HA	1:A:801:GLU:HG3	2.02	0.42
1:A:201:LEU:HD23	1:A:218:GLY:HA3	2.00	0.42
1:A:602:GLN:O	1:A:606:PRO:HG2	2.20	0.42
1:A:415:PHE:CE1	1:A:517:VAL:HG22	2.52	0.42
1:A:199:ASP:HB3	1:A:216:VAL:HG22	2.01	0.42
1:A:23:ASN:OD1	1:A:25:ASN:HB2	2.19	0.42
1:A:43:LEU:O	1:A:44:GLU:C	2.58	0.42
1:A:254:LEU:HB2	1:A:368:PRO:CG	2.50	0.42
1:A:416:ILE:HA	1:A:420:SER:O	2.19	0.42
1:A:843:LEU:HD11	1:A:863:ILE:HG21	2.01	0.42
1:A:165:ARG:O	1:A:166:ASN:HB2	2.20	0.42
1:A:527:VAL:O	1:A:527:VAL:CG1	2.67	0.41
1:A:660:LYS:H	1:A:660:LYS:CD	2.33	0.41
1:A:403:GLN:O	1:A:403:GLN:CG	2.69	0.41
1:A:168:ARG:HG2	1:A:169:ILE:N	2.35	0.41
1:A:471:LEU:CD2	1:A:491:LEU:HD13	2.50	0.41
1:A:578:ASN:HB3	1:A:580:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ILE:HA	1:A:739:PRO:CG	2.50	0.41
1:A:679:HIS:CD2	1:A:726:ASN:ND2	2.88	0.41
1:A:577:THR:HG23	1:A:581:GLY:O	2.20	0.41
1:A:713:ARG:HD2	1:A:781:ASP:OD1	2.20	0.41
1:A:445:VAL:CG1	1:A:554:PRO:HD2	2.51	0.41
1:A:464:LYS:HB3	1:A:464:LYS:HE3	1.83	0.41
1:A:183:GLU:O	1:A:186:ALA:HB3	2.21	0.41
1:A:555:PRO:HB2	1:A:590:TRP:CH2	2.54	0.41
1:A:340:VAL:CG1	1:A:342:MET:HE2	2.50	0.41
1:A:772:LYS:O	1:A:773:GLU:C	2.59	0.41
1:A:174:SER:HB2	1:A:176:ILE:CG1	2.50	0.41
1:A:600:GLU:HA	1:A:604:VAL:CG2	2.51	0.41
1:A:753:PHE:O	1:A:757:GLU:HB2	2.20	0.41
1:A:424:LEU:HG	1:A:526:LEU:HD13	2.02	0.41
1:A:198:PRO:CG	1:A:342:MET:HE1	2.50	0.41
1:A:3:ASN:C	1:A:3:ASN:OD1	2.59	0.41
1:A:496:PHE:CE1	1:A:558:ILE:HG12	2.56	0.41
1:A:246:ARG:HB2	1:A:281:PHE:CE1	2.56	0.41
1:A:723:THR:O	1:A:724:PHE:HB2	2.21	0.41
1:A:102:ASP:OD2	1:A:633:LEU:HD11	2.21	0.41
1:A:202:VAL:HG11	1:A:235:ILE:HD11	2.02	0.41
1:A:464:LYS:CD	1:A:464:LYS:H	2.33	0.41
1:A:560:TYR:CE2	1:A:570:PHE:CZ	3.08	0.41
1:A:835:TYR:CD2	1:A:853:LEU:CD2	3.04	0.41
1:A:595:GLU:O	1:A:598:ALA:HB3	2.21	0.41
1:A:117:ILE:HG13	1:A:232:GLY:HA3	2.02	0.41
1:A:488:MET:HB2	1:A:489:PRO:HD3	2.02	0.41
1:A:396:LYS:HG3	1:A:403:GLN:CB	2.50	0.41
1:A:295:THR:HG23	1:A:440:THR:OG1	2.20	0.41
1:A:550:TYR:HE1	1:A:566:ILE:CD1	2.34	0.40
1:A:373:PRO:HB3	1:A:550:TYR:CZ	2.56	0.40
1:A:101:ARG:HG2	1:A:114:ILE:HB	2.02	0.40
1:A:415:PHE:HE2	1:A:422:PHE:HB2	1.84	0.40
1:A:667:VAL:CG2	1:A:835:TYR:CE1	3.04	0.40
1:A:411:ASP:O	1:A:412:HIS:HB3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	840/908 (92%)	733 (87%)	93 (11%)	14 (2%)	11 46

