



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:44 PM GMT

PDB ID : 3URK  
Title : IspH in complex with propynyl diphosphate (1061)  
Authors : Span, I.; Wang, K.; Wang, W.; Zhang, Y.; Bacher, A.; Eisenreich, W.; Schulz, C.; Oldfield, E.; Groll, M.  
Deposited on : 2011-11-22  
Resolution : 1.50 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  
<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

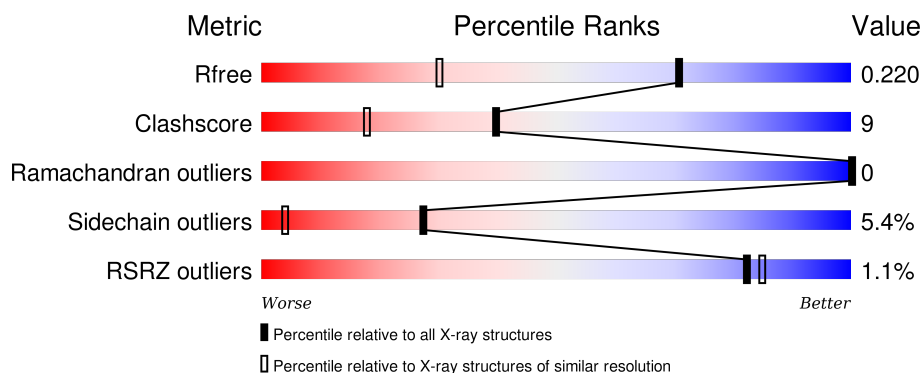
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	324	<div> <div></div> <div>80%12%••5%</div> </div>
1	B	324	<div> <div></div> <div>80%12%••</div> </div>

## 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 4-hydroxy-3-methylbut-2-enyl diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2383	1487	427	459	10			
1	B	310	Total	C	N	O	S	0	0	0
			2390	1492	428	460	10			

There are 16 discrepancies between the modelled and reference sequences:

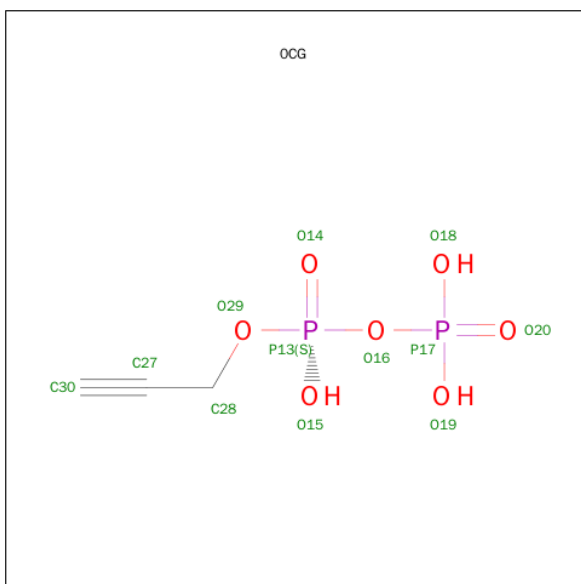
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	EXPRESSION TAG	UNP P62623
A	-6	HIS	-	EXPRESSION TAG	UNP P62623
A	-5	HIS	-	EXPRESSION TAG	UNP P62623
A	-4	HIS	-	EXPRESSION TAG	UNP P62623
A	-3	HIS	-	EXPRESSION TAG	UNP P62623
A	-2	HIS	-	EXPRESSION TAG	UNP P62623
A	-1	GLY	-	EXPRESSION TAG	UNP P62623
A	0	SER	-	EXPRESSION TAG	UNP P62623
B	-7	HIS	-	EXPRESSION TAG	UNP P62623
B	-6	HIS	-	EXPRESSION TAG	UNP P62623
B	-5	HIS	-	EXPRESSION TAG	UNP P62623
B	-4	HIS	-	EXPRESSION TAG	UNP P62623
B	-3	HIS	-	EXPRESSION TAG	UNP P62623
B	-2	HIS	-	EXPRESSION TAG	UNP P62623
B	-1	GLY	-	EXPRESSION TAG	UNP P62623
B	0	SER	-	EXPRESSION TAG	UNP P62623

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is PROP-2-YN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: OCG) (formula:  $C_3H_6O_7P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			12	3	7	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			12	3	7	2		

