



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UJ4  
Title : Crystal structure of the apo-inositol 1,4,5-trisphosphate receptor  
Authors : Ikura, M.; Seo, M.D.; Ishiyama, N.; Stathopulos, P.  
Deposited on : 2011-11-07  
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](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.

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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 : 1.7 (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

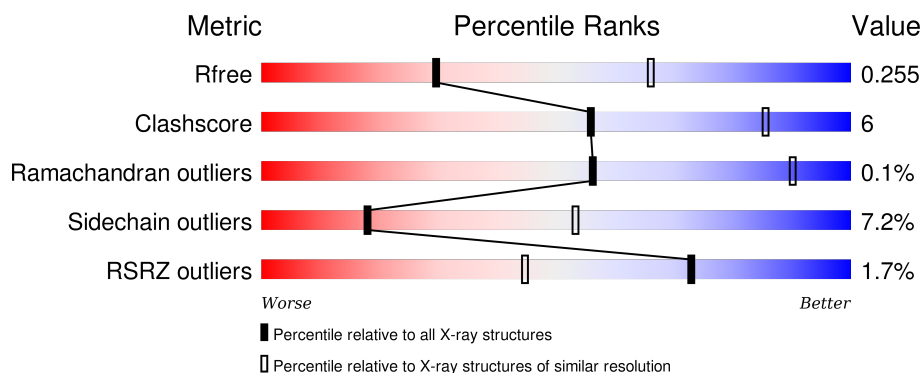
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	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)

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	604	<div> <div> <div></div> <div>67%</div> <div>12%</div> <div>20%</div> </div> <div> <div>2%</div> <div>65%</div> <div>15%</div> <div>19%</div> </div> </div>
1	B	604	<div> <div> <div></div> <div>67%</div> <div>12%</div> <div>20%</div> </div> <div> <div>2%</div> <div>65%</div> <div>15%</div> <div>19%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7454 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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3721	2372	656	688	5			
1	B	490	Total	C	N	O	S	0	0	0
			3700	2351	646	698	5			

There are 26 discrepancies between the modelled and reference sequences:

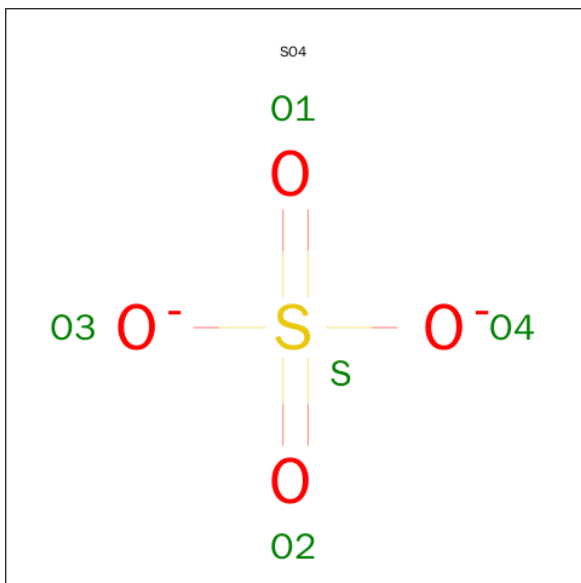
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	CYS	engineered mutation	UNP P29994
A	37	ALA	CYS	engineered mutation	UNP P29994
A	56	ALA	CYS	engineered mutation	UNP P29994
A	61	ALA	CYS	engineered mutation	UNP P29994
A	206	ALA	CYS	engineered mutation	UNP P29994
A	214	ALA	CYS	engineered mutation	UNP P29994
A	253	ALA	CYS	engineered mutation	UNP P29994
A	292	ALA	CYS	engineered mutation	UNP P29994
A	326	ALA	CYS	engineered mutation	UNP P29994
A	394	ALA	CYS	engineered mutation	UNP P29994
A	530	ALA	CYS	engineered mutation	UNP P29994
A	553	ALA	CYS	engineered mutation	UNP P29994
A	556	ALA	CYS	engineered mutation	UNP P29994
B	15	ALA	CYS	engineered mutation	UNP P29994
B	37	ALA	CYS	engineered mutation	UNP P29994
B	56	ALA	CYS	engineered mutation	UNP P29994
B	61	ALA	CYS	engineered mutation	UNP P29994
B	206	ALA	CYS	engineered mutation	UNP P29994
B	214	ALA	CYS	engineered mutation	UNP P29994
B	253	ALA	CYS	engineered mutation	UNP P29994
B	292	ALA	CYS	engineered mutation	UNP P29994
B	326	ALA	CYS	engineered mutation	UNP P29994
B	394	ALA	CYS	engineered mutation	UNP P29994
B	530	ALA	CYS	engineered mutation	UNP P29994
B	553	ALA	CYS	engineered mutation	UNP P29994

