



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:24 PM GMT

PDB ID : 4LI1  
Title : Crystal Structures of Lgr4 and its complex with R-spondin1  
Authors : Xu, Y.; Rajashankar, K.; Robev, D.  
Deposited on : 2013-07-02  
Resolution : 2.66 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

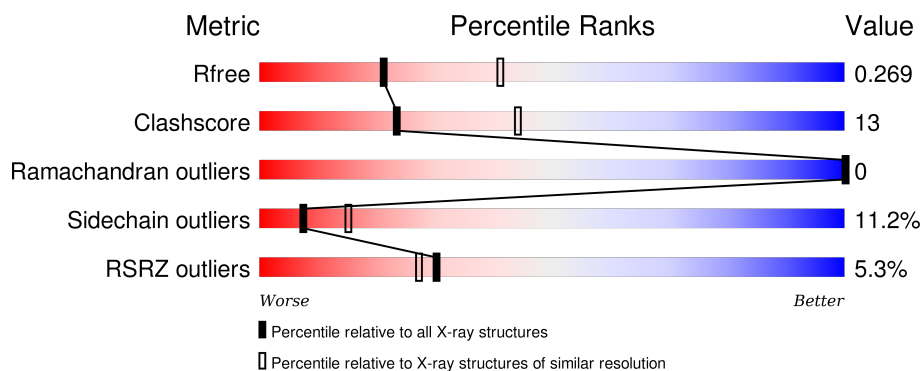
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	432	
1	B	432	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6803 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 Leucine-rich repeat-containing G-protein coupled receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	425	Total	C	N	O	S	0	0	0
			3303	2102	565	625	11			
1	A	424	Total	C	N	O	S	0	0	0
			3298	2099	564	624	11			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

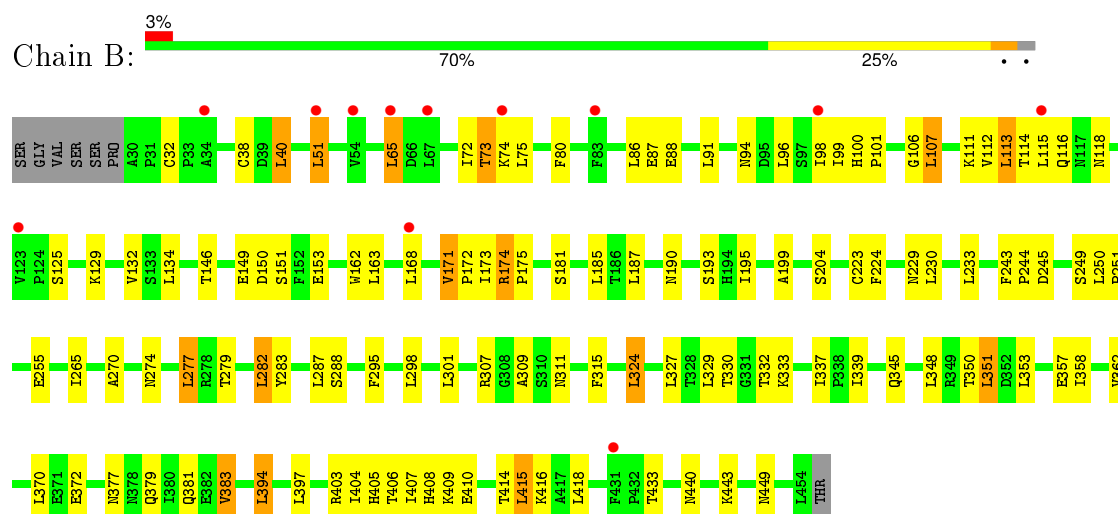
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	114	Total 114	O 114	0	0
3	A	60	Total 60	O 60	0	0

