



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2020 – 10:19 AM JST

PDB ID : 7DH6  
Title : Crystal structure of PLRG1  
Authors : Wang, X.; Xu, C.  
Deposited on : 2020-11-13  
Resolution : 2.58 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
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)	:	2.14.6

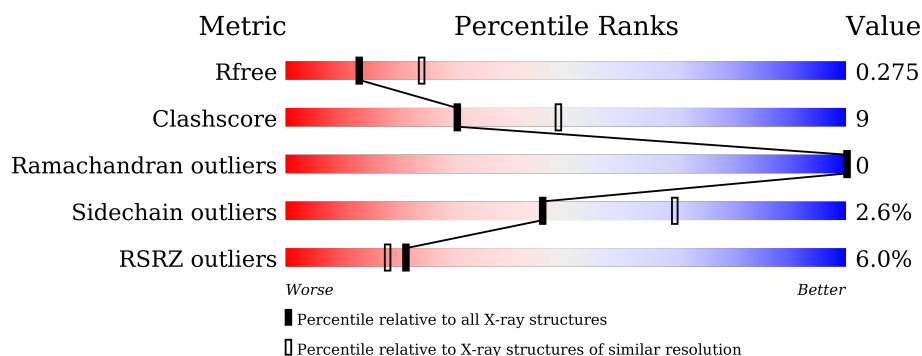
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 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	375	<div> <div>11%</div> <div> <div></div> <div>59%</div> <div>16%</div> <div>•</div> <div>25%</div> </div> </div>
1	B	375	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>14%</div> <div></div> <div>22%</div> </div> </div>
1	C	375	<div> <div></div> <div> <div></div> <div>63%</div> <div>14%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	375	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>17%</div> <div></div> <div>22%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9116 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 Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	4	0
			2180	1395	384	394	7			
1	B	294	Total	C	N	O	S	0	4	0
			2290	1453	410	419	8			
1	C	292	Total	C	N	O	S	0	1	0
			2265	1441	403	414	7			
1	D	291	Total	C	N	O	S	0	2	0
			2238	1426	399	406	7			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

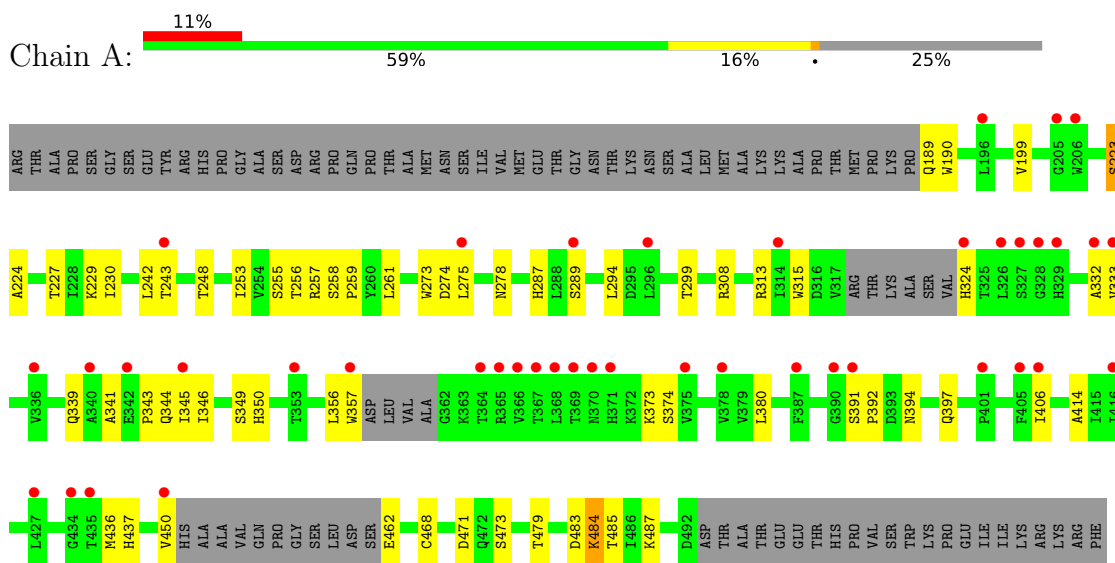
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	31	Total	O	0	0
			31	31		
5	C	37	Total	O	0	0
			37	37		
5	D	39	Total	O	0	0
			39	39		