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Chain	Residue	Modelled	Actual	Comment	Reference
B	556	ALA	CYS	engineered mutation	UNP P29994

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

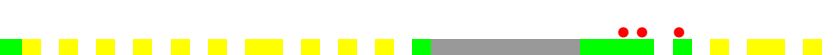


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	14	Total	O	0	0
			14	14		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A: 

- Chain B:
- 
- 2% 65% 15% 19%
- MET SER ASP LYS MET SER F7 S8 L9 I14 S22 S28 T29 Q40 L46 P50 F53 R54 D55 N64 S67 W73 K74 A75 A76 LYS PRO GLY ALA ASN SER THR T84 D85 A86 W87 L88 R91 E106 I121 Q122 H125 L126 K127 S128 W130 V286 V287 Q288 H289 D290 R293 Y298 W299 N300 S301 L302 H307 V318 D319 P320 ASP PHE GLU GLY GLY ALA LEU LEU PHE GLN PRO SER VAL ASP PRO ASP GLN ASP D228 R229 K230 L233 L234 K235 Q247 T252 A285 F283 T287 ARG GLN V352 L355 I364 T374 L376 N385 V386 Q387 V388 R389 L390 R391 A394 T395 N396 S397 W398 E410 K412 K413 V414 M415 T420 K427 A431 I432 V433 P434 D442 A446 L460 E461 K462 G463 T464 K475 L476 L477 T485 G485 GLY THR A551 I552 Y557 L560 R561 H515 S563 Q564 I574 P593 S594

GLN
LYS
GLN
ILE
GLY
TYR
ASP
VAL
LEU
ALA
GLU
ASP
THR
ILE
THR
ALA
LEU
LEU
HIS
ASN
ASN
ARG
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.11Å 77.19Å 101.51Å 105.36° 99.98° 101.04°	Depositor
Resolution (Å)	50.00 – 3.00 46.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.00) 88.7 (46.79-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.256 0.208 , 0.255	Depositor DCC
$R_{free}$ test set	1746 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34772 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	0.50	2/3794 (0.1%)	0.59	0/5153
1	B	0.49	3/3771 (0.1%)	0.57	0/5129
All	All	0.49	5/7565 (0.1%)	0.58	0/10282

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TRP	CD2-CE2	5.19	1.47	1.41
1	B	226	TRP	CD2-CE2	5.17	1.47	1.41
1	B	299	TRP	CD2-CE2	5.08	1.47	1.41
1	B	73	TRP	CD2-CE2	5.04	1.47	1.41
1	A	160	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	3721	0	3629	39	0
1	B	3700	0	3531	53	0
2	B	5	0	0	0	0
3	A	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	0	2	0
All	All	7454	0	7160	90	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 6.