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	648	PHE
1	A	403	GLN
1	A	578	ASN
1	A	746	SER
1	A	397	GLN
1	A	519	GLU
1	A	664	ASP
1	A	67	ASN
1	A	658	PRO
1	A	802	ARG
1	A	16	GLN
1	A	647	PRO
1	A	406	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	723/772 (94%)	676 (94%)	47 (6%)	21 58

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	20	LYS
1	A	21	PHE
1	A	58	GLU
1	A	67	ASN
1	A	125	ASP
1	A	150	ASN
1	A	151	ARG
1	A	176	ILE
1	A	181	ASN
1	A	197	TYR
1	A	237	MET
1	A	247	LEU
1	A	258	THR
1	A	306	THR
1	A	364	LYS
1	A	377	GLN
1	A	380	VAL
1	A	396	LYS
1	A	402	PHE
1	A	407	ASP
1	A	415	PHE
1	A	431	ILE
1	A	447	LEU
1	A	464	LYS
1	A	487	VAL
1	A	492	SER
1	A	513	LEU
1	A	539	GLU
1	A	577	THR
1	A	578	ASN
1	A	619	VAL
1	A	633	LEU
1	A	635	LEU
1	A	653	THR
1	A	654	LEU
1	A	656	LEU
1	A	660	LYS
1	A	698	ASN
1	A	706	PHE
1	A	735	ASN
1	A	758	ARG
1	A	759	TYR

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Mol	Chain	Res	Type
1	A	778	SER
1	A	834	ARG
1	A	837	ILE
1	A	858	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	67	ASN
1	A	181	ASN
1	A	241	GLN
1	A	270	GLN
1	A	332	GLN
1	A	409	HIS
1	A	410	ASN
1	A	679	HIS
1	A	726	ASN
1	A	737	GLN
1	A	743	HIS
1	A	761	GLN
1	A	804	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	28/29 (96%)	6 (21%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	A
2	B	8	C
2	B	9	G
2	B	16	G
2	B	19	C
2	B	27	A

There are no RNA pucker outliers to report.