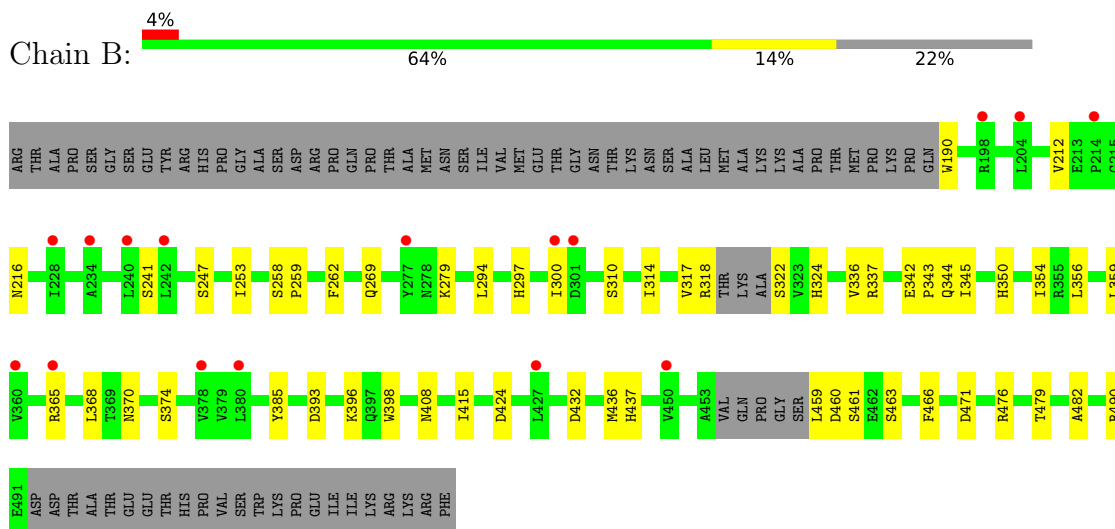
### 3 Residue-property plots [i](#)

