



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4US2 / pdb_00004us2
Title : The crystal structure of H-Ras and SOS in complex with ligands
Authors : Winter, J.J.G.; Anderson, M.; Blades, K.; Brassington, C.; Breeze, A.L.; Chresta, C.; Embrey, K.; Fairley, G.; Faulder, P.; Finlay, M.R.V.; Kettle, J.G.; Nowak, T.; Overman, R.; Patel, S.J.; Perkins, P.; Spadola, L.; Tart, J.; Tucker, J.; Wrigley, G.
Deposited on : 2014-07-02
Resolution : 2.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

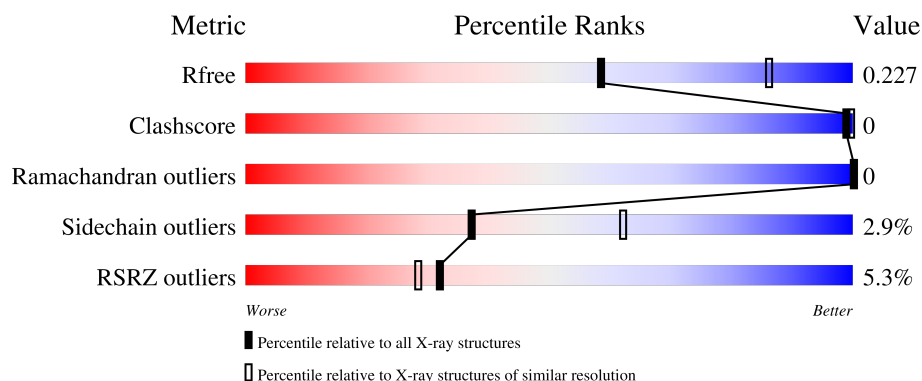
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	R	185	7% 86% • 10%
2	S	487	4% 90% • • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5378 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 GTPASE HRAS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	167	Total	C	N	O	S	0	1	0
			1331	829	230	265	7			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-18	MET	-	expression tag	UNP P01112
R	-17	HIS	-	expression tag	UNP P01112
R	-16	HIS	-	expression tag	UNP P01112
R	-15	HIS	-	expression tag	UNP P01112
R	-14	HIS	-	expression tag	UNP P01112
R	-13	HIS	-	expression tag	UNP P01112
R	-12	HIS	-	expression tag	UNP P01112
R	-11	GLY	-	expression tag	UNP P01112
R	-10	GLY	-	expression tag	UNP P01112
R	-9	GLY	-	expression tag	UNP P01112
R	-8	GLU	-	expression tag	UNP P01112
R	-7	ASN	-	expression tag	UNP P01112
R	-6	LEU	-	expression tag	UNP P01112
R	-5	TYR	-	expression tag	UNP P01112
R	-4	PHE	-	expression tag	UNP P01112
R	-3	GLN	-	expression tag	UNP P01112
R	-2	GLY	-	expression tag	UNP P01112
R	-1	SER	-	expression tag	UNP P01112
R	0	HIS	-	expression tag	UNP P01112

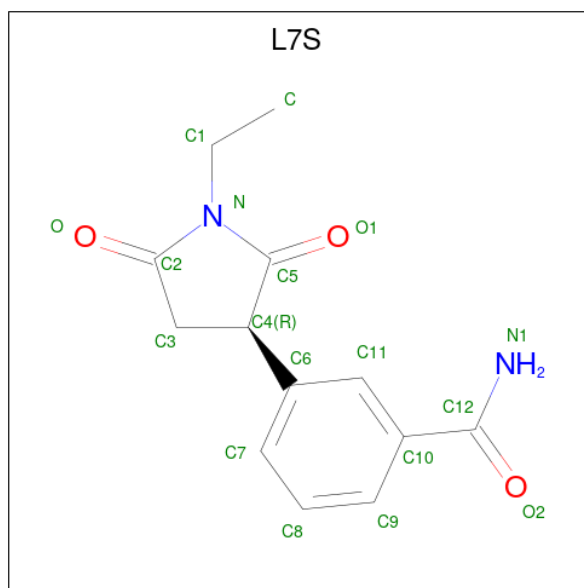
- Molecule 2 is a protein called SON OF SEVENLESS HOMOLOG 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	454	Total	C	N	O	S	0	0	1
			3729	2394	642	679	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	563	MET	-	expression tag	UNP Q07889

- Molecule 3 is 3-[(3R)-1-ethyl-2,5-dioxypyrrolidin-3-yl]benzamide (CCD ID: L7S) (formula: $C_{13}H_{14}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	R	1	Total	C	N	O	0	0
			18	13	2	3		

- Molecule 4 is water.

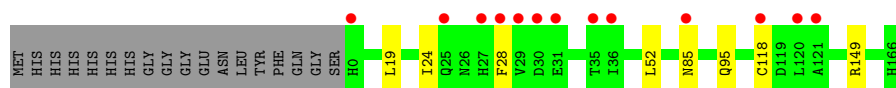
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	114	Total	O	0	0
			114	114		
4	S	186	Total	O	0	0
			186	186		

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.

