



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:36 pm BST

PDB ID : 5Y3S  
Title : Crystal structure of human NLRP1 leucine rich repeat domain  
Authors : Jin, T.; Xiao, T.S.  
Deposited on : 2017-07-30  
Resolution : 2.45 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 : 2.11  
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) : 2.11

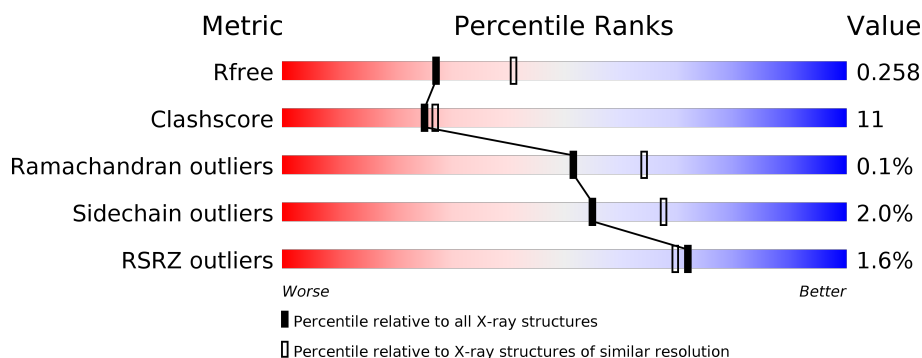
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	205	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	205	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	205	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
1	D	205	<div> <div></div> <div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6228 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 NACHT, LRR and PYD domains-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	1	0
			1550	961	286	291	12			
1	B	198	Total	C	N	O	S	0	0	0
			1540	955	282	291	12			
1	C	201	Total	C	N	O	S	0	1	0
			1569	972	288	297	12			
1	D	199	Total	C	N	O	S	0	1	0
			1550	962	281	295	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	786	GLY	-	expression tag	UNP Q9C000
A	787	SER	-	expression tag	UNP Q9C000
A	788	VAL	-	expression tag	UNP Q9C000
A	789	ASP	-	expression tag	UNP Q9C000
B	786	GLY	-	expression tag	UNP Q9C000
B	787	SER	-	expression tag	UNP Q9C000
B	788	VAL	-	expression tag	UNP Q9C000
B	789	ASP	-	expression tag	UNP Q9C000
C	786	GLY	-	expression tag	UNP Q9C000
C	787	SER	-	expression tag	UNP Q9C000
C	788	VAL	-	expression tag	UNP Q9C000
C	789	ASP	-	expression tag	UNP Q9C000
D	786	GLY	-	expression tag	UNP Q9C000
D	787	SER	-	expression tag	UNP Q9C000
D	788	VAL	-	expression tag	UNP Q9C000
D	789	ASP	-	expression tag	UNP Q9C000

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

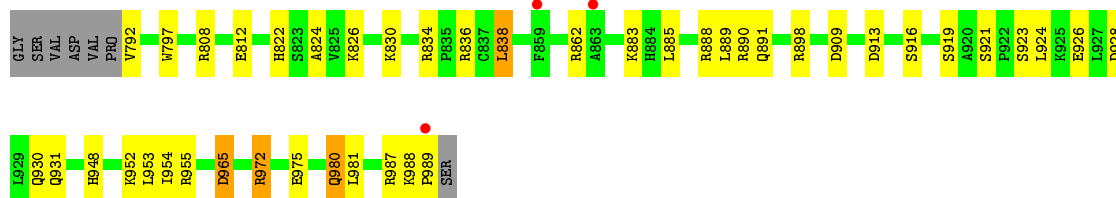
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	D	4	Total	O	0	0
			4	4		

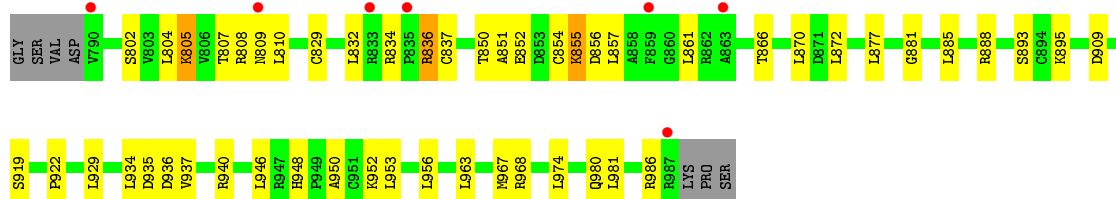
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

