



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 4R6J / pdb_00004r6j
Title : Crystal structure of computaional designed Lucine rich repeats DLRR_H in
space group P212121
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2014-08-25
Resolution : 2.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

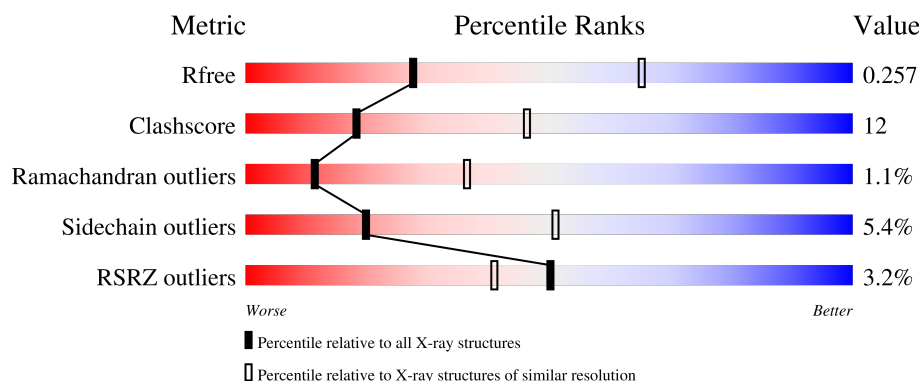
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	254	0.257 86% 11% .
1	B	254	3% 80% 18% .
1	C	254	4% 84% 14% .
1	D	254	5% 67% 26% 6% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7881 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 Lucine rich repeats DLRR_H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	0	0	0
			1968	1241	337	390			
1	B	253	Total	C	N	O	0	0	0
			1968	1241	337	390			
1	C	253	Total	C	N	O	0	0	0
			1968	1241	337	390			
1	D	252	Total	C	N	O	0	0	0
			1961	1237	336	388			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

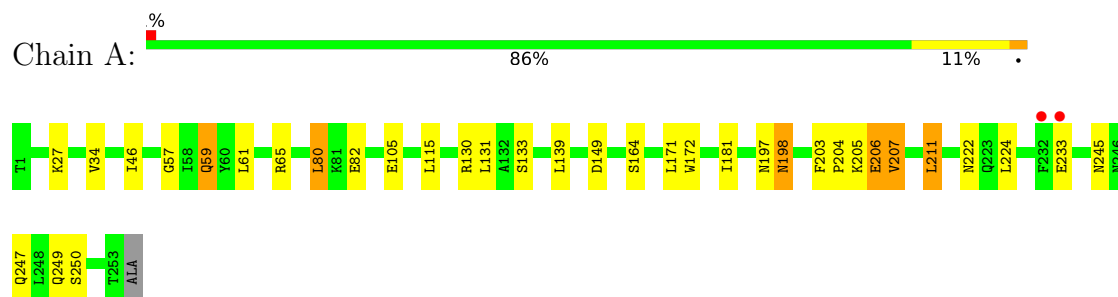
- Molecule 3 is water.

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

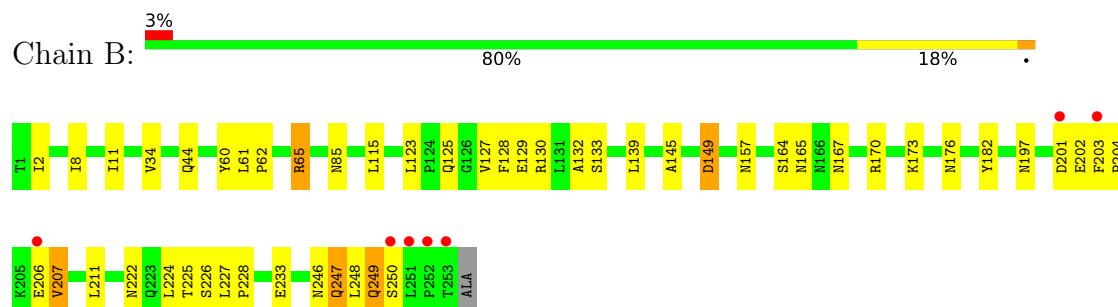
3 Residue-property plots

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.