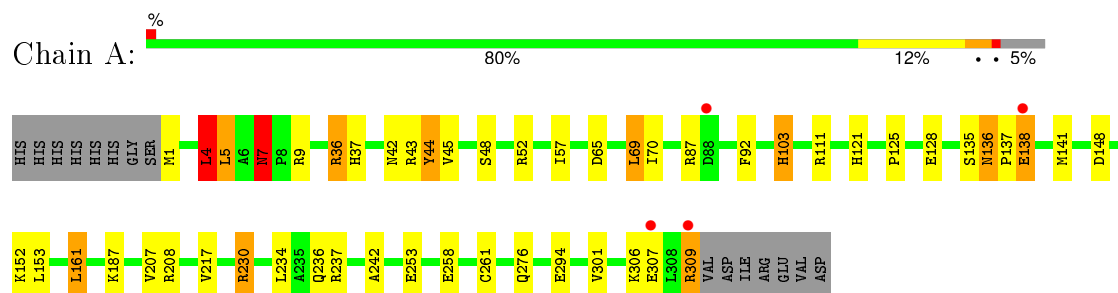
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	0
			279	279		
4	B	286	Total	O	0	0
			286	286		

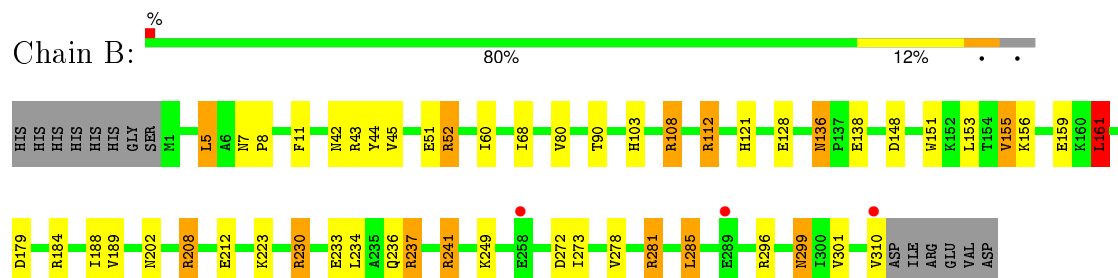
### 3 Residue-property plots [i](#)

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: 4-hydroxy-3-methylbut-2-enyl diphosphate reductase



- Molecule 1: 4-hydroxy-3-methylbut-2-enyl diphosphate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.63Å 80.57Å 111.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.98 – 1.50 47.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.98-1.50) 99.0 (47.98-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.161 , 0.212 0.171 , 0.220	Depositor DCC
$R_{free}$ test set	5082 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 101625 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4531e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, OCG