All (90) 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:251:LEU:HD12	1:A:418:ILE:HD13	1.59	0.83
1:B:204:PRO:HA	3:B:611:HOH:O	1.80	0.82
1:A:251:LEU:HD12	1:A:418:ILE:CD1	2.12	0.79
1:B:64:ASN:H	1:B:122:GLN:NE2	1.86	0.72
1:B:293:ARG:CG	1:B:293:ARG:HH11	2.02	0.72
1:A:64:ASN:H	1:A:122:GLN:NE2	1.88	0.71
1:B:389:ARG:HG3	1:B:427:LYS:HD2	1.73	0.69
1:B:391:ARG:HH11	1:B:396:ASN:HD21	1.41	0.69
1:B:64:ASN:HB2	1:B:122:GLN:HE22	1.58	0.68
1:B:385:ASN:HB3	1:B:434:PRO:HD3	1.77	0.67
1:A:456:ILE:HD13	1:A:473:VAL:HB	1.79	0.65
1:A:300:ASN:HD22	1:A:300:ASN:H	1.44	0.64
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.63	0.63
1:A:114:VAL:HG23	1:B:106:GLU:OE1	2.00	0.62
1:B:288:GLN:HG2	1:B:293:ARG:HB3	1.83	0.61
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.36	0.59
1:A:391:ARG:HH11	1:A:396:ASN:ND2	2.01	0.59
1:A:407:ASP:HB2	1:A:410:GLU:HB2	1.86	0.58
1:B:55:ASP:O	1:B:125:HIS:HE1	1.86	0.57
1:B:121:ILE:HD12	1:B:163:ILE:HB	1.85	0.57
1:B:398:TRP:O	1:B:420:THR:HA	2.05	0.57
1:B:147:MET:HB2	1:B:211:SER:HB3	1.85	0.57
1:A:29:THR:HG23	1:A:125:HIS:CE1	2.40	0.57
1:B:293:ARG:CG	1:B:293:ARG:NH1	2.66	0.57
1:A:251:LEU:CD1	1:A:418:ILE:CD1	2.83	0.56
1:A:288:GLN:HG2	1:A:293:ARG:HB3	1.87	0.56
1:B:364:ILE:HG22	1:B:394:ALA:HB2	1.87	0.56
1:B:557:TYR:HA	1:B:560:LEU:HD12	1.88	0.54
1:A:38:VAL:HB	1:A:206:ALA:HB1	1.90	0.54
1:B:125:HIS:HD2	1:B:128:SER:OG	1.91	0.53
1:A:125:HIS:HD2	1:A:128:SER:H	1.56	0.53
1:B:388:VAL:HG21	1:B:432:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:ND2	1:A:300:ASN:H	2.06	0.53
1:B:28:SER:HB2	1:B:55:ASP:OD1	2.09	0.52
1:A:279:LYS:O	1:A:307:HIS:HE1	1.91	0.52
1:B:14:ILE:HG12	1:B:126:LEU:HD11	1.91	0.51
1:B:247:GLN:HA	1:B:247:GLN:HE21	1.76	0.50
1:A:134:VAL:HG21	1:A:186:PRO:HG3	1.94	0.50
1:A:364:ILE:HG22	1:A:394:ALA:HB2	1.94	0.49
1:B:279:LYS:O	1:B:307:HIS:HE1	1.95	0.48
1:A:64:ASN:HB2	1:A:122:GLN:HE22	1.77	0.48
1:B:230:LYS:O	1:B:235:LYS:HE3	2.14	0.48
1:A:174:ASP:OD1	1:B:67:SER:HB2	2.13	0.48
1:B:385:ASN:HA	1:B:432:ILE:O	2.14	0.47
1:A:298:TYR:O	1:A:301:SER:HB2	2.15	0.47
1:A:24:ASN:O	1:A:41:PRO:HA	2.14	0.47
1:B:501:LYS:HA	1:B:502:PRO:HD3	1.75	0.47
1:B:290:ASP:HB2	1:B:293:ARG:HB2	1.97	0.47
1:B:29:THR:HG23	1:B:125:HIS:CE1	2.51	0.46
1:B:508:LYS:HE3	1:B:511:ARG:HH22	1.80	0.46
1:B:181:LYS:HB3	1:B:217:SER:HB2	1.98	0.46
1:B:285:GLU:CB	3:B:612:HOH:O	2.63	0.46
1:A:202:ASP:OD2	1:A:203:ASN:ND2	2.49	0.46
1:B:9:LEU:HD22	1:B:220:ILE:HD13	1.97	0.45
1:B:178:ILE:HD12	1:B:222:LEU:HG	1.98	0.45
1:B:263:PHE:CD1	1:B:415:MET:HG2	2.52	0.45
1:B:520:PHE:HZ	1:B:574:ILE:HG23	1.82	0.45
1:A:288:GLN:HG2	1:A:293:ARG:CB	2.47	0.44
1:A:171:SER:O	1:A:174:ASP:HB2	2.18	0.44
1:A:564:GLN:HB2	1:A:571:GLN:HG3	2.00	0.43
1:A:504:ARG:HH22	1:A:568:ARG:HH12	1.66	0.43
1:B:226:TRP:CG	1:B:227:SER:N	2.87	0.43
1:A:186:PRO:HB2	1:A:190:GLY:H	1.83	0.43
1:B:167:TYR:HE1	1:B:181:LYS:HD2	1.83	0.43
1:A:14:ILE:HG12	1:A:126:LEU:HD11	1.99	0.43
1:B:551:HIS:CG	1:B:552:ILE:H	2.36	0.43
1:A:125:HIS:CD2	1:A:128:SER:H	2.37	0.42
1:A:466:THR:H	1:A:466:THR:HG1	1.62	0.42
1:B:442:ASP:OD1	1:B:506:ARG:NE	2.53	0.42
1:A:354:SER:HA	1:A:419:GLY:HA2	2.00	0.42
1:B:564:GLN:HE21	1:B:574:ILE:HD12	1.85	0.42
1:A:9:LEU:HG	1:A:115:ILE:HD12	2.02	0.42
1:B:55:ASP:O	1:B:125:HIS:CE1	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ALA:O	1:B:515:ILE:HD11	2.20	0.41
1:B:387:TYR:CE1	1:B:431:ALA:HB2	2.55	0.41
1:B:146:ALA:HB2	1:B:212:VAL:HB	2.01	0.41
1:B:64:ASN:HB2	1:B:122:GLN:NE2	2.31	0.41
1:A:304:ARG:HD3	1:A:366:SER:OG	2.20	0.41
1:B:40:GLN:HG2	1:B:206:ALA:HB2	2.01	0.41
1:B:561:ARG:O	1:B:563:SER:N	2.53	0.41
1:A:223:PHE:O	1:A:293:ARG:O	2.39	0.41
1:B:514:ASN:O	1:B:518:GLN:HG2	2.21	0.41
1:B:185:ASN:HA	1:B:186:PRO:HD3	1.86	0.41
1:A:194:HIS:CD2	1:A:214:ALA:CB	3.04	0.41
1:A:410:GLU:HB3	3:A:612:HOH:O	2.20	0.41
1:A:253:ALA:HB3	1:A:307:HIS:CE1	2.56	0.41
1:B:282:TRP:CZ3	1:B:307:HIS:HB2	2.56	0.41
1:B:298:TYR:O	1:B:301:SER:HB2	2.20	0.40
1:A:510:MET:HE2	1:A:510:MET:HA	2.03	0.40
1:B:50:PRO:O	1:B:53:PHE:HB2	2.22	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	472/604 (78%)	447 (95%)	25 (5%)	0	100	100
1	B	472/604 (78%)	443 (94%)	28 (6%)	1 (0%)	52	88
All	All	944/1208 (78%)	890 (94%)	53 (6%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	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	384/520 (74%)	354 (92%)	30 (8%)	16	49
1	B	377/520 (72%)	352 (93%)	25 (7%)	21	57
All	All	761/1040 (73%)	706 (93%)	55 (7%)	18	53