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: Pleiotropic regulator 1

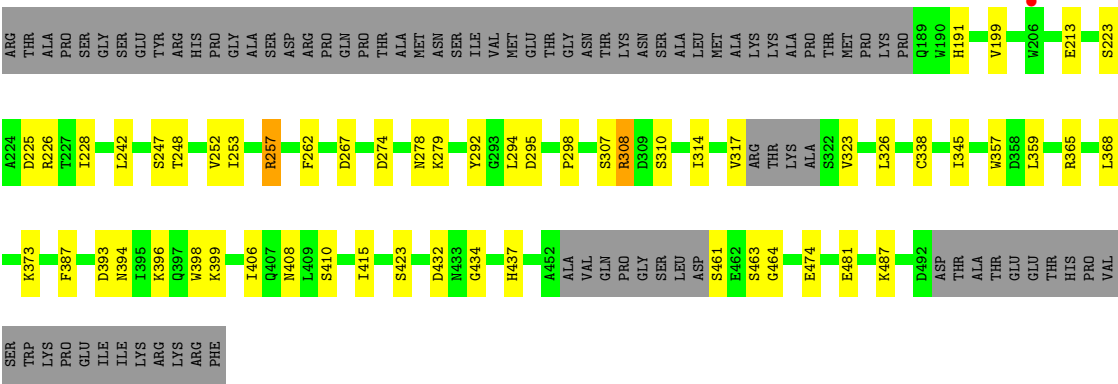


#### • Molecule 1: Pleiotropic regulator 1

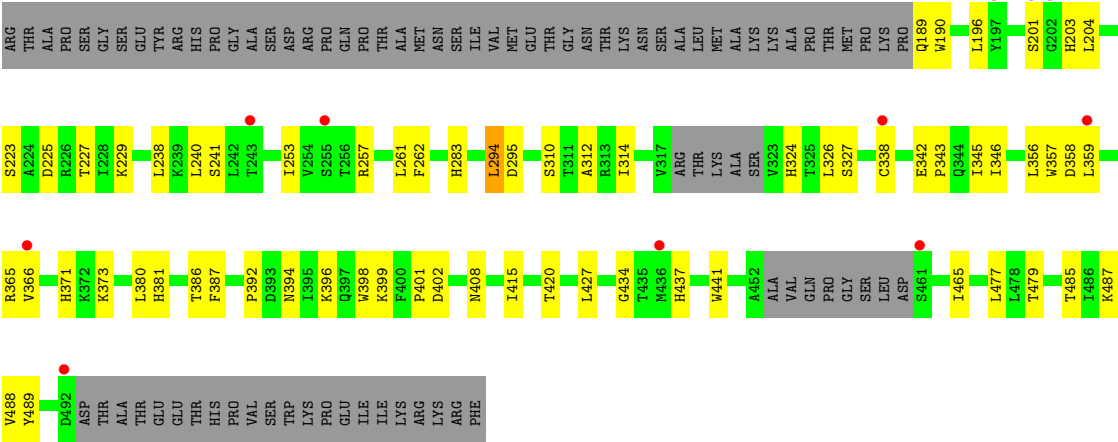


#### • Molecule 1: Pleiotropic regulator 1





• Molecule 1: Pleiotropic regulator 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.00Å 82.12Å 99.39Å 90.00° 99.44° 90.00°	Depositor
Resolution (Å)	38.16 – 2.58 48.53 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.16-2.58) 98.9 (48.53-2.58)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.226 , 0.276 0.226 , 0.275	Depositor DCC
$R_{free}$ test set	1705 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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 32.05 % 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 1.0008e-03. 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, 0.333 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: NI, CA, 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	0.37	0/2244	0.55	0/3068
1	B	0.29	0/2346	0.52	0/3200
1	C	0.28	0/2324	0.51	0/3173
1	D	0.28	0/2298	0.52	0/3139
All	All	0.31	0/9212	0.52	0/12580

There are no bond length outliers.