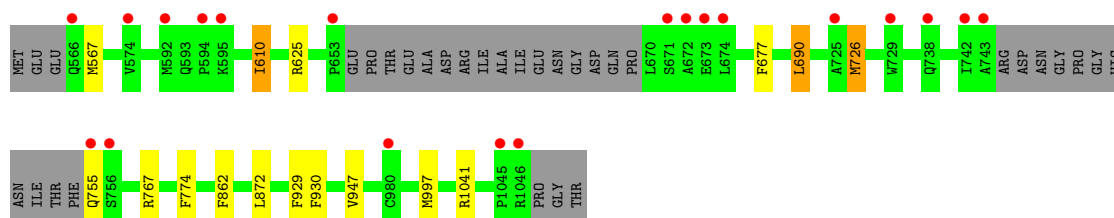
- Molecule 1: GTPASE HRAS

Chain R: 



- Molecule 2: SON OF SEVENLESS HOMOLOG 1

Chain S: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.71Å 149.71Å 200.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.93 – 2.48 52.93 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.8 (52.93-2.48) 96.8 (52.93-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.190 , 0.228 0.188 , 0.227	Depositor DCC
R_{free} test set	1963 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5378	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: L7S

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	R	0.89	0/1352	1.05	0/1823
2	S	0.84	2/3820 (0.1%)	1.14	2/5173 (0.0%)
All	All	0.85	2/5172 (0.0%)	1.12	2/6996 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	610	ILE	CG1-CD1	-5.70	1.29	1.51
2	S	997	MET	SD-CE	-5.29	1.66	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	774	PHE	CA-CB-CG	6.44	120.24	113.80
2	S	862	PHE	CA-CB-CG	5.36	119.16	113.80

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	R	1331	0	1305	1	0
2	S	3729	0	3707	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	18	0	12	1	0
4	R	114	0	0	0	0
4	S	186	0	0	0	0
All	All	5378	0	5024	4	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 0.

All (4) 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:R:85:ASN:HB2	3:R:1167:L7S:O	2.04	0.58
2:S:567:MET:CE	2:S:677:PHE:HA	2.48	0.42
2:S:690:LEU:HD22	2:S:726:MET:HE2	2.02	0.42
2:S:872:LEU:HD12	2:S:929:PHE:HB2	2.01	0.41

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	R	166/185 (90%)	163 (98%)	3 (2%)	0	100	100
2	S	448/487 (92%)	442 (99%)	6 (1%)	0	100	100
All	All	614/672 (91%)	605 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	R	144/159 (91%)	136 (94%)	8 (6%)	19	37
2	S	413/452 (91%)	404 (98%)	9 (2%)	45	70
All	All	557/611 (91%)	540 (97%)	17 (3%)	37	60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	19	LEU
1	R	24	ILE
1	R	28	PHE
1	R	52	LEU
1	R	95	GLN
1	R	118	CYS
1	R	149[A]	ARG
1	R	149[B]	ARG
2	S	610	ILE
2	S	625	ARG
2	S	690	LEU
2	S	726	MET
2	S	755	GLN
2	S	767	ARG
2	S	930	PHE
2	S	947	VAL
2	S	1041	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	25	GLN
1	R	61	GLN
1	R	116	ASN
2	S	764	HIS
2	S	770	HIS

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Mol	Chain	Res	Type
2	S	869	ASN
2	S	879	ASN
2	S	999	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	L7S	R	1167	1	19,19,19	0.60	0	26,27,27	2.08	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	L7S	R	1167	1	-	6/10/26/26	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1167	L7S	C4-C3-C2	-7.62	100.42	105.67
3	R	1167	L7S	C3-C4-C6	6.03	126.36	115.42
3	R	1167	L7S	C3-C4-C5	2.56	104.79	103.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1167	L7S	C9-C10-C12-N1
3	R	1167	L7S	C9-C10-C12-O2
3	R	1167	L7S	C11-C10-C12-N1
3	R	1167	L7S	C11-C10-C12-O2
3	R	1167	L7S	C3-C4-C6-C7
3	R	1167	L7S	C3-C4-C6-C11

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1167	L7S	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	167/185 (90%)	-0.04	13 (7%) 19 16	27, 40, 76, 90	1 (0%)
2	S	454/487 (93%)	0.10	20 (4%) 39 35	29, 48, 86, 112	0
All	All	621/672 (92%)	0.06	33 (5%) 32 28	27, 45, 85, 112	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	743	ALA	6.2
2	S	594	PRO	5.3
1	R	29	VAL	5.1
2	S	673	GLU	4.7
2	S	1046	ARG	4.7
1	R	118	CYS	4.4
1	R	120	LEU	4.3
2	S	729	TRP	4.1
1	R	27	HIS	3.9
2	S	672	ALA	3.5
2	S	980	CYS	3.2
2	S	742	ILE	3.1
2	S	574	VAL	3.0
1	R	28	PHE	2.9
2	S	755	GLN	2.9
1	R	30	ASP	2.7
2	S	674	LEU	2.7
2	S	725	ALA	2.7
2	S	595	LYS	2.6
2	S	756	SER	2.6
2	S	671	SER	2.6
1	R	31	GLU	2.5
1	R	0	HIS	2.5
1	R	121	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	85	ASN	2.5
2	S	653	PRO	2.5
2	S	566	GLN	2.3
1	R	35	THR	2.3
2	S	1045	PRO	2.2
1	R	25	GLN	2.1
2	S	738	GLN	2.1
1	R	36	ILE	2.0
2	S	592	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	L7S	R	1167	18/18	0.76	0.26	64,72,73,75	18

6.5 Other polymers [i](#)

There are no such residues in this entry.