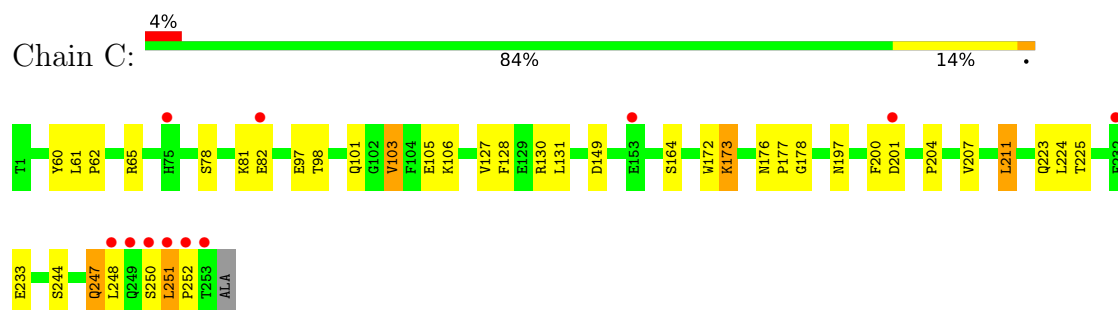
- Molecule 1: Lucine rich repeats DLRR_H



- Molecule 1: Lucine rich repeats DLRR_H



- Molecule 1: Lucine rich repeats DLRR_H



- Molecule 1: Lucine rich repeats DLRR_H





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.78Å 96.50Å 136.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.90) 99.7 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.219 , 0.256 0.218 , 0.257	Depositor DCC
R_{free} test set	1389 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7881	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.92	0/1996	0.92	3/2721 (0.1%)
1	B	0.90	0/1996	0.95	3/2721 (0.1%)
1	C	0.86	0/1996	0.93	2/2721 (0.1%)
1	D	1.17	2/1989 (0.1%)	0.99	3/2711 (0.1%)
All	All	0.97	2/7977 (0.0%)	0.95	11/10874 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	THR	C-N	26.34	1.70	1.33
1	D	74	LEU	C-N	24.18	1.69	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ASN	N-CA-C	-8.77	94.59	109.24
1	D	74	LEU	O-C-N	-8.01	113.17	123.02
1	B	207	VAL	N-CA-C	7.46	117.54	110.53
1	C	103	VAL	CB-CA-C	-6.73	104.84	111.30
1	B	176	ASN	N-CA-C	-6.48	101.89	109.93
1	D	50	SER	N-CA-C	-6.40	100.99	110.46
1	C	101	GLN	CB-CA-C	-6.07	101.45	110.67
1	B	249	GLN	N-CA-C	5.89	119.26	109.96
1	A	198	ASN	O-C-N	-5.72	116.30	123.27
1	A	249	GLN	N-CA-C	-5.45	101.69	110.14
1	D	55	VAL	CB-CA-C	-5.26	106.14	112.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1968	0	2007	23	0
1	B	1968	0	2007	49	0
1	C	1968	0	2007	20	1
1	D	1961	0	2000	103	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	4	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	7881	0	8021	193	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 12.