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	2180	0	2056	49	0
1	B	2290	0	2192	32	0
1	C	2265	0	2172	40	0
1	D	2238	0	2136	43	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	26	0	0	3	0
5	B	31	0	0	3	0
5	C	37	0	0	3	0
5	D	39	0	0	2	0
All	All	9116	0	8556	161	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 (161) 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:D:358:ASP:HB3	5:D:701:HOH:O	1.70	0.91
1:B:342:GLU:HB3	1:B:365:ARG:HH22	1.47	0.78
1:D:366:VAL:HG21	1:D:402:ASP:HA	1.66	0.77
1:D:342:GLU:HB3	1:D:365:ARG:HH12	1.51	0.76
1:B:269:GLN:HG3	5:B:708:HOH:O	1.90	0.71
1:A:242:LEU:HD11	1:A:275:LEU:HD23	1.71	0.71
1:C:257:ARG:NH1	1:C:298:PRO:O	2.25	0.68
1:A:483:ASP:O	1:A:484:LYS:HG3	1.94	0.68
1:A:339:GLN:NE2	1:A:341:ALA:O	2.27	0.68
1:C:199:VAL:HG22	1:C:487:LYS:HG2	1.76	0.67
1:D:201:SER:HB3	1:D:485:THR:HG22	1.75	0.67
1:C:253:ILE:CG2	1:C:294:LEU:HD13	2.24	0.67
1:A:462:GLU:N	5:A:702:HOH:O	2.30	0.65
1:A:373:LYS:HB2	1:A:392:PRO:HD2	1.79	0.64
1:A:199:VAL:HG22	1:A:487:LYS:HG2	1.80	0.63
1:C:415:ILE:HB	1:C:432:ASP:HB2	1.80	0.63
1:A:274:ASP:O	1:A:278:ASN:N	2.31	0.62
1:A:414:ALA:N	5:A:701:HOH:O	2.33	0.61
1:B:415:ILE:HB	1:B:432:ASP:HB2	1.82	0.60
1:B:314:ILE:HD12	1:B:324:HIS:HB2	1.84	0.60
1:A:242:LEU:HD13	1:A:273:TRP:CE3	2.38	0.59
1:D:386:THR:HG22	1:D:399:LYS:HA	1.84	0.59
1:B:396:LYS:NZ	1:B:408:ASN:OD1	2.33	0.58
1:A:289:SER:HB3	1:A:308[B]:ARG:HG2	1.86	0.58
1:C:365:ARG:NH1	5:C:702:HOH:O	2.22	0.58
1:D:240:LEU:HD12	1:D:241:SER:H	1.68	0.58
1:A:261:LEU:HB3	1:A:275:LEU:HD11	1.86	0.57
1:D:225:ASP:OD1	1:D:227[B]:THR:HG22	2.03	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLN:HG2	1:D:190:TRP:H	1.70	0.57
1:D:240:LEU:HD12	1:D:241:SER:N	2.20	0.56
1:A:242:LEU:HD11	1:A:275:LEU:CD2	2.36	0.56
1:B:258:SER:CB	1:B:259:PRO:CD	2.84	0.56
1:A:257:ARG:NH2	1:A:299:THR:HG22	2.21	0.56
1:B:336:VAL:O	1:B:337:ARG:NH1	2.39	0.56
1:D:343:PRO:HD3	1:D:401:PRO:HB3	1.87	0.56
1:D:434:GLY:HA2	1:D:465:ILE:HG13	1.88	0.55
1:A:257:ARG:HH21	1:A:299:THR:HG22	1.70	0.55
1:D:373:LYS:HD2	1:D:392:PRO:HB2	1.88	0.55
1:C:423:SER:OG	1:C:474:GLU:OE1	2.22	0.55
1:D:253:ILE:HB	1:D:294:LEU:HD11	1.88	0.55
1:B:476:ARG:HG2	1:B:490:ARG:HD3	1.89	0.55
1:A:313:ARG:HG3	1:A:324:HIS:O	2.07	0.54
1:A:230:ILE:CD1	1:A:275:LEU:HD22	2.36	0.54
1:B:345:ILE:HD11	1:B:359:LEU:HD13	1.88	0.54
1:B:350:HIS:HA	1:B:374:SER:HB3	1.90	0.54
1:A:256:THR:HG23	1:A:257:ARG:HG3	1.88	0.54
1:D:295:ASP:OD2	1:D:338:CYS:N	2.41	0.53
1:A:289:SER:CB	1:A:308[B]:ARG:HG2	2.38	0.53
1:B:297:HIS:HB3	1:B:300:ILE:O	2.09	0.53
1:A:227[B]:THR:HG21	1:A:229:LYS:NZ	2.24	0.53
1:A:230:ILE:HD11	1:A:275:LEU:HD22	1.90	0.52
1:D:283:HIS:NE2	5:D:703:HOH:O	2.24	0.52
