



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8BE9  
Title : Crystal structure of SOS1-HRas-peptidomimetic5  
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Deposited on : 2022-10-21  
Resolution : 2.51 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.2  
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) : 2.32.2

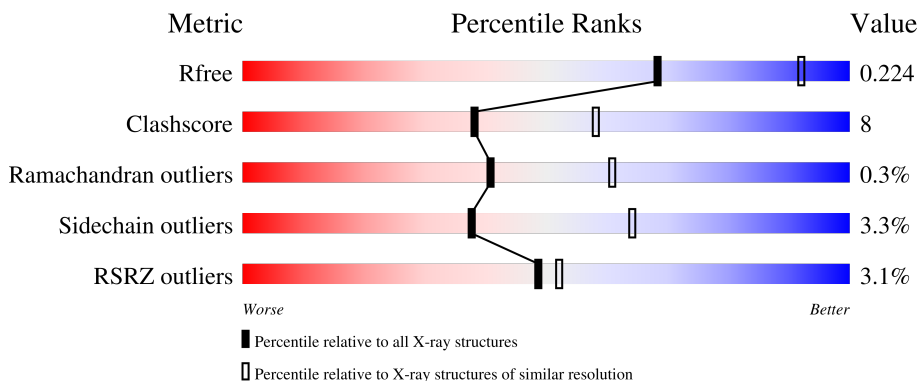
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	186	 2% 76% 13% 11%
2	S	507	 3% 69% 18% 12%
3	P	9	 11% 33% 33% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XSN	P	9	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5382 atoms, of which 86 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
			Total	C	N	O	S			
1	R	166	1322	824	228	263	7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-19	MET	-	initiating methionine	UNP P01112
R	-18	GLY	-	expression tag	UNP P01112
R	-17	SER	-	expression tag	UNP P01112
R	-16	SER	-	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	HIS	-	expression tag	UNP P01112
R	-10	HIS	-	expression tag	UNP P01112
R	-9	SER	-	expression tag	UNP P01112
R	-8	SER	-	expression tag	UNP P01112
R	-7	GLY	-	expression tag	UNP P01112
R	-6	LEU	-	expression tag	UNP P01112
R	-5	VAL	-	expression tag	UNP P01112
R	-4	PRO	-	expression tag	UNP P01112
R	-3	ARG	-	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
			Total	C	N	O	S			
2	S	446	3724	2396	641	673	14	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	543	MET	-	initiating methionine	UNP Q07889
S	544	GLY	-	expression tag	UNP Q07889
S	545	SER	-	expression tag	UNP Q07889
S	546	SER	-	expression tag	UNP Q07889
S	547	HIS	-	expression tag	UNP Q07889
S	548	HIS	-	expression tag	UNP Q07889
S	549	HIS	-	expression tag	UNP Q07889
S	550	HIS	-	expression tag	UNP Q07889
S	551	HIS	-	expression tag	UNP Q07889
S	552	HIS	-	expression tag	UNP Q07889
S	553	SER	-	expression tag	UNP Q07889
S	554	SER	-	expression tag	UNP Q07889
S	555	GLY	-	expression tag	UNP Q07889
S	556	LEU	-	expression tag	UNP Q07889
S	557	VAL	-	expression tag	UNP Q07889
S	558	PRO	-	expression tag	UNP Q07889
S	559	ARG	-	expression tag	UNP Q07889
S	560	GLY	-	expression tag	UNP Q07889
S	561	SER	-	expression tag	UNP Q07889
S	562	HIS	-	expression tag	UNP Q07889
S	563	MET	-	expression tag	UNP Q07889

- Molecule 3 is a protein called SOS1-HRas-peptidomimetic5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	N	O		
3	P	9	153	53	72	17	11	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	R	3	3	3	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	R	1	4	1	1	2	0	0
5	R	1	4	1	1	2	0	0
5	R	1	4	1	1	2	0	0
5	R	1	4	1	1	2	0	0
5	R	1	4	1	1	2	0	0
5	R	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0
5	S	1	4	1	1	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	37	Total 37	O 37	0	0
6	S	85	Total 85	O 85	0	0
6	P	2	Total 2	O 2	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.41Å 150.41Å 200.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.51 48.65 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.65-2.51) 99.2 (48.65-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.190 , 0.229 0.189 , 0.224	Depositor DCC
$R_{free}$ test set	1968 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, FMT, XSN, 7XC