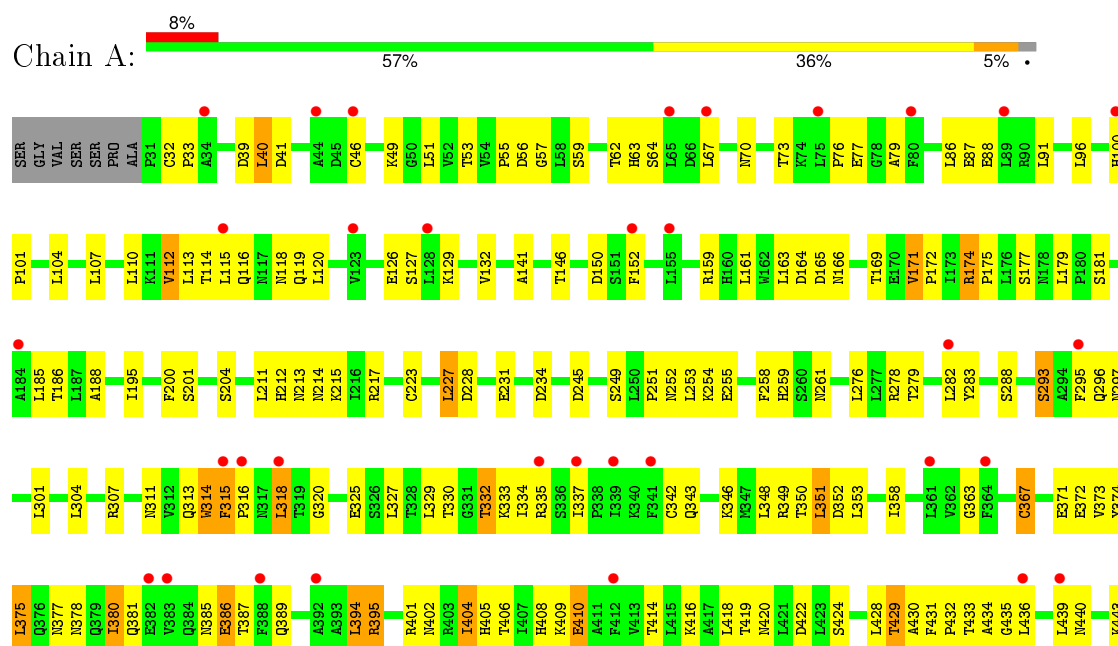
### 3 Residue-property plots

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: Leucine-rich repeat-containing G-protein coupled receptor 4



- Molecule 1: Leucine-rich repeat-containing G-protein coupled receptor 4



L444	
N449	
F450	
K451	
P452	
T453	
L454	
THR	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.29 Å   158.58 Å   227.61 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	79.29 – 2.66 79.29 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.29-2.66) 93.9 (79.29-2.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.65 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.216 , 0.272 0.211 , 0.269	Depositor DCC
$R_{free}$ test set	1512 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 31899 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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: NAG

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	0.43	0/3365	0.71	0/4578
1	B	0.48	0/3370	0.74	1/4586 (0.0%)
All	All	0.45	0/6735	0.73	1/9164 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	394	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	GLY	Peptide

### 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	3298	0	3317	109	0
1	B	3303	0	3319	69	0
2	B	28	0	26	1	0
3	A	60	0	0	5	0
3	B	114	0	0	4	0
All	All	6803	0	6662	177	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 13.