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	1.25	5/2418 (0.2%)	1.60	18/3273 (0.5%)
1	B	1.22	5/2425 (0.2%)	1.60	30/3283 (0.9%)
All	All	1.24	10/4843 (0.2%)	1.60	48/6556 (0.7%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	ARG	CZ-NH2	9.57	1.45	1.33
1	A	230	ARG	CD-NE	-8.91	1.31	1.46
1	A	7	ASN	CB-CG	-7.63	1.33	1.51
1	B	230	ARG	CD-NE	-7.45	1.33	1.46
1	B	237	ARG	CD-NE	-7.32	1.34	1.46
1	A	7	ASN	CG-ND2	6.28	1.48	1.32
1	A	138	GLU	CG-CD	6.23	1.61	1.51
1	A	44	TYR	CE2-CZ	-5.73	1.31	1.38
1	B	189	VAL	CB-CG2	-5.61	1.41	1.52
1	B	278	VAL	CB-CG2	-5.06	1.42	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH1	-49.06	95.77	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH2	36.51	138.55	120.30
1	B	230	ARG	NE-CZ-NH1	-34.26	103.17	120.30
1	B	230	ARG	NE-CZ-NH2	24.10	132.35	120.30
1	B	184	ARG	NE-CZ-NH1	-23.25	108.68	120.30
1	B	281	ARG	NE-CZ-NH1	21.78	131.19	120.30
1	B	237	ARG	NE-CZ-NH2	18.18	129.39	120.30
1	A	230	ARG	CD-NE-CZ	14.62	144.07	123.60
1	B	184	ARG	NE-CZ-NH2	13.36	126.98	120.30
1	B	281	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	A	36	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	A	161	LEU	CB-CG-CD2	10.66	129.12	111.00
1	B	281	ARG	CD-NE-CZ	10.29	138.00	123.60
1	B	52	ARG	NE-CZ-NH2	10.09	125.35	120.30
1	B	241	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	B	230	ARG	CD-NE-CZ	9.84	137.38	123.60
1	B	230	ARG	CG-CD-NE	-9.52	91.80	111.80
1	B	52	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	B	241	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	B	237	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	A	230	ARG	CG-CD-NE	-8.19	94.60	111.80
1	B	237	ARG	CB-CG-CD	7.97	132.31	111.60
1	A	4	LEU	CB-CG-CD1	7.38	123.55	111.00
1	A	237	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	223	LYS	CD-CE-NZ	6.99	127.79	111.70
1	A	43	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	285	LEU	CB-CG-CD1	6.91	122.74	111.00
1	B	161	LEU	CB-CG-CD2	6.87	122.68	111.00
1	A	5	LEU	CB-CG-CD1	6.86	122.67	111.00
1	A	208	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	A	69	LEU	CB-CG-CD1	6.21	121.55	111.00
1	B	281	ARG	CB-CG-CD	6.18	127.67	111.60
1	B	151	TRP	CA-CB-CG	6.03	125.15	113.70
1	A	65	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	234	LEU	CB-CG-CD2	5.77	120.81	111.00
1	A	141	MET	CG-SD-CE	5.74	109.39	100.20
1	A	9	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	208	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	43	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	5	LEU	CB-CG-CD2	5.47	120.31	111.00
1	B	5	LEU	CB-CG-CD1	5.46	120.28	111.00
1	B	155	VAL	CA-CB-CG1	5.34	118.91	110.90
1	B	208	ARG	NE-CZ-NH1	-5.28	117.66	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	B	179	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	234	LEU	CB-CG-CD2	5.12	119.71	111.00
1	A	87	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	296	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ASN	Sidechain

## 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	2383	0	2395	50	0
1	B	2390	0	2404	36	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	12	0	5	0	0
3	B	12	0	6	0	0
4	A	279	0	0	32	0
4	B	286	0	0	16	0
All	All	5378	0	4810	85	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 (85) 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:276:GLN:HG2	4:A:529:HOH:O	1.20	1.33
1:B:121:HIS:HD2	4:B:377:HOH:O	1.15	1.29
1:A:121:HIS:HD2	4:A:566:HOH:O	0.88	1.22