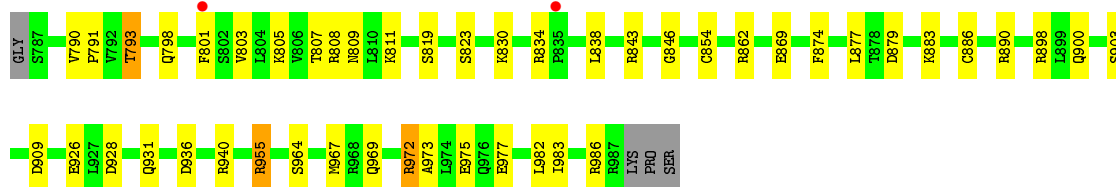
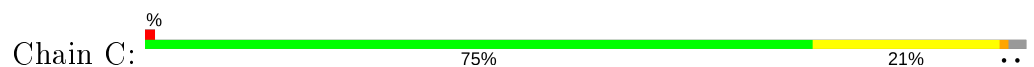
- Molecule 1: NACHT, LRR and PYD domains-containing protein 1



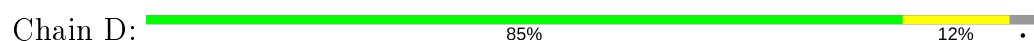
- Molecule 1: NACHT, LRR and PYD domains-containing protein 1

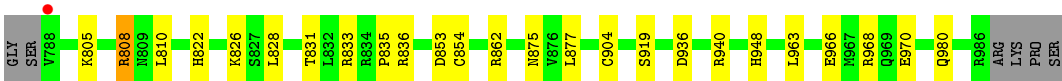


- Molecule 1: NACHT, LRR and PYD domains-containing protein 1



- Molecule 1: NACHT, LRR and PYD domains-containing protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.48 Å   141.48 Å   294.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	33.76 – 2.45 47.06 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.76-2.45) 92.8 (47.06-2.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.45 Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, $R_{free}$	0.211   ,   0.259 0.211   ,   0.258	Depositor DCC
$R_{free}$ test set	2062 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4

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	0/1568	0.64	0/2113
1	B	0.43	0/1555	0.66	0/2098
1	C	0.44	0/1587	0.64	2/2141 (0.1%)
1	D	0.46	0/1568	0.65	0/2117
All	All	0.44	0/6278	0.65	2/8469 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	955	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	C	862	ARG	NE-CZ-NH2	5.18	122.89	120.30

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	1550	0	1617	45	1
1	B	1540	0	1600	44	1
1	C	1569	0	1630	34	0
1	D	1550	0	1608	19	0
2	A	5	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
All	All	6228	0	6455	135	1

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 11.

