



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 12:16 PM JST

PDB ID : 8HPP
Title : Crystal structure of human INTS3 with SAGE1
Authors : Deng, W.; Wu, J.; Lei, M.
Deposited on : 2022-12-12
Resolution : 3.00 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) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

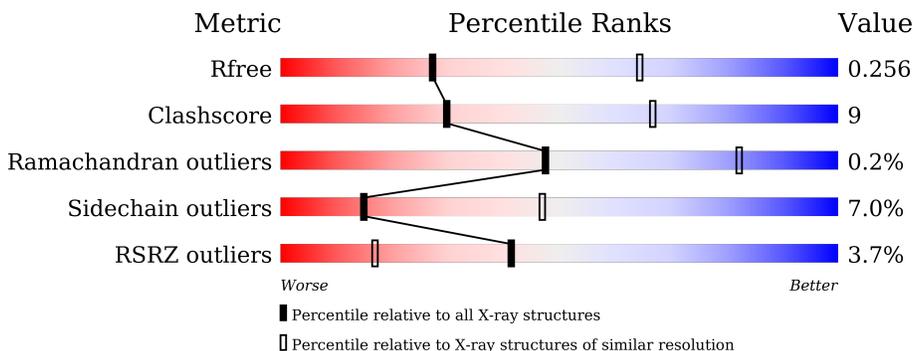
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	471	 3% 59% 21% • 16%
1	B	471	 4% 61% 21% • 16%
2	C	90	 71% 20% •••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7102 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 Integrator complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3195	2026	528	615	26	0	0	0
1	B	394	3189	2023	527	613	26	0	0	0

- Molecule 2 is a protein called Sarcoma antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	86	718	461	131	122	4	0	0	0

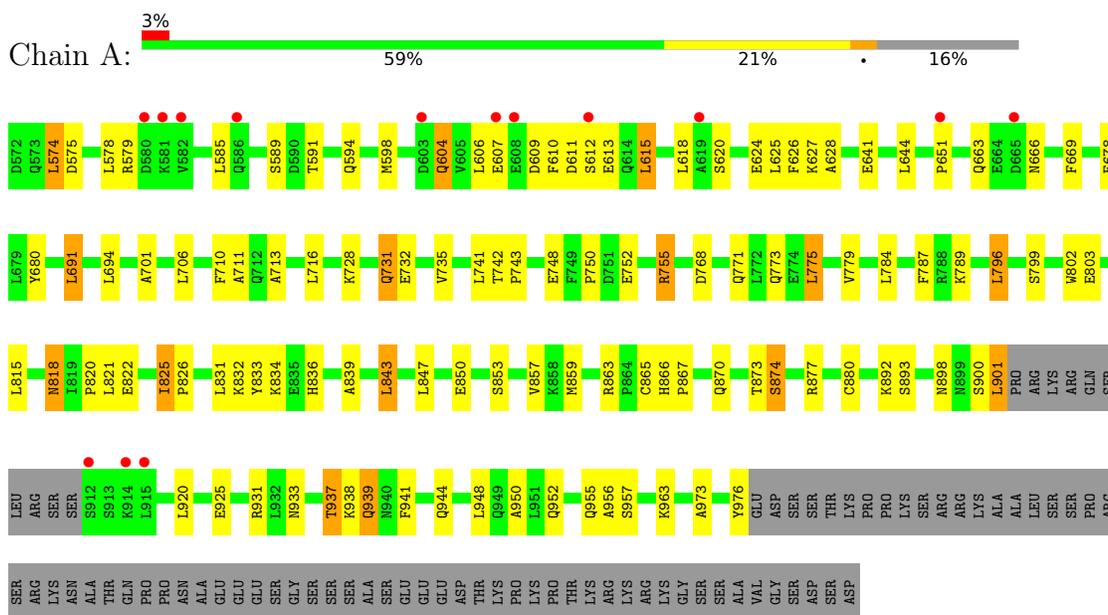
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	815	PRO	-	expression tag	UNP Q9NXZ1
C	816	GLY	-	expression tag	UNP Q9NXZ1
C	817	SER	-	expression tag	UNP Q9NXZ1