All (177) 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:B:408:HIS:ND1	1:B:409:LYS:O	2.05	0.89
1:B:195:ILE:HG22	1:B:223:CYS:HB2	1.64	0.78
1:A:255:GLU:HG3	1:A:279:THR:HB	1.65	0.78
1:A:119:GLN:O	3:A:524:HOH:O	2.06	0.73
1:B:255:GLU:HG3	1:B:279:THR:HB	1.70	0.72
1:B:348:LEU:HD21	1:B:351:LEU:HG	1.74	0.68
1:B:174:ARG:HG2	1:B:175:PRO:HD3	1.75	0.68
1:A:350:THR:HG22	1:A:372:GLU:HB2	1.76	0.66
1:B:204:SER:O	1:B:229:ASN:ND2	2.29	0.66
1:A:88:GLU:HG2	1:A:112:VAL:HG13	1.79	0.65
1:B:91:LEU:O	1:B:94:ASN:ND2	2.29	0.65
1:B:171:VAL:HG22	1:B:173:ILE:HD13	1.77	0.64
1:A:419:THR:OG1	1:A:420:ASN:OD1	2.12	0.64
1:A:283:TYR:HB2	1:A:307:ARG:HB2	1.80	0.64
1:B:383:VAL:HG13	1:B:407:ILE:HG12	1.79	0.63
1:A:315:PHE:CG	1:A:316:PRO:HD2	2.33	0.63
1:A:434:ALA:HB1	1:A:435:GLY:HA2	1.79	0.62
1:A:258:PHE:O	1:A:261:ASN:ND2	2.31	0.62
1:B:350:THR:HG22	1:B:372:GLU:HB2	1.81	0.62
1:A:293:SER:HB3	1:A:296:GLN:HE21	1.66	0.61
1:B:274:ASN:HB2	1:B:277:LEU:HD22	1.82	0.61
1:B:283:TYR:HB2	1:B:307:ARG:HB2	1.83	0.60
1:A:348:LEU:HD21	1:A:351:LEU:HG	1.83	0.60
1:A:76:PRO:HG2	1:A:79:ALA:HB2	1.82	0.60
1:B:73:THR:O	1:B:96:LEU:HA	2.02	0.60
1:A:159:ARG:NH2	1:A:181:SER:O	2.32	0.60
1:B:440:ASN:O	1:A:440:ASN:ND2	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:HA	1:A:394:LEU:HA	1.84	0.59
1:B:287:LEU:HB2	1:B:309:ALA:HB1	1.83	0.59
1:A:381:GLN:NE2	3:A:526:HOH:O	2.28	0.59
1:B:414:THR:O	1:B:416:LYS:NZ	2.36	0.58
1:A:231:GLU:HB3	1:A:254:LYS:HG2	1.83	0.58
1:A:386:GLU:HA	1:A:389:GLN:HB2	1.84	0.58
1:A:316:PRO:HB2	1:A:318:LEU:HD23	1.85	0.58
1:A:215:LYS:HE3	1:A:217:ARG:HH12	1.66	0.58
1:A:342:CYS:HB3	1:A:367:CYS:N	2.19	0.57
1:B:415:LEU:HD23	1:B:418:LEU:HD22	1.86	0.56
1:A:186:THR:HG22	1:A:188:ALA:H	1.69	0.56
1:A:432:PRO:O	3:A:540:HOH:O	2.17	0.56
1:A:46:CYS:SG	1:A:55:PRO:HG2	2.45	0.56
1:A:385:ASN:OD1	1:A:410:GLU:HG3	2.06	0.56
1:A:228:ASP:O	1:A:252:ASN:ND2	2.39	0.56
1:B:125:SER:HB2	1:B:151:SER:HA	1.88	0.55
1:A:212:HIS:HB3	1:A:234:ASP:OD1	2.06	0.55
1:A:181:SER:HB2	3:A:544:HOH:O	2.06	0.54
1:B:174:ARG:HD3	1:B:174:ARG:H	1.72	0.54
1:A:314:TRP:HA	1:A:334:ILE:HG13	1.88	0.54
1:A:385:ASN:HD21	1:A:408:HIS:CE1	2.25	0.54
1:B:80:PHE:HB3	1:B:107:LEU:HD21	1.89	0.54
1:B:333:LYS:HA	1:B:357:GLU:HG2	1.90	0.53
1:A:174:ARG:O	1:A:177:SER:OG	2.22	0.53
1:A:164:ASP:O	1:A:166:ASN:ND2	2.41	0.53
1:A:450:PHE:O	1:A:453:THR:OG1	2.25	0.53
1:B:96:LEU:HB2	1:B:118:ASN:OD1	2.08	0.53
1:A:174:ARG:HB2	1:A:175:PRO:HD3	1.90	0.53
1:A:254:LYS:HE3	1:A:278:ARG:HG3	1.91	0.53
1:A:49:LYS:H	1:A:70:ASN:HD21	1.55	0.52
1:B:88:GLU:HG2	1:B:112:VAL:HG13	1.89	0.52
1:B:65:LEU:HB2	1:B:86:LEU:HD11	1.91	0.52
1:A:380:ILE:HG13	1:A:404:ILE:HG22	1.92	0.52
1:B:381:GLN:O	1:B:404:ILE:HA	2.10	0.52