All (135) 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:809:ASN:N	1:B:836:ARG:HH21	1.57	1.02
1:B:808:ARG:HA	1:B:836:ARG:NH2	1.77	0.98
1:B:808:ARG:HA	1:B:836:ARG:CZ	1.98	0.93
1:D:808:ARG:HE	1:D:836:ARG:HH11	1.09	0.92
1:B:807:THR:O	1:B:836:ARG:NH1	2.03	0.91
1:A:808:ARG:HA	1:A:836:ARG:HH12	1.36	0.88
1:B:808:ARG:CA	1:B:836:ARG:NH2	2.37	0.87
1:D:805:LYS:O	1:D:836:ARG:NH2	2.17	0.77
1:B:857:LEU:O	1:B:861:LEU:HD12	1.85	0.76
1:B:809:ASN:H	1:B:836:ARG:HH21	1.31	0.74
1:A:808:ARG:CA	1:A:836:ARG:HH12	2.02	0.72
1:B:963:LEU:O	1:B:968:ARG:NH2	2.23	0.72
1:A:923:SER:HA	1:A:952:LYS:HE3	1.72	0.71
1:A:862:ARG:HG3	1:A:888:ARG:CZ	2.20	0.71
1:C:879:ASP:O	1:C:883:LYS:HG2	1.90	0.71
1:B:809:ASN:N	1:B:836:ARG:NH2	2.36	0.70
1:B:940:ARG:HG3	1:B:967:MET:CE	2.21	0.70
1:A:987:ARG:NH2	1:C:926:GLU:OE1	2.25	0.70
1:C:807:THR:HG22	1:D:810:LEU:HD13	1.75	0.68
1:B:854:CYS:SG	1:B:877:LEU:HD22	2.34	0.68
1:C:808:ARG:NE	1:C:809:ASN:H	1.93	0.66
1:B:940:ARG:HG3	1:B:967:MET:HE1	1.78	0.66
1:D:963:LEU:O	1:D:968:ARG:NH1	2.30	0.64
1:B:808:ARG:C	1:B:836:ARG:NH2	2.51	0.63
1:B:834:ARG:O	1:B:837:CYS:N	2.29	0.62
1:A:836:ARG:NH1	1:A:838:LEU:HD11	2.15	0.61
1:A:988:LYS:HD3	1:A:989:PRO:HD2	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:GLN:NE2	1:C:928:ASP:OD2	2.33	0.61
1:A:952:LYS:NZ	1:A:952:LYS:HB2	2.13	0.61
1:C:898[B]:ARG:HG2	1:C:900:GLN:HE22	1.64	0.61
1:B:852:GLU:O	1:B:855:LYS:HG3	2.01	0.61
1:C:809:ASN:HD22	1:C:811:LYS:HE3	1.66	0.59
1:C:808:ARG:HE	1:C:809:ASN:H	1.51	0.58
1:D:808:ARG:HE	1:D:836:ARG:HD2	1.68	0.58
1:D:808:ARG:NE	1:D:836:ARG:HD2	2.19	0.58
1:B:837:CYS:O	1:B:866:THR:HG21	2.04	0.57
1:A:808:ARG:HA	1:A:836:ARG:NH1	2.13	0.57
1:A:988:LYS:HA	2:C:1001:PO4:O4	2.05	0.56
1:C:973:ALA:O	1:C:977:GLU:HG3	2.06	0.55
1:C:940:ARG:CZ	1:C:967:MET:HE1	2.37	0.55
1:A:822:HIS:O	1:A:826:LYS:HG3	2.07	0.55
1:B:855:LYS:NZ	1:B:856:ASP:OD2	2.27	0.55
1:B:968:ARG:NH2	4:B:1001:HOH:O	2.40	0.54
1:A:987:ARG:HD2	1:C:986:ARG:HH22	1.72	0.53
1:B:946:LEU:HD11	1:B:956:LEU:HD22	1.89	0.53
1:C:791:PRO:HB2	1:C:793:THR:HB	1.90	0.53
1:A:954:ILE:HG13	1:A:955:ARG:HG3	1.91	0.53
1:B:980:GLN:N	1:B:980:GLN:OE1	2.41	0.53
1:A:923:SER:CA	1:A:952:LYS:HE3	2.39	0.52
1:D:833:ARG:HD3	1:D:862:ARG:NH1	2.24	0.52
1:B:870:LEU:HD11	1:B:872:LEU:HD21	1.91	0.52
1:B:922:PRO:HA	1:B:952:LYS:HE3	1.92	0.52
1:B:805:LYS:O	1:B:808:ARG:NH1	2.42	0.52
1:C:791:PRO:O	1:C:798:GLN:NE2	2.43	0.52
1:C:898[B]:ARG:HG3	1:C:926:GLU:HB3	1.91	0.52
1:B:832:LEU:HA	1:B:837:CYS:SG	2.51	0.51
1:B:946:LEU:HD21	1:B:953:LEU:HD23	1.93	0.51
1:C:843:ARG:NH2	1:C:869:GLU:OE2	2.42	0.51
1:A:862:ARG:HG3	1:A:888:ARG:NH2	2.25	0.51
1:D:980:GLN:CD	1:D:980:GLN:H	2.15	0.50
1:B:802:SER:O	1:B:805:LYS:HG3	2.12	0.50
1:A:972:ARG:HA	1:A:975:GLU:HG2	1.94	0.50
1:C:926:GLU:HG3	1:C:955:ARG:HB2	1.94	0.50
1:D:936:ASP:HB3	1:D:940:ARG:NH1	2.27	0.50
1:B:829:CYS:HA	1:B:832:LEU:HD12	1.94	0.49
1:B:807:THR:O	1:B:836:ARG:CZ	2.58	0.49
1:D:966:GLU:O	1:D:970:GLU:HG3	2.11	0.49
1:A:888:ARG:HH21	1:A:891:GLN:HG3	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:TRP:CD1	1:A:824:ALA:HB2	2.47	0.48