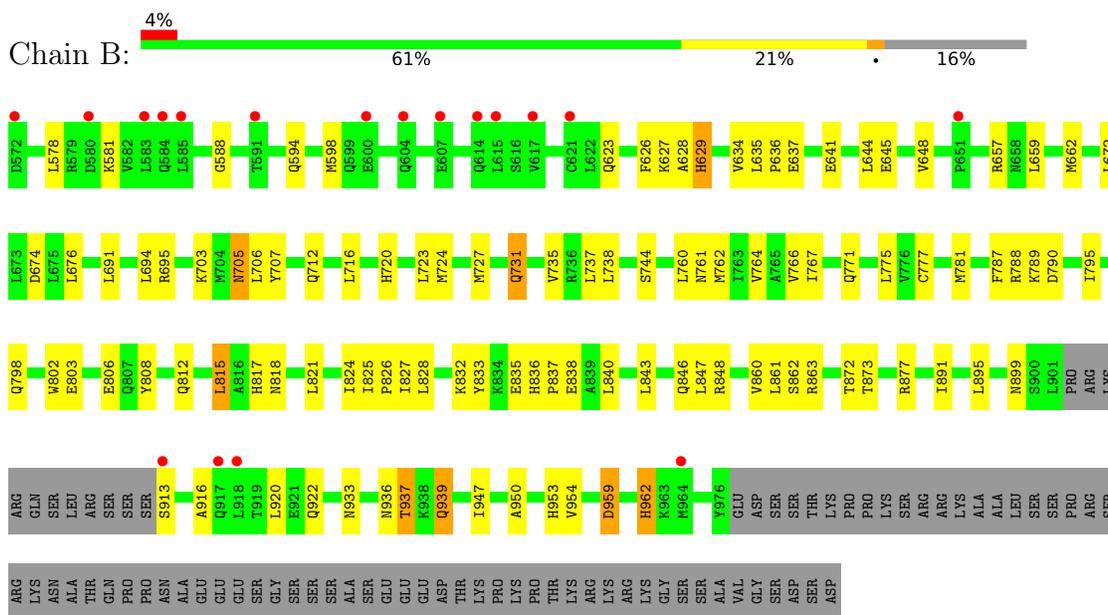
3 Residue-property plots [i](#)

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: Integrator complex subunit 3



- Molecule 1: Integrator complex subunit 3



● Molecule 2: Sarcoma antigen 1

Chain C:  71% 20% . . .

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	260.12Å 46.24Å 103.10Å 90.00° 113.28° 90.00°	Depositor
Resolution (Å)	47.40 – 3.00 47.35 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.40-3.00) 96.9 (47.35-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.215 , 0.257 0.216 , 0.256	Depositor DCC
R_{free} test set	1102 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtrriage
Anisotropy	0.782	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.022 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7102	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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	0.26	0/3251	0.65	7/4392 (0.2%)
1	B	0.26	0/3245	0.63	2/4384 (0.0%)
2	C	0.25	0/728	0.80	2/965 (0.2%)
All	All	0.26	0/7224	0.66	11/9741 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	ALA	CB-CA-C	15.55	133.43	110.10
1	B	629	HIS	N-CA-CB	-10.99	90.81	110.60
1	A	900	SER	N-CA-C	10.95	140.56	111.00
2	C	847	ILE	CB-CA-C	10.07	131.75	111.60
1	A	701	ALA	CB-CA-C	9.40	124.20	110.10
1	A	901	LEU	N-CA-CB	-8.40	93.60	110.40
1	A	900	SER	CB-CA-C	-8.14	94.62	110.10
1	A	956	ALA	CB-CA-C	7.68	121.62	110.10
2	C	848	LEU	N-CA-CB	-7.10	96.19	110.40
1	A	957	SER	N-CA-CB	-7.03	99.95	110.50
1	A	701	ALA	N-CA-C	-6.56	93.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3195	0	3178	65	0
1	B	3189	0	3173	61	0
2	C	718	0	763	12	0
All	All	7102	0	7114	134	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 9.