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:HIS:HB3	4:B:514:HOH:O	1.05	1.19
1:A:36:ARG:HH21	1:A:36:ARG:HG2	1.02	1.12
1:A:121:HIS:CD2	4:A:566:HOH:O	1.71	1.04
1:A:36:ARG:NH2	1:A:36:ARG:HG2	1.64	0.95
1:B:237:ARG:HD3	4:B:532:HOH:O	1.67	0.94
1:A:36:ARG:CG	1:A:36:ARG:HH21	1.78	0.89
1:B:51:GLU:OE2	1:B:52:ARG:HD2	1.77	0.85
1:A:128:GLU:HG3	4:A:429:HOH:O	1.79	0.82
1:A:121:HIS:CE1	4:A:409:HOH:O	2.31	0.82
1:A:148:ASP:HB3	4:A:481:HOH:O	1.81	0.81
1:A:128:GLU:CG	4:A:429:HOH:O	2.29	0.81
1:B:7:ASN:HB3	4:B:599:HOH:O	1.80	0.79
1:B:121:HIS:CD2	4:B:377:HOH:O	2.03	0.79
1:B:7:ASN:CB	4:B:599:HOH:O	2.31	0.79
1:B:68:ILE:HD13	1:B:90:THR:HB	1.64	0.79
1:B:42:ASN:HD22	1:B:45:VAL:H	1.30	0.78
1:B:236:GLN:HG2	4:B:404:HOH:O	1.81	0.78
1:A:7:ASN:ND2	4:A:402:HOH:O	2.11	0.77
1:A:7:ASN:CG	4:A:551:HOH:O	2.21	0.77
1:B:112:ARG:HG3	1:B:112:ARG:HH21	1.55	0.71
1:B:103:HIS:HD2	4:B:449:HOH:O	1.73	0.70
1:B:272:ASP:OD2	4:B:580:HOH:O	2.10	0.69
1:A:42:ASN:HD22	1:A:45:VAL:H	1.39	0.68
1:B:241:ARG:HD3	4:B:604:HOH:O	1.93	0.68
1:A:306:LYS:HA	1:A:309:ARG:HD3	1.75	0.67
1:A:253:GLU:HG3	4:A:489:HOH:O	1.96	0.66
1:A:48:SER:C	4:A:584:HOH:O	2.34	0.65
1:A:103:HIS:HD2	4:A:514:HOH:O	1.80	0.63
1:A:136:ASN:ND2	1:A:138:GLU:H	1.96	0.63
1:A:52:ARG:CD	4:A:584:HOH:O	2.47	0.62
1:B:136:ASN:ND2	1:B:138:GLU:H	1.99	0.60
1:B:249:LYS:HD3	4:B:564:HOH:O	2.02	0.60
1:A:37:HIS:CG	4:A:568:HOH:O	2.55	0.59
1:A:148:ASP:CB	4:A:481:HOH:O	2.45	0.58
1:B:136:ASN:HD22	1:B:138:GLU:H	1.50	0.58
1:A:52:ARG:HD3	4:A:584:HOH:O	2.03	0.57
1:B:108:ARG:CZ	1:B:108:ARG:HB2	2.34	0.57
1:A:128:GLU:HG2	4:A:429:HOH:O	2.01	0.56
1:B:112:ARG:CG	1:B:112:ARG:HH21	2.19	0.56
1:A:135:SER:O	1:A:137:PRO:HD3	2.05	0.56
1:B:128:GLU:HG2	4:B:434:HOH:O	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:HD22	1:A:138:GLU:H	1.51	0.56
1:A:52:ARG:NH1	4:A:494:HOH:O	2.39	0.56
1:A:276:GLN:CG	4:A:529:HOH:O	2.05	0.55
1:A:136:ASN:HD22	1:A:136:ASN:C	2.10	0.54
1:A:307:GLU:CG	4:A:370:HOH:O	2.56	0.53
1:A:7:ASN:HB2	4:A:402:HOH:O	2.08	0.53
1:B:237:ARG:CD	4:B:532:HOH:O	2.38	0.53
1:B:233:GLU:O	1:B:237:ARG:HG3	2.09	0.52
1:A:307:GLU:HG3	4:A:370:HOH:O	2.10	0.51
1:A:306:LYS:O	1:A:309:ARG:HG2	2.10	0.51
1:B:60:ILE:HD11	1:B:80:VAL:HG13	1.92	0.50
1:B:103:HIS:HE1	4:B:331:HOH:O	1.95	0.49
1:A:52:ARG:HD2	4:A:584:HOH:O	2.11	0.49
1:A:103:HIS:HE1	4:A:324:HOH:O	1.96	0.49
1:B:42:ASN:HD21	1:B:44:TYR:HB3	1.78	0.48
1:A:7:ASN:CB	4:A:551:HOH:O	2.58	0.48
1:A:152:LYS:HE3	4:A:582:HOH:O	2.13	0.48
1:B:310:VAL:O	1:B:310:VAL:HG12	2.14	0.47
1:B:161:LEU:HB3	1:B:188:ILE:HG13	1.98	0.46
1:A:1:MET:N	4:A:502:HOH:O	2.48	0.46
1:A:4:LEU:HD22	1:A:261:CYS:SG	2.56	0.46
1:B:68:ILE:CD1	1:B:90:THR:HB	2.39	0.46
1:A:48:SER:HB3	4:A:584:HOH:O	2.15	0.45
1:B:299:ASN:HD22	1:B:299:ASN:C	2.20	0.45
1:A:42:ASN:HD21	1:A:44:TYR:HB3	1.82	0.45
1:B:212:GLU:CG	4:B:479:HOH:O	2.66	0.44
1:B:136:ASN:C	1:B:136:ASN:HD22	2.20	0.44
1:A:217:VAL:O	1:A:242:ALA:HA	2.18	0.43
1:A:125:PRO:HB3	4:A:568:HOH:O	2.17	0.43
1:B:8:PRO:HG2	1:B:202:ASN:HB3	1.99	0.43
1:A:301:VAL:HB	1:B:301:VAL:HB	1.99	0.43
1:A:236:GLN:HG3	1:A:242:ALA:HB3	2.00	0.42
1:A:111:ARG:HG3	4:A:381:HOH:O	2.19	0.42
1:A:36:ARG:NH2	1:A:36:ARG:CG	2.43	0.41
1:A:7:ASN:OD1	4:A:551:HOH:O	2.22	0.41
1:A:70:ILE:HA	1:A:92:PHE:O	2.21	0.41
1:A:152:LYS:CE	4:A:582:HOH:O	2.67	0.41
1:A:136:ASN:HD21	1:A:138:GLU:HB2	1.85	0.41
1:B:208:ARG:O	1:B:212:GLU:HG3	2.21	0.41
1:B:310:VAL:O	1:B:310:VAL:CG1	2.69	0.41
1:B:156:LYS:HE3	4:B:602:HOH:O	2.20	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	307/324 (95%)	303 (99%)	4 (1%)	0	100	100
1	B	308/324 (95%)	305 (99%)	3 (1%)	0	100	100
All	All	615/648 (95%)	608 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	257/271 (95%)	243 (95%)	14 (5%)	27	4
1	B	258/271 (95%)	244 (95%)	14 (5%)	27	4
All	All	515/542 (95%)	487 (95%)	28 (5%)	27	4