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	67	SER
1	A	98	LEU
1	A	169	LEU
1	A	185	ASN
1	A	200	LEU
1	A	201	VAL
1	A	210	ASN
1	A	251	LEU
1	A	252	THR
1	A	277	SER
1	A	286	VAL
1	A	293	ARG
1	A	300	ASN
1	A	302	LEU
1	A	319	ASP
1	A	384	ARG
1	A	389	ARG
1	A	390	LEU
1	A	396	ASN
1	A	407	ASP
1	A	408	LYS
1	A	418	ILE
1	A	465	ILE
1	A	505	GLU
1	A	509	LEU
1	A	522	LEU

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Mol	Chain	Res	Type
1	A	523	LEU
1	A	567	TYR
1	A	568	ARG
1	B	22	SER
1	B	46	LEU
1	B	74	LYS
1	B	121	ILE
1	B	129	ASN
1	B	210	ASN
1	B	215	ASN
1	B	222	LEU
1	B	228	ASP
1	B	233	ILE
1	B	252	THR
1	B	286	VAL
1	B	293	ARG
1	B	301	SER
1	B	302	LEU
1	B	318	VAL
1	B	355	LEU
1	B	374	THR
1	B	389	ARG
1	B	396	ASN
1	B	432	ILE
1	B	460	LEU
1	B	475	LYS
1	B	477	LEU
1	B	509	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	125	HIS
1	A	129	ASN
1	A	185	ASN
1	A	210	ASN
1	A	300	ASN
1	A	307	HIS
1	A	396	ASN
1	A	507	GLN
1	A	514	ASN

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Mol	Chain	Res	Type
1	A	564	GLN
1	B	122	GLN
1	B	125	HIS
1	B	129	ASN
1	B	185	ASN
1	B	247	GLN
1	B	261	HIS
1	B	307	HIS
1	B	312	HIS
1	B	396	ASN
1	B	564	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](#)

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](#)

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	$\# Z  > 2$
2	SO4	B	605	-	4,4,4	0.26	0	6,6,6	0.14	0

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	SO4	B	605	-	-	0/0/0/0	0/0/0/0

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	A	486/604 (80%)	-0.30	5 (1%) 84 60	47, 71, 149, 226	0
1	B	490/604 (81%)	-0.19	12 (2%) 62 32	51, 88, 154, 189	0
All	All	976/1208 (80%)	-0.24	17 (1%) 73 45	47, 78, 153, 226	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	THR	4.8
1	B	88	LEU	4.5
1	B	463	GLY	3.9
1	B	76	ALA	3.4
1	A	87	VAL	3.4
1	A	91	LYS	3.4
1	B	462	LYS	3.1
1	A	268	GLY	2.9
1	B	86	ALA	2.8
1	B	502	PRO	2.6
1	B	460	LEU	2.6
1	B	522	LEU	2.5
1	A	377	GLY	2.4
1	A	88	LEU	2.4
1	B	91	LYS	2.2
1	B	414	VAL	2.2
1	B	189	ALA	2.1

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

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	SO4	B	605	5/5	0.97	0.10	-1.33	72,72,72,72	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.