All (134) 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:832:LYS:H	1:A:836:HIS:HD2	0.99	0.97
1:B:727:MET:HB3	1:B:762:MET:HE1	1.53	0.89
1:B:832:LYS:H	1:B:836:HIS:HD2	1.19	0.89
1:A:832:LYS:H	1:A:836:HIS:CD2	1.90	0.86
1:B:777:CYS:O	1:B:781:MET:HG2	1.76	0.85
1:A:825:ILE:N	1:A:826:PRO:HD2	1.94	0.82
1:B:825:ILE:N	1:B:826:PRO:HD2	1.95	0.82
1:B:821:LEU:HD23	1:B:847:LEU:HD23	1.60	0.81
1:A:821:LEU:HD21	1:A:847:LEU:HD23	1.60	0.81
1:B:695:ARG:HH11	1:B:744:SER:HB2	1.50	0.77
1:A:832:LYS:N	1:A:836:HIS:HD2	1.80	0.77
1:A:898:ASN:HB3	1:A:920:LEU:HD12	1.69	0.74
1:B:821:LEU:HD21	1:B:846:GLN:HB3	1.71	0.72
1:B:645:GLU:HA	1:B:648:VAL:HG22	1.74	0.70
1:A:831:LEU:O	1:A:863:ARG:NH2	2.25	0.69
1:B:832:LYS:H	1:B:836:HIS:CD2	2.09	0.68
1:A:821:LEU:CD2	1:A:847:LEU:HD23	2.23	0.68
1:A:866:HIS:HD2	1:A:867:PRO:HD2	1.59	0.68
2:C:843:GLU:O	2:C:847:ILE:HG23	1.93	0.68
1:A:803:GLU:HG2	2:C:874:LYS:O	1.95	0.66
1:A:615:LEU:HA	1:A:618:LEU:HB3	1.77	0.65
1:A:820:PRO:HB2	1:A:822:GLU:HG2	1.76	0.65
1:B:634:VAL:HG21	1:B:737:LEU:HD22	1.78	0.65
1:B:766:VAL:O	2:C:872:ARG:NH2	2.31	0.64
2:C:849:LEU:O	2:C:852:VAL:HG12	1.97	0.64
1:A:937:THR:HG22	1:A:938:LYS:H	1.62	0.64
1:A:743:PRO:HA	1:A:784:LEU:HD13	1.78	0.63
1:A:825:ILE:N	1:A:826:PRO:CD	2.63	0.62
1:B:825:ILE:N	1:B:826:PRO:CD	2.62	0.62
1:B:828:LEU:HG	1:B:863:ARG:HD2	1.82	0.61
1:B:635:LEU:HD23	1:B:636:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:ALA:O	1:B:954:VAL:HG23	2.03	0.59
1:B:824:ILE:C	1:B:826:PRO:HD2	2.23	0.57
1:B:899:ASN:HA	1:B:920:LEU:HD11	1.87	0.57
1:A:952:GLN:HE22	1:A:976:TYR:HD1	1.51	0.56
1:A:941:PHE:O	1:A:944:GLN:HG2	2.06	0.56
1:B:694:LEU:HD21	1:B:706:LEU:HD23	1.86	0.56
1:B:815:LEU:HD11	1:B:846:GLN:HG3	1.86	0.56
1:B:899:ASN:HD22	1:B:953:HIS:CD2	2.24	0.55
1:A:853:SER:O	1:A:857:VAL:HG23	2.05	0.55
1:A:626:PHE:C	1:A:628:ALA:H	2.09	0.55
1:A:892:LYS:HG3	1:A:950:ALA:HB2	1.90	0.54
1:B:641:GLU:HA	1:B:644:LEU:HD12	1.90	0.53
1:B:861:LEU:O	1:B:922:GLN:NE2	2.41	0.53
1:A:877:ARG:HD2	1:A:933:ASN:OD1	2.08	0.53
1:A:620:SER:O	1:A:624:GLU:HG2	2.09	0.53