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	57	ILE
1	A	69	LEU
1	A	103	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	136	ASN
1	A	153	LEU
1	A	161	LEU
1	A	187	LYS
1	A	207	VAL
1	A	230	ARG
1	A	258	GLU
1	A	294	GLU
1	A	309	ARG
1	B	5	LEU
1	B	108	ARG
1	B	112	ARG
1	B	136	ASN
1	B	148	ASP
1	B	153	LEU
1	B	155	VAL
1	B	159	GLU
1	B	161	LEU
1	B	230	ARG
1	B	273	ILE
1	B	281	ARG
1	B	285	LEU
1	B	299	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	59	GLN
1	A	103	HIS
1	A	121	HIS
1	A	136	ASN
1	A	229	ASN
1	A	236	GLN
1	A	277	ASN
1	B	42	ASN
1	B	78	GLN
1	B	103	HIS
1	B	121	HIS
1	B	133	GLN
1	B	136	ASN
1	B	276	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	277	ASN
1	B	283	GLN
1	B	299	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z  > 2$
2	SF4	A	317	1,4	0,12,12	0.00	-	0,24,24	0.00	-
3	0CG	A	318	-	9,11,11	1.60	2 (22%)	13,16,16	1.10	0
2	SF4	B	317	1,4	0,12,12	0.00	-	0,24,24	0.00	-
3	0CG	B	318	-	9,11,11	1.67	2 (22%)	13,16,16	1.19	1 (7%)

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
2	SF4	A	317	1,4	-	0/0/48/48	0/6/5/5
3	0CG	A	318	-	-	1/10/11/11	0/0/0/0
2	SF4	B	317	1,4	-	0/0/48/48	0/6/5/5
3	0CG	B	318	-	-	0/10/11/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	318	0CG	P17-O20	-2.06	1.44	1.51
3	A	318	0CG	P13-O15	-2.01	1.46	1.54
3	A	318	0CG	C27-C30	3.69	1.26	1.17
3	B	318	0CG	C27-C30	3.99	1.27	1.17

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	318	0CG	O29-C28-C27	2.55	120.25	108.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	318	0CG	P13-O29-C28-C27

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 [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, 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	A	309/324 (95%)	-0.14	4 (1%) 79 82	7, 15, 26, 43	0
1	B	310/324 (95%)	-0.16	3 (0%) 84 86	8, 16, 28, 41	0
All	All	619/648 (95%)	-0.15	7 (1%) 82 85	7, 15, 28, 43	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	VAL	4.2
1	A	88	ASP	3.0
1	A	309	ARG	2.4
1	B	289	GLU	2.3
1	A	138	GLU	2.2
1	B	258	GLU	2.2
1	A	307	GLU	2.1

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	B	317	8/8	0.99	0.08	0.57	8,9,10,16	0
2	SF4	A	317	8/8	0.99	0.08	0.03	8,8,10,17	0
3	OCG	B	318	12/12	0.99	0.06	-0.72	8,9,11,12	0
3	OCG	A	318	12/12	1.00	0.06	-1.02	8,9,13,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.