1:A:436:MET:HB3	1:A:450:VAL:CG1	2.40	0.52
1:B:342:GLU:HB3	1:B:365:ARG:NH2	2.22	0.52
1:C:396:LYS:NZ	1:C:408:ASN:OD1	2.42	0.51
1:C:253:ILE:HG21	1:C:294:LEU:HD13	1.92	0.51
1:B:343:PRO:HG3	1:B:356:LEU:HB3	1.92	0.51
1:A:350:HIS:HA	1:A:374:SER:HB3	1.91	0.51
1:A:391:SER:HG	1:A:394:ASN:H	1.53	0.51
1:D:196:LEU:HD12	1:D:488:VAL:O	2.12	0.51
1:D:223:SER:HB3	1:D:225:ASP:OD1	2.12	0.50
1:A:255:SER:HB3	1:A:258:SER:HB2	1.92	0.50
1:A:313:ARG:HD2	1:A:315:TRP:CZ2	2.46	0.50
1:C:310:SER:O	5:C:701:HOH:O	2.20	0.50
1:A:243:THR:O	1:A:273:TRP:HH2	1.95	0.50
1:A:287:HIS:HB2	5:A:705:HOH:O	2.11	0.50
1:D:345:ILE:HD11	1:D:359:LEU:HD13	1.94	0.50
1:B:466:PHE:CE2	1:B:482:ALA:HB2	2.47	0.50
1:D:312:ALA:HB3	1:D:326:LEU:HB2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LYS:HB2	1:D:392:PRO:HD2	1.94	0.49
1:C:399:LYS:HG3	1:C:406:ILE:HD11	1.95	0.49
1:A:483:ASP:OD1	1:A:485:THR:OG1	2.30	0.48
1:C:481:GLU:OE2	1:C:487:LYS:HD2	2.13	0.48
1:C:345:ILE:HB	1:C:357:TRP:HB2	1.94	0.48
1:A:346:ILE:HD13	1:A:380:LEU:HD21	1.95	0.48
1:B:459:LEU:HD23	1:B:460:ASP:H	1.78	0.48
1:C:314:ILE:HB	1:C:323:VAL:HG22	1.95	0.48
1:A:313:ARG:HD2	1:A:315:TRP:CH2	2.49	0.48
1:C:406:ILE:HG12	1:D:204:LEU:HD11	1.95	0.48
1:D:326:LEU:HG	1:D:357:TRP:CE3	2.48	0.48
1:C:345:ILE:HD11	1:C:359:LEU:HD12	1.95	0.48
1:C:326:LEU:HB3	1:C:357:TRP:CZ3	2.48	0.48
1:C:387:PHE:CE1	1:C:398:TRP:HB2	2.49	0.48
1:D:387:PHE:CE1	1:D:398:TRP:HB2	2.49	0.47
1:A:258:SER:HB3	1:A:259:PRO:CD	2.42	0.47
1:C:253:ILE:HB	1:C:294:LEU:CD1	2.45	0.47
1:D:381:HIS:HD2	1:D:441:TRP:CE2	2.32	0.47
1:B:216:ASN:OD1	1:B:471:ASP:HB2	2.14	0.47
1:D:477:LEU:HB3	1:D:489:TYR:HB2	1.96	0.47
1:C:481:GLU:OE1	1:C:487:LYS:NZ	2.45	0.47
1:B:459:LEU:HD23	1:B:460:ASP:N	2.30	0.47
1:C:262:PHE:HZ	1:C:317:VAL:HG11	1.80	0.46
1:D:294:LEU:O	1:D:294:LEU:HD12	2.15	0.46
1:A:289:SER:HB3	1:A:308[B]:ARG:NH2	2.30	0.46
1:D:227[B]:THR:HG21	1:D:229:LYS:NZ	2.31	0.46
1:B:190:TRP:N	5:B:704:HOH:O	2.49	0.46
1:A:189:GLN:HG2	1:A:190:TRP:H	1.81	0.46
1:A:468[A]:CYS:SG	1:A:479:THR:HG22	2.56	0.46
1:B:342:GLU:CB	1:B:365:ARG:HH22	2.25	0.46
1:C:274:ASP:O	1:C:278:ASN:N	2.46	0.45
1:B:212:VAL:HG21	1:B:471:ASP:HA	1.98	0.45
1:B:253:ILE:HG22	1:B:262:PHE:HB2	1.99	0.45
1:A:471:ASP:OD2	1:A:473:SER:OG	2.25	0.45
1:C:223:SER:HB3	1:C:225:ASP:OD1	2.16	0.45
1:A:299:THR:HG21	1:D:310:SER:HB2	1.99	0.45
1:B:466:PHE:HE2	1:B:482:ALA:HB2	1.81	0.45
1:C:253:ILE:CG2	1:C:294:LEU:CD1	2.94	0.45
1:B:436:MET:HE1	1:B:479:THR:HG21	1.99	0.44
1:C:434:GLY:N	1:C:464:GLY:HA2	2.32	0.44
1:C:481:GLU:CD	1:C:487:LYS:HZ2	2.20	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:THR:O	1:D:427:LEU:HD12	2.17	0.44
1:A:345:ILE:HB	1:A:357:TRP:HB2	2.00	0.44