1:A:939:GLN:HE21	1:A:939:GLN:N	2.07	0.53
1:A:680:TYR:CD1	1:A:710:PHE:HZ	2.28	0.52
1:A:870:GLN:NE2	1:A:870:GLN:HA	2.24	0.51
2:C:860:ARG:HB2	2:C:889:ILE:HG21	1.91	0.51
1:A:606:LEU:O	1:A:607:GLU:C	2.49	0.51
1:B:913:SER:HA	1:B:916:ALA:HB3	1.93	0.51
1:A:666:ASN:HB3	1:A:669:PHE:HB2	1.92	0.51
1:A:799:SER:HA	1:A:802:TRP:CD2	2.46	0.50
1:B:795:ILE:O	1:B:798:GLN:HB2	2.12	0.50
2:C:841:ASN:OD1	2:C:843:GLU:HG2	2.10	0.50
1:B:731:GLN:CB	1:B:738:LEU:HD22	2.42	0.50
2:C:857:LYS:O	2:C:861:GLN:HG3	2.11	0.50
1:B:727:MET:CB	1:B:762:MET:HE1	2.34	0.50
1:B:788:ARG:HD3	1:B:790:ASP:OD1	2.10	0.50
1:B:862:SER:C	1:B:922:GLN:HE22	2.15	0.50
1:B:838:GLU:H	1:B:838:GLU:CD	2.14	0.50
1:B:824:ILE:O	1:B:827:ILE:HG22	2.11	0.50
1:B:933:ASN:O	1:B:936:ASN:ND2	2.42	0.49
2:C:815:PRO:N	2:C:821:LYS:HZ2	2.10	0.49
1:B:731:GLN:HB2	1:B:738:LEU:HD22	1.95	0.48
1:A:578:LEU:HD21	1:A:604:GLN:HB3	1.95	0.48
2:C:845:ILE:O	2:C:848:LEU:HB3	2.13	0.48
1:A:748:GLU:C	1:A:750:PRO:HD3	2.35	0.48
1:B:803:GLU:HB2	1:B:806:GLU:CD	2.33	0.48
1:A:865:CYS:SG	1:A:925:GLU:HB3	2.53	0.47
1:B:764:VAL:O	1:B:806:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:LEU:HA	1:B:662:MET:HE2	1.95	0.47
1:B:891:ILE:O	1:B:895:LEU:HB2	2.15	0.47
1:A:641:GLU:HA	1:A:644:LEU:HD12	1.96	0.47
1:B:937:THR:HB	1:B:939:GLN:HG3	1.96	0.46
1:B:835:GLU:C	1:B:837:PRO:HD3	2.36	0.46
1:A:585:LEU:HD22	1:A:625:LEU:HD21	1.96	0.46
1:A:663:GLN:HG3	1:A:666:ASN:HB2	1.98	0.46
1:B:626:PHE:O	1:B:629:HIS:HB3	2.16	0.46
1:A:694:LEU:HD21	1:A:706:LEU:HD23	1.98	0.46
1:B:954:VAL:HG12	1:B:954:VAL:O	2.15	0.46
2:C:879:ILE:O	2:C:883:GLU:HG2	2.16	0.46
1:A:711:ALA:C	1:A:713:ALA:H	2.19	0.45
1:A:589:SER:HA	1:A:594:GLN:NE2	2.32	0.45
1:A:691:LEU:HD12	1:A:691:LEU:HA	1.79	0.45
1:B:802:TRP:HB3	1:B:806:GLU:OE1	2.17	0.45
1:A:626:PHE:C	1:A:628:ALA:N	2.70	0.44
1:B:891:ILE:HB	1:B:947:ILE:HD11	1.99	0.44
1:A:598:MET:HG3	1:A:651:PRO:HB3	2.00	0.44
1:A:818:ASN:ND2	1:B:848:ARG:HH12	2.15	0.44
1:A:825:ILE:HG23	1:A:859:MET:HG3	1.99	0.44
1:A:768:ASP:OD1	1:A:771:GLN:HG3	2.18	0.43
1:A:574:LEU:HB3	1:A:579:ARG:HD2	1.99	0.43