1:A:282:LEU:HD21	1:A:295:PHE:HZ	1.75	0.52
1:A:293:SER:HB3	1:A:296:GLN:NE2	2.24	0.51
1:B:224:PHE:HB3	1:B:250:LEU:HD21	1.92	0.51
1:A:307:ARG:HG2	1:A:330:THR:OG1	2.10	0.51
1:A:381:GLN:O	1:A:404:ILE:HA	2.11	0.51
1:A:297:ASN:H	1:A:320:GLY:H	1.58	0.51
1:A:114:THR:HB	1:A:116:GLN:OE1	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASN:OD1	1:A:401:ARG:NE	2.30	0.50
1:A:405:HIS:CE1	1:A:406:THR:HG22	2.46	0.50
1:A:51:LEU:HD21	1:A:55:PRO:HG3	1.94	0.50
1:A:385:ASN:O	3:A:557:HOH:O	2.20	0.50
1:B:403:ARG:NH1	3:B:648:HOH:O	2.44	0.50
1:B:87:GLU:OE2	1:B:111:LYS:NZ	2.44	0.50
1:A:195:ILE:HG22	1:A:223:CYS:HB2	1.94	0.50
1:B:40:LEU:HD12	1:B:40:LEU:H	1.76	0.49
1:B:187:LEU:O	1:B:190:ASN:ND2	2.37	0.49
1:B:287:LEU:HB2	1:B:309:ALA:CB	2.43	0.49
1:B:114:THR:HB	1:B:116:GLN:OE1	2.12	0.49
1:A:405:HIS:ND1	1:A:406:THR:HG22	2.28	0.49
1:A:126:GLU:O	1:A:129:LYS:HB2	2.12	0.49
1:A:49:LYS:H	1:A:70:ASN:ND2	2.11	0.48
1:A:380:ILE:HG23	1:A:402:ASN:OD1	2.13	0.48
1:A:297:ASN:H	1:A:320:GLY:N	2.12	0.48
1:A:126:GLU:HA	1:A:129:LYS:HD3	1.95	0.48
1:B:243:PHE:CZ	1:B:270:ALA:HB1	2.48	0.48
1:A:46:CYS:HB2	1:A:67:LEU:HD23	1.95	0.47
1:A:429:THR:O	1:A:449:ASN:ND2	2.47	0.47
1:A:372:GLU:HB3	1:A:374:TYR:CE2	2.50	0.47
1:A:428:LEU:HD13	1:A:430:ALA:O	2.15	0.47
1:A:371:GLU:HB3	1:A:395:ARG:HE	1.80	0.46
1:A:373:VAL:HG12	1:A:375:LEU:HD22	1.98	0.46
1:A:293:SER:HA	1:A:296:GLN:HG3	1.97	0.46
1:A:408:HIS:HD2	1:A:409:LYS:H	1.62	0.46
1:B:51:LEU:O	1:B:72:ILE:HG13	2.16	0.46
1:A:51:LEU:CD2	1:A:55:PRO:HG3	2.46	0.46
1:B:91:LEU:HA	1:B:91:LEU:HD23	1.77	0.46
1:A:307:ARG:NH2	1:A:352:ASP:OD2	2.48	0.46
1:B:32:CYS:SG	1:B:38:CYS:N	2.89	0.46
1:A:152:PHE:HB3	1:A:179:LEU:HD21	1.97	0.46
1:A:363:GLY:HA2	1:A:387:THR:HA	1.98	0.46
1:B:171:VAL:HA	1:B:172:PRO:HD3	1.82	0.45
1:B:113:LEU:HB2	1:B:134:LEU:HD11	1.97	0.45
1:B:249:SER:O	1:B:251:PRO:HD3	2.16	0.45
1:A:49:LYS:HA	1:A:49:LYS:HD3	1.70	0.45
1:A:211:LEU:O	1:A:214:ASN:ND2	2.49	0.45
1:A:171:VAL:HA	1:A:172:PRO:HD3	1.57	0.45
1:A:39:ASP:HB2	1:A:40:LEU:HD12	1.97	0.45
1:A:343:GLN:O	1:A:346:LYS:HE2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ARG:CD	1:B:174:ARG:H	2.29	0.45
1:A:342:CYS:HB3	1:A:367:CYS:H	1.81	0.45
1:A:325:GLU:HG2	1:A:349:ARG:HD3	1.99	0.45
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.83	0.45
1:A:63:HIS:O	1:A:86:LEU:HD12	2.17	0.44
1:A:358:ILE:HB	1:A:378:ASN:ND2	2.31	0.44
1:B:337:ILE:HD11	1:B:358:ILE:HD13	1.98	0.44
1:A:107:LEU:HB3	1:A:110:LEU:HB2	2.00	0.44
1:A:335:ARG:HA	1:A:358:ILE:HA	1.98	0.44
1:A:96:LEU:HB2	1:A:118:ASN:OD1	2.18	0.44
1:A:451:LYS:HA	1:A:454:LEU:HD22	2.00	0.44
1:A:431:PHE:CE1	1:A:444:LEU:HB3	2.53	0.44
1:A:77:GLU:HG2	1:A:100:HIS:CE1	2.53	0.44
1:B:149:GLU:HG2	1:B:174:ARG:CZ	2.48	0.43