1:A:391:SER:OG	1:A:394:ASN:O	2.26	0.44
1:C:253:ILE:HB	1:C:294:LEU:HD11	1.99	0.44
1:A:343:PRO:CG	1:A:356:LEU:HB3	2.48	0.44
1:D:253:ILE:O	1:D:261:LEU:HD12	2.18	0.44
1:D:229:LYS:HG3	1:D:238:LEU:HD11	2.00	0.44
1:B:424:ASP:OD2	1:C:373:LYS:NZ	2.50	0.43
1:B:459:LEU:HD22	1:B:461:SER:H	1.83	0.43
1:C:228:ILE:HB	1:C:242:LEU:HB2	2.00	0.43
1:C:368:LEU:HD13	1:C:398:TRP:CE3	2.53	0.43
1:A:339:GLN:HB3	1:A:344:GLN:HA	2.00	0.43
1:C:294:LEU:O	1:C:294:LEU:HD12	2.19	0.43
1:B:436:MET:CE	1:B:479:THR:HG21	2.49	0.43
1:D:203:HIS:CE1	1:D:229:LYS:HD3	2.54	0.43
1:C:326:LEU:HD22	1:C:357:TRP:CE3	2.54	0.43
1:A:253:ILE:O	1:A:261:LEU:HD12	2.19	0.43
1:B:370:ASN:HB2	1:B:398:TRP:HH2	1.84	0.43
1:B:317:VAL:O	1:B:318:ARG:HB2	2.19	0.42
1:C:292:TYR:CZ	1:C:308:ARG:HB2	2.54	0.42
1:D:343:PRO:HG3	1:D:356:LEU:HD13	2.01	0.42
1:C:393:ASP:OD1	1:C:394:ASN:N	2.52	0.42
1:D:346:ILE:HD13	1:D:380:LEU:HD21	2.01	0.42
1:A:333:VAL:HA	1:A:349:SER:HA	2.02	0.42
1:C:247:SER:OG	1:C:248:THR:N	2.53	0.42
1:B:322:SER:N	5:B:705:HOH:O	2.52	0.42
1:A:339:GLN:HE21	1:A:339:GLN:HB3	1.71	0.42
1:D:257:ARG:HG2	1:D:257:ARG:H	1.68	0.42
1:D:392:PRO:HG3	1:D:415:ILE:HD13	2.02	0.42
1:D:479:THR:OG1	1:D:487:LYS:HB2	2.19	0.42
1:A:261:LEU:CB	1:A:275:LEU:HD11	2.50	0.42
1:D:371:HIS:CE1	1:D:396:LYS:HG3	2.55	0.42
1:A:397:GLN:HB3	1:A:406:ILE:HB	2.02	0.42
1:C:252:VAL:HA	1:C:262:PHE:O	2.20	0.42
1:A:332:ALA:HB3	1:A:350:HIS:ND1	2.35	0.41
1:D:253:ILE:HB	1:D:294:LEU:CD1	2.50	0.41
1:D:312:ALA:O	1:D:326:LEU:N	2.49	0.41
1:C:247:SER:HB3	1:C:267:ASP:HB3	2.02	0.41
1:A:223:SER:OG	1:A:224:ALA:N	2.53	0.41
1:C:295:ASP:OD2	1:C:338:CYS:N	2.53	0.41
1:A:484:LYS:O	1:A:484:LYS:HD2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:OD1	1:B:393:ASP:N	2.51	0.41
1:C:307:SER:OG	1:C:308:ARG:N	2.52	0.41
1:B:354:ILE:HB	1:B:368:LEU:HD12	2.02	0.41
1:B:344:GLN:NE2	1:B:359:LEU:HB3	2.35	0.41
1:C:253:ILE:HG22	1:C:294:LEU:HD13	2.01	0.40
1:D:394:ASN:OD1	1:D:408:ASN:HB3	2.21	0.40
1:C:191:HIS:HB3	5:C:722:HOH:O	2.21	0.40
1:D:253:ILE:HG22	1:D:262:PHE:HB2	2.04	0.40
1:A:224:ALA:HA	1:A:248:THR:HG23	2.03	0.40
1:D:314:ILE:HD12	1:D:324:HIS:HB2	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	A	279/375 (74%)	267 (96%)	12 (4%)	0	100	100
1	B	291/375 (78%)	282 (97%)	9 (3%)	0	100	100
1	C	287/375 (76%)	278 (97%)	9 (3%)	0	100	100
1	D	287/375 (76%)	277 (96%)	10 (4%)	0	100	100
All	All	1144/1500 (76%)	1104 (96%)	40 (4%)	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	223/322 (69%)	219 (98%)	4 (2%)	59	78
1	B	240/322 (74%)	232 (97%)	8 (3%)	38	61
1	C	239/322 (74%)	230 (96%)	9 (4%)	33	57
1	D	231/322 (72%)	228 (99%)	3 (1%)	69	85
All	All	933/1288 (72%)	909 (97%)	24 (3%)	46	69