1:A:752:GLU:HA	1:A:755:ARG:NH2	2.33	0.43
1:A:850:GLU:OE1	1:A:850:GLU:HA	2.19	0.43
1:A:948:LEU:HD22	1:A:973:ALA:HA	2.00	0.43
1:A:839:ALA:O	1:A:843:LEU:HB2	2.18	0.43
1:A:939:GLN:HE21	1:A:939:GLN:H	1.67	0.43
1:A:892:LYS:O	1:A:893:SER:C	2.56	0.43
1:B:720:HIS:O	1:B:724:MET:HG2	2.18	0.43
1:B:767:ILE:HA	1:B:771:GLN:OE1	2.18	0.43
1:B:594:GLN:O	1:B:598:MET:HB2	2.18	0.43
1:B:703:LYS:HB3	1:B:705:ASN:OD1	2.18	0.43
1:B:808:TYR:O	1:B:812:GLN:HG2	2.19	0.43
1:A:833:TYR:CD2	1:A:866:HIS:CE1	3.06	0.42
1:A:870:GLN:O	1:A:874:SER:HB2	2.18	0.42
1:B:860:VAL:HG13	1:B:872:THR:HG23	2.00	0.42
1:A:775:LEU:HD12	1:A:775:LEU:HA	1.82	0.42
1:B:760:LEU:HD23	1:B:802:TRP:HH2	1.84	0.42
1:B:787:PHE:HD2	1:B:817:HIS:ND1	2.18	0.42
1:B:821:LEU:CD2	1:B:847:LEU:HD23	2.43	0.42
1:A:611:ASP:HB3	1:A:612:SER:H	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:ASN:HB2	1:B:802:TRP:CZ2	2.55	0.42
1:A:755:ARG:H	1:A:755:ARG:HG3	1.76	0.41
1:A:773:GLN:NE2	1:B:840:LEU:HB3	2.34	0.41
2:C:856:MET:HE1	2:C:889:ILE:HG23	2.01	0.41
1:A:585:LEU:HA	1:A:594:GLN:HG2	2.02	0.41
2:C:886:LEU:HD12	2:C:886:LEU:HA	1.87	0.41
1:A:728:LYS:HE3	1:A:731:GLN:OE1	2.19	0.41
1:B:877:ARG:NH1	1:B:936:ASN:HD21	2.18	0.41
1:A:731:GLN:HG3	1:A:732:GLU:N	2.33	0.41
1:A:931:ARG:HH11	1:A:931:ARG:HG2	1.85	0.41
1:B:860:VAL:CG1	1:B:872:THR:HG23	2.50	0.41
1:B:672:LEU:HD12	1:B:672:LEU:HA	1.85	0.41
1:B:764:VAL:HG23	1:B:806:GLU:HB3	2.02	0.41
1:A:779:VAL:HG23	1:A:784:LEU:HD23	2.03	0.41
1:B:707:TYR:OH	1:B:723:LEU:HA	2.20	0.41
1:A:741:LEU:O	1:A:742:THR:C	2.59	0.40
1:B:578:LEU:HD23	1:B:581:LYS:HG3	2.03	0.40
1:A:955:GLN:O	1:A:963:LYS:HE2	2.21	0.40
1:A:575:ASP:HB3	1:A:578:LEU:HD12	2.04	0.40
1:A:796:LEU:HD12	1:A:796:LEU:HA	1.93	0.40
1:B:959:ASP:H	1:B:962:HIS:CE1	2.40	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	391/471 (83%)	355 (91%)	35 (9%)	1 (0%)	41	76
1	B	390/471 (83%)	364 (93%)	25 (6%)	1 (0%)	41	76
2	C	84/90 (93%)	84 (100%)	0	0	100	100
All	All	865/1032 (84%)	803 (93%)	60 (7%)	2 (0%)	47	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	THR
1	B	588	GLY