1:B:243:PHE:HA	1:B:244:PRO:HD3	1.75	0.43
1:B:288:SER:HA	1:B:311:ASN:HB2	1.99	0.43
1:A:200:PHE:HB3	1:A:227:LEU:HD21	1.99	0.43
1:A:422:ASP:OD1	1:A:424:SER:OG	2.26	0.43
1:B:162:TRP:N	1:B:162:TRP:CD1	2.86	0.43
1:B:324:LEU:HB2	1:B:345:GLN:OE1	2.19	0.43
1:B:91:LEU:HB2	1:B:115:LEU:HD23	1.99	0.43
1:B:80:PHE:CB	1:B:107:LEU:HD21	2.49	0.43
1:B:339:ILE:HA	1:B:362:VAL:HG11	2.00	0.43
1:B:307:ARG:HG2	1:B:330:THR:OG1	2.18	0.42
1:A:91:LEU:HB2	1:A:115:LEU:HD23	2.01	0.42
1:A:315:PHE:CD1	1:A:316:PRO:HD2	2.54	0.42
1:A:428:LEU:HD11	1:A:431:PHE:CD1	2.54	0.42
1:B:100:HIS:HA	1:B:101:PRO:HD2	1.88	0.42
1:A:353:LEU:HA	1:A:353:LEU:HD23	1.77	0.42
1:A:249:SER:O	1:A:251:PRO:HD3	2.20	0.42
1:A:59:SER:O	1:A:62:THR:HG23	2.19	0.42
1:B:72:ILE:O	1:B:94:ASN:HB3	2.19	0.42
1:B:74:LYS:HE3	1:B:98:ILE:H	1.85	0.42
1:A:51:LEU:HG	1:A:53:THR:O	2.19	0.42
1:A:301:LEU:HD21	1:A:304:LEU:HD22	2.00	0.42
1:B:150:ASP:O	1:B:153:GLU:HB2	2.19	0.42
1:B:73:THR:O	1:B:96:LEU:HD23	2.20	0.42
1:A:315:PHE:CZ	1:A:337:ILE:HG22	2.55	0.42
1:B:409:LYS:O	1:B:410:GLU:HB2	2.20	0.42
1:B:173:ILE:HD12	1:B:199:ALA:HA	2.02	0.42
1:A:351:LEU:HD22	1:A:353:LEU:HG	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD22	1:B:353:LEU:HG	2.01	0.41
1:A:386:GLU:CD	1:A:386:GLU:H	2.23	0.41
1:A:101:PRO:O	1:A:127:SER:HA	2.20	0.41
1:B:149:GLU:CD	1:B:174:ARG:HG3	2.40	0.41
1:B:282:LEU:N	1:B:282:LEU:HD12	2.35	0.41
1:B:370:LEU:HD23	1:B:370:LEU:HA	1.94	0.41
1:A:313:GLN:HA	1:A:333:LYS:HB3	2.01	0.41
1:A:254:LYS:NZ	1:A:276:LEU:O	2.44	0.41
1:A:87:GLU:C	1:A:110:LEU:HD12	2.41	0.41
1:A:418:LEU:O	1:A:439:LEU:HD22	2.20	0.41
1:A:325:GLU:O	1:A:348:LEU:HD12	2.21	0.41
1:A:332:THR:OG1	1:A:334:ILE:HD12	2.19	0.41
1:A:288:SER:HA	1:A:311:ASN:HB2	2.01	0.41
1:B:149:GLU:OE1	1:B:174:ARG:NE	2.52	0.41
1:B:282:LEU:HD21	1:B:295:PHE:HZ	1.85	0.41
1:B:405:HIS:HD2	3:B:709:HOH:O	2.04	0.41
1:B:408:HIS:CE1	2:B:502:NAG:H82	2.55	0.41
1:A:150:ASP:OD1	1:A:150:ASP:N	2.52	0.41
1:A:141:ALA:H	1:A:165:ASP:HB3	1.86	0.41
1:B:408:HIS:HD2	3:B:710:HOH:O	2.04	0.40
1:A:380:ILE:O	1:A:380:ILE:HG13	2.20	0.40
1:B:397:LEU:HD12	1:B:397:LEU:HA	1.86	0.40
1:B:174:ARG:HB2	3:B:665:HOH:O	2.21	0.40
1:A:245:ASP:OD1	1:A:245:ASP:N	2.53	0.40
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.90	0.40
1:A:33:PRO:HD3	1:A:57:GLY:O	2.21	0.40
1:A:161:LEU:HB3	1:A:185:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	422/432 (98%)	409 (97%)	13 (3%)	0	100	100
1	B	423/432 (98%)	410 (97%)	13 (3%)	0	100	100
All	All	845/864 (98%)	819 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/384 (98%)	333 (88%)	45 (12%)	6	13
1	B	378/384 (98%)	338 (89%)	40 (11%)	8	17
All	All	756/768 (98%)	671 (89%)	85 (11%)	7	15