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	294	LEU
1	A	437	HIS
1	A	484	LYS
1	B	241	SER
1	B	247	SER
1	B	279	LYS
1	B	294	LEU
1	B	310	SER
1	B	385	TYR
1	B	437	HIS
1	B	463	SER
1	C	213	GLU
1	C	226	ARG
1	C	257	ARG
1	C	279	LYS
1	C	308	ARG
1	C	410	SER
1	C	437	HIS
1	C	461	SER
1	C	463	SER
1	D	294	LEU
1	D	327	SER
1	D	437	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\# Z  > 2$
3	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.09	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 ⓘ

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	283/375 (75%)	0.72	42 (14%) 2 1	25, 57, 89, 108	0
1	B	294/375 (78%)	0.34	16 (5%) 25 22	25, 46, 66, 82	0
1	C	292/375 (77%)	0.04	1 (0%) 94 94	22, 37, 52, 66	0
1	D	291/375 (77%)	0.35	11 (3%) 40 36	24, 44, 75, 110	0
All	All	1160/1500 (77%)	0.36	70 (6%) 21 18	22, 45, 78, 110	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	6.3
1	A	369	THR	5.5
1	A	370	ASN	4.5
1	D	202	GLY	4.5
1	A	416	ILE	4.4
1	A	326	LEU	4.4
1	A	206	TRP	4.3
1	A	406	ILE	4.3
1	D	338	CYS	4.3
1	A	328	GLY	4.2
1	A	450	VAL	4.2
1	A	333	VAL	3.8
1	A	401	PRO	3.7
1	B	228	ILE	3.6
1	B	300	ILE	3.5
1	A	275	LEU	3.5
1	B	240	LEU	3.5
1	A	368	LEU	3.4
1	A	366	VAL	3.3
1	A	378	VAL	3.2
1	A	364	THR	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	450	VAL	3.0
1	A	329	HIS	3.0
1	B	198	ARG	3.0
1	A	391	SER	3.0
1	A	314	ILE	3.0
1	B	214	PRO	3.0
1	B	380	LEU	2.9
1	A	434	GLY	2.9
1	D	461	SER	2.8
1	A	289	SER	2.8
1	B	204	LEU	2.8
1	A	327	SER	2.8
1	A	357	TRP	2.8
1	A	427	LEU	2.8
1	A	332	ALA	2.8
1	D	243	THR	2.7
1	A	367	THR	2.7
1	A	205	GLY	2.6
1	A	387	PHE	2.5
1	D	436	MET	2.5
1	A	342	GLU	2.5
1	A	405	PHE	2.5
1	A	371	HIS	2.4
1	D	197	TYR	2.4
1	A	324	HIS	2.4
1	B	378	VAL	2.4
1	A	340	ALA	2.4
1	D	366	VAL	2.4
1	A	435	THR	2.4
1	A	296	LEU	2.4
1	A	390	GLY	2.3
1	B	301	ASP	2.3
1	B	242	LEU	2.3
1	D	255	SER	2.3
1	A	365	ARG	2.3
1	B	427	LEU	2.2
1	A	196	LEU	2.2
1	D	359	LEU	2.2
1	B	365	ARG	2.2
1	D	201	SER	2.2
1	A	336	VAL	2.1
1	B	234	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	360	VAL	2.1
1	A	353	THR	2.1
1	D	492	ASP	2.1
1	B	277	TYR	2.1
1	C	206	TRP	2.1
1	A	243	THR	2.0
1	A	345	ILE	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](#)

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( $\text{\AA}^2$ )	Q<0.9
4	CA	B	601	1/1	0.88	0.12	58,58,58,58	0
4	CA	C	602	1/1	0.95	0.13	51,51,51,51	0
3	SO4	A	602	5/5	0.96	0.14	74,76,76,76	0
4	CA	D	601	1/1	0.96	0.09	50,50,50,50	0
2	NI	A	601	1/1	0.99	0.11	36,36,36,36	0
2	NI	C	601	1/1	0.99	0.07	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.