1:A:836:ARG:CZ	1:A:838:LEU:HD11	2.42	0.48
1:C:808:ARG:NH1	1:C:838:LEU:HD12	2.28	0.48
1:D:808:ARG:NE	1:D:836:ARG:HH11	1.92	0.48
1:A:952:LYS:HB2	1:A:952:LYS:HZ3	1.78	0.48
1:B:940:ARG:HG3	1:B:967:MET:HE3	1.95	0.48
1:A:928:ASP:OD1	1:A:930:GLN:HG3	2.14	0.48
1:B:974:LEU:HD22	1:B:981:LEU:HD23	1.95	0.48
1:A:980:GLN:O	1:A:980:GLN:HG3	2.13	0.48
1:D:822:HIS:HD2	1:D:853:ASP:OD1	1.97	0.48
1:B:950:ALA:O	1:B:952:LYS:NZ	2.38	0.47
1:A:909:ASP:HA	1:D:835:PRO:HD2	1.96	0.47
1:D:822:HIS:O	1:D:826:LYS:HG3	2.15	0.47
1:C:846:GLY:HA2	1:C:874:PHE:O	2.15	0.47
1:C:803:VAL:O	1:C:807:THR:HG23	2.14	0.47
1:D:828:LEU:O	1:D:831:THR:HG22	2.14	0.47
1:B:804:LEU:HA	1:B:804:LEU:HD23	1.71	0.47
1:A:921:SER:O	1:A:952:LYS:NZ	2.47	0.47
1:B:929:LEU:HD13	1:B:934:LEU:HD11	1.98	0.46
1:A:808:ARG:CB	1:A:836:ARG:HH12	2.29	0.46
1:A:836:ARG:NH1	1:A:838:LEU:CD1	2.80	0.45
1:A:885:LEU:O	1:A:889:LEU:HG	2.16	0.45
1:D:919:SER:HB2	1:D:948:HIS:CD2	2.51	0.45
1:A:830:LYS:HA	1:A:830:LYS:HD3	1.68	0.45
1:A:987:ARG:NH1	1:C:955:ARG:HD2	2.32	0.45
1:B:893:SER:O	1:B:895:LYS:HE2	2.17	0.45
1:A:890:ARG:NE	1:A:916:SER:OG	2.49	0.44
1:C:898[B]:ARG:HG2	1:C:900:GLN:NE2	2.31	0.44
1:A:919:SER:HB2	1:A:948:HIS:CG	2.52	0.44
1:C:969:GLN:HA	1:C:972:ARG:HG2	1.98	0.44
1:B:935:ASP:OD1	1:B:937:VAL:HG22	2.17	0.44
1:A:898:ARG:HG2	1:A:926:GLU:HB2	1.98	0.44
1:D:936:ASP:HB3	1:D:940:ARG:HH12	1.83	0.44
1:C:975:GLU:HG3	1:C:983:ILE:HD12	2.00	0.44
1:C:805:LYS:HD2	1:C:805:LYS:N	2.33	0.44
1:C:886:CYS:O	1:C:890:ARG:HG2	2.17	0.44
1:A:792:VAL:HG13	1:A:797:TRP:NE1	2.33	0.43
1:C:790:VAL:HG22	1:C:823:SER:HB3	2.00	0.43
1:A:836:ARG:HH11	1:A:838:LEU:HD11	1.83	0.43
1:A:919:SER:HB2	1:A:948:HIS:CD2	2.54	0.43
1:B:881:GLY:O	1:B:885:LEU:HD22	2.18	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:955:ARG:HH21	1:C:982:LEU:HB3	1.83	0.43
1:A:808:ARG:HB3	1:A:836:ARG:HH12	1.84	0.43
1:C:834:ARG:HH11	1:C:834:ARG:HB3	1.83	0.43
1:B:850:THR:HG22	1:B:851:ALA:N	2.34	0.42
1:A:898:ARG:HG2	1:A:926:GLU:CB	2.49	0.42
1:C:830:LYS:HB2	1:C:830:LYS:HE2	1.94	0.42
1:B:922:PRO:C	1:B:952:LYS:HE3	2.40	0.42
1:B:953:LEU:HA	1:B:953:LEU:HD12	1.88	0.42
1:C:936:ASP:OD2	1:C:964:SER:OG	2.24	0.42
1:A:812:GLU:HG2	1:B:808:ARG:HB2	2.02	0.42
1:A:836:ARG:CZ	1:A:838:LEU:CD1	2.98	0.42
1:C:854:CYS:SG	1:C:877:LEU:HD22	2.60	0.41
1:B:810:LEU:HA	1:B:810:LEU:HD12	1.82	0.41
1:A:883:LYS:HG3	1:A:913:ASP:OD2	2.20	0.41
1:B:919:SER:HB2	1:B:948:HIS:CD2	2.56	0.41
1:D:854:CYS:SG	1:D:877:LEU:HD22	2.60	0.41
1:C:808:ARG:HH11	1:C:838:LEU:HD12	1.85	0.41
1:A:924:LEU:HG	1:A:953:LEU:HD21	2.03	0.41
1:B:936:ASP:HA	1:B:967:MET:HE2	2.03	0.41
1:A:834:ARG:HA	1:A:834:ARG:HD3	1.85	0.41
1:B:854:CYS:SG	1:B:885:LEU:HD21	2.61	0.41
1:A:836:ARG:NE	1:A:838:LEU:HD11	2.37	0.40
1:A:965:ASP:OD1	1:A:965:ASP:N	2.54	0.40
1:C:903:SER:HA	1:C:931:GLN:O	2.21	0.40
1:C:940:ARG:HG3	1:C:967:MET:HE3	2.04	0.40
1:D:875:ASN:O	1:D:904:CYS:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:O	1:B:986:ARG:NH2[17_434]	2.01	0.19