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	LEU
1	B	51	LEU
1	B	65	LEU
1	B	73	THR
1	B	75	LEU
1	B	99	ILE
1	B	107	LEU
1	B	113	LEU
1	B	129	LYS
1	B	132	VAL
1	B	146	THR
1	B	168	LEU
1	B	171	VAL
1	B	174	ARG
1	B	181	SER
1	B	185	LEU
1	B	193	SER
1	B	230	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	233	LEU
1	B	245	ASP
1	B	265	ILE
1	B	277	LEU
1	B	282	LEU
1	B	298	LEU
1	B	301	LEU
1	B	315	PHE
1	B	324	LEU
1	B	327	LEU
1	B	329	LEU
1	B	332	THR
1	B	351	LEU
1	B	377	ASN
1	B	379	GLN
1	B	383	VAL
1	B	394	LEU
1	B	406	THR
1	B	415	LEU
1	B	433	THR
1	B	443	LYS
1	B	449	ASN
1	A	32	CYS
1	A	40	LEU
1	A	41	ASP
1	A	56	ASP
1	A	64	SER
1	A	73	THR
1	A	104	LEU
1	A	112	VAL
1	A	113	LEU
1	A	120	LEU
1	A	132	VAL
1	A	146	THR
1	A	169	THR
1	A	171	VAL
1	A	174	ARG
1	A	201	SER
1	A	204	SER
1	A	213	ASN
1	A	227	LEU
1	A	253	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	259	HIS
1	A	293	SER
1	A	314	TRP
1	A	315	PHE
1	A	318	LEU
1	A	327	LEU
1	A	329	LEU
1	A	332	THR
1	A	351	LEU
1	A	367	CYS
1	A	375	LEU
1	A	380	ILE
1	A	386	GLU
1	A	394	LEU
1	A	395	ARG
1	A	404	ILE
1	A	410	GLU
1	A	414	THR
1	A	416	LYS
1	A	429	THR
1	A	433	THR
1	A	436	LEU
1	A	443	LYS
1	A	449	ASN
1	A	454	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	449	ASN
1	A	222	HIS
1	A	239	ASN
1	A	296	GLN
1	A	408	HIS
1	A	440	ASN
1	A	449	ASN