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	0.47	0/1341	0.63	0/1810
2	S	0.46	0/3813	0.61	0/5153
3	P	3.31	8/60 (13.3%)	1.80	1/80 (1.2%)
All	All	0.58	8/5214 (0.2%)	0.64	1/7043 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	4	PRO	N-CD	-10.56	1.33	1.47
3	P	4	PRO	CA-CB	-9.36	1.34	1.53
3	P	7	VAL	C-N	8.52	1.53	1.34
3	P	6	SER	C-N	7.63	1.51	1.34
3	P	4	PRO	N-CA	7.53	1.60	1.47
3	P	4	PRO	C-N	6.87	1.49	1.34
3	P	3	HIS	C-N	6.32	1.46	1.34
3	P	3	HIS	CB-CG	5.15	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	LYS	CB-CA-C	-7.04	96.31	110.40

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	1322	0	1296	16	0
2	S	3724	0	3752	61	0
3	P	81	72	62	3	0
4	R	3	0	0	0	0
5	R	18	6	6	0	0
5	S	24	8	8	0	0
6	P	2	0	0	0	0
6	R	37	0	0	1	0
6	S	85	0	0	1	0
All	All	5296	86	5124	78	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 8.

All (78) 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)
2:S:741:LYS:O	2:S:742:ILE:HG13	1.64	0.98
2:S:576:ARG:HD3	2:S:646:GLU:OE2	1.64	0.97
2:S:1043:SER:O	2:S:1044:ASN:HB2	1.82	0.79
1:R:119:ASP:HB3	1:R:121:ALA:H	1.53	0.71
2:S:598:ILE:HG23	2:S:599:PRO:HD2	1.73	0.70
1:R:26:ASN:HB2	1:R:29:VAL:CG2	2.24	0.67
1:R:84:ILE:HD12	1:R:123:ARG:CZ	2.24	0.67
2:S:1033:TYR:HB2	2:S:1034:PRO:HD2	1.79	0.65
2:S:586:ILE:HD11	2:S:608:LYS:HB3	1.79	0.63
2:S:589:GLU:HG2	2:S:592:MET:SD	2.39	0.62
2:S:847:GLU:HG2	2:S:1035:LEU:HD11	1.83	0.61
1:R:29:VAL:HG13	6:R:302:HOH:O	2.01	0.60
2:S:735:LYS:HD3	2:S:735:LYS:C	2.23	0.59
2:S:724:LYS:O	2:S:724:LYS:HD3	2.03	0.57
1:R:26:ASN:HB2	1:R:29:VAL:HG23	1.86	0.57
3:P:8:ALA:O	3:P:9:XSN:N1	2.38	0.56
2:S:674:LEU:O	2:S:678:ARG:HG3	2.05	0.56
1:R:26:ASN:HB2	1:R:29:VAL:HG21	1.89	0.54
2:S:716:GLU:O	2:S:720:THR:HG23	2.08	0.54
2:S:677:PHE:CE2	2:S:682:ILE:HD11	2.43	0.54
3:P:2:7XC:O	3:P:3:HIS:HB2	2.09	0.53
2:S:1020:ASN:N	2:S:1021:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:616:HIS:HB3	2:S:685:VAL:HG23	1.92	0.52
2:S:1019:ARG:C	2:S:1021:PRO:HD2	2.30	0.51
2:S:796:TYR:CE1	2:S:928:PRO:HG2	2.46	0.50
2:S:763:TRP:CE2	2:S:768:PRO:HG3	2.47	0.50
2:S:683:GLN:HB3	2:S:684:PRO:HD3	1.93	0.50
2:S:606:VAL:O	2:S:610:ILE:HG12	2.11	0.49
2:S:697:VAL:HG12	2:S:736:ILE:CG2	2.42	0.49
2:S:782:ILE:HD11	2:S:1040:VAL:C	2.33	0.49
2:S:807:SER:HA	2:S:809:TRP:CZ3	2.48	0.49
2:S:683:GLN:HB3	2:S:684:PRO:CD	2.43	0.49
2:S:586:ILE:HG13	2:S:608:LYS:HG3	1.93	0.49
3:P:1:LYS:O	3:P:1:LYS:HG3	2.12	0.48
1:R:24:ILE:HD12	1:R:39:SER:O	2.12	0.48
2:S:674:LEU:H	2:S:674:LEU:HD22	1.78	0.48
2:S:598:ILE:CG2	2:S:599:PRO:HD2	2.40	0.48
1:R:157:TYR:O	1:R:161:ARG:HG3	2.14	0.48
2:S:872:LEU:HD12	2:S:929:PHE:HB2	1.95	0.48
2:S:771:ILE:HD11	2:S:986:ASP:CG	2.34	0.48
2:S:1033:TYR:HB2	2:S:1034:PRO:CD	2.43	0.47
1:R:73:ARG:NH1	2:S:879:ASN:O	2.48	0.47
2:S:583:GLU:HA	2:S:583:GLU:OE1	2.15	0.47
2:S:915:TYR:CE2	2:S:932:ILE:HD12	2.50	0.46
2:S:735:LYS:HD3	2:S:735:LYS:O	2.14	0.46
2:S:764:HIS:CE1	2:S:1038:PRO:HD3	2.50	0.46
2:S:586:ILE:CG1	2:S:608:LYS:HB3	2.46	0.46
2:S:1024:LEU:HD12	2:S:1025:PRO:HD2	1.98	0.46
2:S:586:ILE:CD1	2:S:608:LYS:HB3	2.44	0.45
2:S:938:LEU:HD11	2:S:942:GLU:OE2	2.17	0.45
1:R:24:ILE:CD1	1:R:40:TYR:HA	2.47	0.45
2:S:675:LYS:HD3	2:S:676:ARG:N	2.32	0.45
1:R:67:MET:HG2	2:S:876:SER:OG	2.16	0.44
2:S:582:SER:H	2:S:585:ASN:HB2	1.82	0.44
2:S:724:LYS:NZ	2:S:727:LYS:HD2	2.32	0.44
2:S:898:LYS:HE3	6:S:1212:HOH:O	2.16	0.44
2:S:941:GLU:HA	2:S:960:LYS:HE2	2.00	0.44
2:S:906:GLU:OE1	2:S:909:GLU:HG3	2.17	0.44
2:S:764:HIS:CD2	2:S:765:ILE:HG13	2.52	0.44
2:S:1043:SER:O	2:S:1044:ASN:CB	2.57	0.44
2:S:754:PHE:CD1	2:S:755:GLN:N	2.87	0.43
1:R:24:ILE:CD1	1:R:39:SER:O	2.67	0.43
2:S:733:ILE:O	2:S:737:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:27:HIS:HA	1:R:149:ARG:NH1	2.34	0.43
2:S:679:LYS:O	2:S:679:LYS:HG3	2.18	0.43
2:S:684:PRO:O	2:S:688:ARG:HG2	2.19	0.43
2:S:724:LYS:O	2:S:724:LYS:CD	2.66	0.43
2:S:742:ILE:O	2:S:742:ILE:HG22	2.17	0.43
2:S:796:TYR:CZ	2:S:928:PRO:HG2	2.54	0.43
2:S:1023:PRO:O	2:S:1025:PRO:HD3	2.20	0.42
2:S:911:HIS:O	2:S:912:TYR:HB2	2.19	0.42
1:R:117:LYS:O	1:R:117:LYS:HG2	2.20	0.42
2:S:634:PHE:CD1	2:S:956:ILE:HD13	2.55	0.42
2:S:926:CYS:HA	2:S:979:TYR:OH	2.20	0.41
1:R:141:TYR:OH	1:R:143:GLU:HG2	2.21	0.41
2:S:809:TRP:CZ2	2:S:934:LEU:HB3	2.56	0.40
1:R:22:GLN:HE22	1:R:146:ALA:HA	1.85	0.40
2:S:947:VAL:HG21	2:S:954:GLU:HG2	2.03	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	R	164/186 (88%)	161 (98%)	3 (2%)	0	100	100
2	S	439/507 (87%)	428 (98%)	11 (2%)	0	100	100
3	P	6/9 (67%)	4 (67%)	0	2 (33%)	0	0
All	All	609/702 (87%)	593 (97%)	14 (2%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	3	HIS
3	P	7	VAL