## 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	197/205 (96%)	188 (95%)	9 (5%)	0	100	100
1	B	196/205 (96%)	182 (93%)	14 (7%)	0	100	100
1	C	200/205 (98%)	190 (95%)	9 (4%)	1 (0%)	29	34
1	D	198/205 (97%)	193 (98%)	5 (2%)	0	100	100
All	All	791/820 (96%)	753 (95%)	37 (5%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	793	THR

### 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	178/183 (97%)	174 (98%)	4 (2%)	52	64
1	B	177/183 (97%)	172 (97%)	5 (3%)	43	56
1	C	181/183 (99%)	177 (98%)	4 (2%)	52	64
1	D	179/183 (98%)	178 (99%)	1 (1%)	86	91
All	All	715/732 (98%)	701 (98%)	14 (2%)	55	67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	838	LEU
1	A	965	ASP
1	A	972	ARG
1	A	980	GLN
1	B	805	LYS
1	B	836	ARG
1	B	855	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	888	ARG
1	B	909	ASP
1	C	801	PHE
1	C	819	SER
1	C	909	ASP
1	C	972	ARG
1	D	808	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	798	GLN
1	A	809	ASN
1	A	960	GLN
1	B	809	ASN
1	B	865	GLN
1	C	809	ASN
1	C	900	GLN
1	D	822	HIS
1	D	980	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
2	PO4	A	1001	-	4,4,4	0.78	0	6,6,6	0.54	0
2	PO4	C	1001	-	4,4,4	0.93	0	6,6,6	0.50	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	PO4	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	198/205 (96%)	0.07	3 (1%) 73 71	48, 71, 97, 110	0
1	B	198/205 (96%)	0.24	7 (3%) 44 40	54, 76, 99, 108	0
1	C	201/205 (98%)	0.02	2 (0%) 82 83	50, 69, 96, 108	0
1	D	199/205 (97%)	-0.14	1 (0%) 91 92	42, 57, 79, 101	0
All	All	796/820 (97%)	0.05	13 (1%) 72 69	42, 69, 96, 110	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	863	ALA	4.3
1	B	790	VAL	4.0
1	A	989	PRO	3.8
1	B	987	ARG	3.2
1	A	859	PHE	3.2
1	A	863	ALA	3.1
1	B	835	PRO	2.9
1	B	859	PHE	2.5
1	B	833	ARG	2.5
1	C	801	PHE	2.5
1	D	788	VAL	2.5
1	C	835	PRO	2.4
1	B	809	ASN	2.2

### 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. 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
2	PO4	C	1001	5/5	0.71	0.22	92,101,107,115	0
2	PO4	A	1001	5/5	0.88	0.12	101,103,109,121	0
3	NA	A	1002	1/1	0.94	0.13	73,73,73,73	0

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

There are no such residues in this entry.