### 5.3.3 RNA ⓘ

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](#)

2 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	NAG	B	501	1	14,14,15	0.24	0	15,19,21	0.57	0
2	NAG	B	502	1	14,14,15	0.55	0	15,19,21	0.47	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	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	424/432 (98%)	0.52	33 (7%)	16 13	36, 70, 104, 112	0
1	B	425/432 (98%)	0.28	12 (2%)	56 55	32, 52, 85, 106	0
All	All	849/864 (98%)	0.40	45 (5%)	30 27	32, 60, 100, 112	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	ALA	4.7
1	A	439	LEU	4.7
1	A	388	PHE	4.3
1	A	152	PHE	4.0
1	A	75	LEU	3.9
1	B	67	LEU	3.8
1	A	316	PRO	3.8
1	A	412	PHE	3.5
1	B	51	LEU	3.5
1	A	339	ILE	3.4
1	A	155	LEU	3.2
1	A	341	PHE	3.2
1	A	383	VAL	3.2
1	B	34	ALA	3.1
1	B	54	VAL	3.0
1	A	337	ILE	2.9
1	A	115	LEU	2.8
1	A	436	LEU	2.8
1	A	315	PHE	2.8
1	A	89	LEU	2.7
1	A	295	PHE	2.7
1	B	98	ILE	2.7
1	A	335	ARG	2.6
1	B	431	PHE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	128	LEU	2.6
1	A	318	LEU	2.6
1	A	67	LEU	2.5
1	A	46	CYS	2.5
1	A	65	LEU	2.5
1	A	361	LEU	2.5
1	B	65	LEU	2.4
1	A	123	VAL	2.4
1	A	364	PHE	2.3
1	A	392	ALA	2.3
1	A	80	PHE	2.2
1	B	74	LYS	2.2
1	B	115	LEU	2.2
1	A	44	ALA	2.2
1	B	123	VAL	2.1
1	B	168	LEU	2.1
1	A	382	GLU	2.1
1	A	184	ALA	2.1
1	A	282	LEU	2.0
1	A	100	HIS	2.0
1	B	83	PHE	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 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(Å <sup>2</sup> )	Q<0.9
2	NAG	B	502	14/15	0.87	0.14	-0.72	62,68,72,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	501	14/15	0.82	0.17	-	60,73,77,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.