### 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	R	144/161 (89%)	140 (97%)	4 (3%)	43	70
2	S	419/469 (89%)	405 (97%)	14 (3%)	38	64
3	P	6/6 (100%)	5 (83%)	1 (17%)	2	4
All	All	569/636 (90%)	550 (97%)	19 (3%)	38	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	30	ASP
1	R	38	ASP
1	R	112	VAL
1	R	120	LEU
2	S	579	GLU
2	S	615	TYR
2	S	673	GLU
2	S	727	LYS
2	S	728	LYS
2	S	739	ARG
2	S	808	VAL
2	S	830	ASN
2	S	930	PHE
2	S	947	VAL
2	S	953	LYS
2	S	960	LYS
2	S	973	GLN
2	S	1041	ARG
3	P	1	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	897	GLN
2	S	923	ASN

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Mol	Chain	Res	Type
2	S	973	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	XSN	P	9	3	7,7,8	2.85	2 (28%)	7,8,10	1.76	2 (28%)
3	7XC	P	2	3	14,15,16	2.96	6 (42%)	16,19,21	1.04	2 (12%)

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	XSN	P	9	3	-	6/7/7/8	-
3	7XC	P	2	3	-	2/9/10/12	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	2	7XC	C10-N2	8.31	1.47	1.37
3	P	9	XSN	C-N1	6.43	1.49	1.32
3	P	2	7XC	CB-CG	4.30	1.61	1.51
3	P	9	XSN	CB-CG	3.23	1.58	1.49
3	P	2	7XC	CZ-N2	2.81	1.47	1.41
3	P	2	7XC	C10-N4	2.71	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	2	7XC	CD1-CG	2.41	1.44	1.38
3	P	2	7XC	CE2-CZ	2.20	1.42	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	9	XSN	O-C-N1	-3.12	117.58	123.00
3	P	9	XSN	CA-C-N1	2.85	121.58	116.68
3	P	2	7XC	CZ-N2-C10	-2.72	121.27	127.85
3	P	2	7XC	CG-CB-CA	2.65	119.46	114.10