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	366/433 (84%)	338 (92%)	28 (8%)	13	42
1	B	365/433 (84%)	342 (94%)	23 (6%)	18	51
2	C	78/82 (95%)	72 (92%)	6 (8%)	13	42
All	All	809/948 (85%)	752 (93%)	57 (7%)	15	47

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	574	LEU
1	A	604	GLN
1	A	609	ASP
1	A	610	PHE
1	A	613	GLU
1	A	615	LEU
1	A	627	LYS
1	A	678	GLU
1	A	691	LEU
1	A	716	LEU
1	A	731	GLN
1	A	735	VAL
1	A	755	ARG
1	A	775	LEU
1	A	787	PHE
1	A	789	LYS
1	A	796	LEU
1	A	815	LEU
1	A	818	ASN

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Mol	Chain	Res	Type
1	A	825	ILE
1	A	834	LYS
1	A	843	LEU
1	A	873	THR
1	A	874	SER
1	A	880	CYS
1	A	901	LEU
1	A	937	THR
1	A	939	GLN
1	B	623	GLN
1	B	627	LYS
1	B	637	GLU
1	B	657	ARG
1	B	674	ASP
1	B	676	LEU
1	B	691	LEU
1	B	705	ASN
1	B	712	GLN
1	B	716	LEU
1	B	731	GLN
1	B	735	VAL
1	B	775	LEU
1	B	789	LYS
1	B	815	LEU
1	B	818	ASN
1	B	833	TYR
1	B	843	LEU
1	B	873	THR
1	B	937	THR
1	B	939	GLN
1	B	959	ASP
1	B	962	HIS
2	C	844	ARG
2	C	847	ILE
2	C	852	VAL
2	C	858	VAL
2	C	860	ARG
2	C	900	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	623	GLN
1	A	663	GLN
1	A	689	HIS
1	A	818	ASN
1	A	836	HIS
1	A	866	HIS
1	A	870	GLN
1	A	939	GLN
1	A	940	ASN
1	A	952	GLN
1	A	953	HIS
1	B	586	GLN
1	B	604	GLN
1	B	689	HIS
1	B	731	GLN
1	B	761	ASN
1	B	836	HIS
1	B	870	GLN
1	B	899	ASN
1	B	922	GLN
1	B	949	GLN
1	B	953	HIS
2	C	861	GLN
2	C	892	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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, 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	395/471 (83%)	-0.04	14 (3%) 44 18	44, 102, 200, 240	0
1	B	394/471 (83%)	0.02	18 (4%) 32 12	41, 108, 203, 239	0
2	C	86/90 (95%)	-0.39	0 100 100	43, 67, 105, 152	0
All	All	875/1032 (84%)	-0.05	32 (3%) 41 17	41, 98, 201, 240	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	GLU	5.9
1	B	580	ASP	5.0
1	B	604	GLN	4.4
1	B	621	CYS	4.3
1	B	918	LEU	4.1
1	A	914	LYS	4.0
1	B	572	ASP	3.9
1	B	591	THR	3.7
1	B	917	GLN	3.3
1	A	912	SER	3.1
1	B	614	GLN	3.1
1	A	651	PRO	3.1
1	A	612	SER	3.1
1	A	607	GLU	2.9
1	A	603	ASP	2.8
1	B	615	LEU	2.7
1	A	581	LYS	2.6
1	B	651	PRO	2.6
1	B	584	GLN	2.5
1	B	583	LEU	2.5
1	A	582	VAL	2.5
1	A	915	LEU	2.5
1	B	607	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	580	ASP	2.4
1	A	608	GLU	2.4
1	B	617	VAL	2.4
1	A	619	ALA	2.3
1	B	913	SER	2.2
1	A	665	ASP	2.2
1	B	964	MET	2.1
1	A	586	GLN	2.1
1	B	585	LEU	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.