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	848/908 (93%)	1.03	161 (18%) 2 1	74, 119, 158, 173	0
2	B	29/29 (100%)	0.91	3 (10%) 9 3	98, 115, 133, 136	0
All	All	877/937 (93%)	1.03	164 (18%) 2 1	74, 118, 158, 173	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	656	LEU	6.6
1	A	583	GLN	6.2
1	A	889	LYS	6.1
1	A	564	GLY	6.0
1	A	791	GLY	5.9
1	A	838	ILE	5.7
1	A	563	ALA	5.3
1	A	688	ARG	5.2
1	A	572	LYS	5.1
1	A	701	LEU	4.9
1	A	786	GLY	4.8
1	A	416	ILE	4.8
1	A	654	LEU	4.7
1	A	788	PHE	4.7
1	A	794	ALA	4.7
1	A	215	GLY	4.7
1	A	860	GLN	4.6
1	A	888	ALA	4.6
1	A	793	LYS	4.6
1	A	560	TYR	4.5
1	A	547	ARG	4.2
1	A	681	SER	4.1
1	A	545	ASN	4.1
1	A	394	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	584	VAL	4.0
1	A	698	ASN	3.9
1	A	784	ALA	3.9
1	A	723	THR	3.9
1	A	734	LEU	3.9
1	A	782	TRP	3.8
1	A	523	GLN	3.8
1	A	785	LYS	3.7
1	A	703	PRO	3.7
1	A	413	LYS	3.7
1	A	722	GLY	3.6
1	A	742	ILE	3.6
1	A	565	THR	3.6
1	A	462	ASN	3.6
1	A	213	GLY	3.5
1	A	106	LYS	3.5
1	A	559	ALA	3.5
1	A	812	GLY	3.4
1	A	585	PHE	3.4
1	A	811	MET	3.3
1	A	787	PRO	3.3
1	A	421	GLU	3.3
1	A	423	THR	3.3
1	A	685	ASN	3.3
1	A	349	PRO	3.3
1	A	429	VAL	3.3
1	A	562	ILE	3.3
1	A	426	HIS	3.2
1	A	581	GLY	3.2
1	A	412	HIS	3.1
1	A	424	LEU	3.1
1	A	147	PHE	3.1
1	A	310	PHE	3.1
1	A	766	LEU	3.1
1	A	736	LYS	3.1
1	A	710	GLY	3.1
1	A	561	ALA	3.0
1	A	655	ASP	3.0
1	A	684	GLY	3.0
1	A	702	THR	3.0
1	A	200	SER	2.9
1	A	396	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	105	LYS	2.9
1	A	430	VAL	2.9
1	A	155	GLU	2.9
1	A	212	ASP	2.8
1	A	216	VAL	2.8
1	A	18	GLY	2.8
1	A	38	SER	2.8
1	A	630	SER	2.8
1	A	256	THR	2.8
1	A	781	ASP	2.8
1	A	706	PHE	2.8
1	A	536	ARG	2.8
1	A	218	GLY	2.8
1	A	783	ALA	2.7
1	A	311	PRO	2.7
1	A	635	LEU	2.7
1	A	746	SER	2.7
1	A	308	THR	2.7
1	A	747	GLY	2.7
1	A	400	LYS	2.7
1	A	289	SER	2.6
1	A	279	GLU	2.6
1	A	521	ILE	2.6
1	A	580	LYS	2.6
1	A	700	GLY	2.6
1	A	632	LYS	2.6
1	A	659	PRO	2.6
2	B	3	A	2.6
1	A	697	THR	2.6
1	A	859	PHE	2.6
1	A	309	PHE	2.5
1	A	295	THR	2.5
1	A	555	PRO	2.5
1	A	522	THR	2.5
1	A	406	PRO	2.5
1	A	403	GLN	2.5
1	A	749	THR	2.5
1	A	291	ALA	2.5
1	A	297	ALA	2.5
1	A	682	PRO	2.5
1	A	347	SER	2.5
1	A	840	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	2.4
1	A	709	TYR	2.4
1	A	652	LEU	2.4
1	A	257	SER	2.4
1	A	428	SER	2.4
1	A	415	PHE	2.4
1	A	331	LYS	2.4
1	A	93	SER	2.3
1	A	278	VAL	2.3
1	A	17	PRO	2.3
1	A	292	ASP	2.3
1	A	557	VAL	2.3
1	A	577	THR	2.3
1	A	587	ARG	2.3
1	A	198	PRO	2.3
1	A	391	SER	2.3
1	A	399	PHE	2.3
1	A	705	GLU	2.3
1	A	553	SER	2.3
1	A	554	PRO	2.3
1	A	210	MET	2.2
1	A	704	ARG	2.2
1	A	850	GLN	2.2
2	B	24	C	2.2
1	A	199	ASP	2.2
1	A	764	HIS	2.2
1	A	789	LEU	2.2
1	A	853	LEU	2.2
1	A	419	ASP	2.2
1	A	758	ARG	2.2
1	A	750	LEU	2.2
1	A	211	ILE	2.2
1	A	407	ASP	2.2
1	A	556	LEU	2.2
1	A	639	LYS	2.1
1	A	217	LEU	2.1
1	A	255	VAL	2.1
1	A	417	TYR	2.1
1	A	857	LYS	2.1
1	A	280	PHE	2.1
1	A	730	LEU	2.1
1	A	566	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	532	LEU	2.1
1	A	806	SER	2.1
1	A	767	ILE	2.1
2	B	2	G	2.1
1	A	699	ARG	2.1
1	A	107	LEU	2.1
1	A	719	MET	2.0
1	A	469	THR	2.0
1	A	667	VAL	2.0
1	A	540	GLY	2.0
1	A	558	ILE	2.0
1	A	19	LYS	2.0
1	A	574	PRO	2.0
1	A	745	PRO	2.0

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

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

6.3 Carbohydrates (i)

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.