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	9	XSN	O-C-CA-CB
3	P	9	XSN	N1-C-CA-N
3	P	9	XSN	N1-C-CA-CB
3	P	9	XSN	C-CA-CB-CG
3	P	9	XSN	N-CA-CB-CG
3	P	9	XSN	O-C-CA-N
3	P	2	7XC	CA-CB-CG-CD1
3	P	2	7XC	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	9	XSN	1	0
3	P	2	7XC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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
5	FMT	S	1104	-	2,2,2	0.61	0	1,1,1	0.30	0
5	FMT	R	208	-	2,2,2	0.60	0	1,1,1	0.36	0
5	FMT	R	206	-	2,2,2	0.66	0	1,1,1	0.42	0
5	FMT	S	1101	-	2,2,2	0.69	0	1,1,1	0.51	0
5	FMT	S	1102	-	2,2,2	0.71	0	1,1,1	0.43	0
5	FMT	R	207	-	2,2,2	0.66	0	1,1,1	0.30	0
5	FMT	S	1105	-	2,2,2	0.64	0	1,1,1	0.39	0
5	FMT	S	1108	-	2,2,2	0.66	0	1,1,1	0.41	0
5	FMT	R	204	-	2,2,2	0.67	0	1,1,1	0.40	0
5	FMT	S	1103	-	2,2,2	0.66	0	1,1,1	0.38	0
5	FMT	S	1107	-	2,2,2	0.60	0	1,1,1	0.28	0
5	FMT	R	209	-	2,2,2	0.60	0	1,1,1	0.28	0
5	FMT	R	205	-	2,2,2	0.68	0	1,1,1	0.24	0
5	FMT	S	1106	-	2,2,2	0.67	0	1,1,1	0.39	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	R	166/186 (89%)	0.07	4 (2%) 59 62	45, 54, 82, 104	0
2	S	446/507 (87%)	0.22	15 (3%) 45 48	43, 60, 96, 121	0
3	P	7/9 (77%)	0.46	0 100 100	53, 61, 103, 112	0
All	All	619/702 (88%)	0.19	19 (3%) 49 52	43, 58, 96, 121	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	118	CYS	4.2
1	R	27	HIS	4.0
2	S	573	ASP	3.8
2	S	591	ASN	3.5
2	S	653	PRO	3.5
1	R	30	ASP	3.4
1	R	120	LEU	3.3
2	S	677	PHE	3.2
2	S	572	ALA	3.1
2	S	569	LEU	3.0
2	S	574	VAL	2.9
2	S	674	LEU	2.8
2	S	1022	LYS	2.8
2	S	1020	ASN	2.4
2	S	568	ARG	2.1
2	S	673	GLU	2.1
2	S	678	ARG	2.1
2	S	680	GLU	2.0
2	S	679	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	XSN	P	9	8/9	0.78	0.34	118,128,147,148	0
3	7XC	P	2	15/16	0.86	0.25	70,80,99,102	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
5	FMT	S	1104	3/3	0.59	0.27	78,80,84,100	0
5	FMT	R	207	3/3	0.71	0.30	84,86,92,111	0
5	FMT	S	1105	3/3	0.83	0.14	80,80,81,97	0
5	FMT	S	1103	3/3	0.87	0.35	69,80,84,96	0
5	FMT	R	205	3/3	0.87	0.33	67,71,73,88	0
4	CL	R	203	1/1	0.87	0.15	86,86,86,86	0
5	FMT	S	1107	3/3	0.87	0.21	66,73,77,92	0
5	FMT	S	1106	3/3	0.88	0.17	76,77,77,92	0
5	FMT	R	209	3/3	0.89	0.19	65,72,74,87	0
4	CL	R	201	1/1	0.89	0.10	79,79,79,79	0
5	FMT	R	208	3/3	0.89	0.27	74,75,79,89	0
5	FMT	S	1108	3/3	0.90	0.27	77,80,82,96	0
5	FMT	S	1102	3/3	0.93	0.22	74,78,79,94	0
4	CL	R	202	1/1	0.94	0.08	79,79,79,79	0
5	FMT	R	206	3/3	0.94	0.13	67,77,82,92	0
5	FMT	R	204	3/3	0.94	0.17	72,74,75,89	0
5	FMT	S	1101	3/3	0.97	0.22	59,65,69,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.