All (193) 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:74:LEU:C	1:D:75:HIS:N	1.69	1.48
1:D:98:THR:C	1:D:99:LEU:N	1.70	1.47
1:D:149:ASP:HB3	1:D:181:ILE:HD11	1.23	1.19
1:C:200:PHE:O	1:C:224:LEU:HD12	1.44	1.14
1:D:60:TYR:O	1:D:62:PRO:HD3	1.48	1.10
1:D:17:PHE:HZ	1:D:58:ILE:HD12	1.13	1.07
1:D:17:PHE:CZ	1:D:58:ILE:HD12	1.92	1.04
1:B:203:PHE:CZ	1:B:228:PRO:HD3	1.92	1.03
1:B:60:TYR:O	1:B:62:PRO:HD3	1.59	1.02
1:D:221:ASN:OD1	1:D:245:ASN:ND2	1.94	1.00
1:B:203:PHE:CZ	1:B:228:PRO:CD	2.45	0.99
1:B:203:PHE:CZ	1:B:227:LEU:HA	1.96	0.99
1:B:203:PHE:CE2	1:B:228:PRO:CD	2.48	0.96
1:D:149:ASP:CB	1:D:181:ILE:HD11	1.96	0.94
1:D:55:VAL:HG12	1:D:58:ILE:HB	1.48	0.94
1:D:149:ASP:HB3	1:D:181:ILE:CD1	1.98	0.94
1:B:203:PHE:CE2	1:B:228:PRO:HD2	2.07	0.90
1:D:77:ILE:HD12	1:D:103:VAL:HG21	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:THR:HA	1:B:247:GLN:O	1.76	0.85
1:D:59:GLN:N	1:D:59:GLN:OE1	2.10	0.84
1:B:203:PHE:CZ	1:B:227:LEU:HD23	2.16	0.81
1:B:203:PHE:CZ	1:B:228:PRO:HD2	2.15	0.81
1:D:60:TYR:O	1:D:62:PRO:CD	2.28	0.81
1:C:78:SER:HB2	1:C:81:LYS:HE3	1.62	0.80
1:D:81:LYS:HZ1	1:D:105:GLU:HB2	1.49	0.78
1:B:203:PHE:CE2	1:B:228:PRO:HD3	2.16	0.78
1:D:221:ASN:OD1	1:D:245:ASN:CB	2.33	0.77
1:D:104:PHE:HD1	1:D:107:LEU:HD12	1.49	0.77
1:D:221:ASN:OD1	1:D:245:ASN:HB2	1.85	0.76
1:D:81:LYS:HZ1	1:D:105:GLU:CB	1.98	0.76
1:D:129:GLU:HG3	1:D:130:ARG:HD3	1.66	0.76
1:D:81:LYS:HG3	1:D:103:VAL:HA	1.67	0.76
1:D:81:LYS:NZ	1:D:105:GLU:CB	2.49	0.76
1:B:203:PHE:CZ	1:B:227:LEU:CD2	2.70	0.75
1:D:11:ILE:HG23	1:D:60:TYR:CE1	2.22	0.75
1:D:55:VAL:CG1	1:D:58:ILE:HD13	2.16	0.75
1:D:55:VAL:HG11	1:D:58:ILE:HD13	1.68	0.74
1:D:2:ILE:HG22	1:D:36:GLN:OE1	1.87	0.73
1:D:77:ILE:CD1	1:D:103:VAL:HG21	2.19	0.73
1:A:171:LEU:HD22	1:A:181:ILE:HD12	1.71	0.72
1:B:203:PHE:HZ	1:B:227:LEU:HA	1.48	0.71
1:D:94:ASN:HB2	1:D:96:LEU:CD1	2.21	0.71
1:B:129:GLU:HG3	1:B:130:ARG:H	1.57	0.69
1:C:78:SER:CB	1:C:81:LYS:HE3	2.22	0.69
1:D:81:LYS:NZ	1:D:105:GLU:HB3	2.07	0.69
1:B:60:TYR:O	1:B:62:PRO:CD	2.39	0.69
1:B:203:PHE:CE1	1:B:227:LEU:HA	2.28	0.69
1:B:11:ILE:HG23	1:B:60:TYR:CE1	2.28	0.68
1:D:180:PRO:HG2	1:D:182:TYR:OH	1.94	0.68
1:C:82:GLU:OE1	1:C:106:LYS:HE2	1.94	0.67
1:D:221:ASN:CG	1:D:245:ASN:HD22	2.02	0.67
1:C:200:PHE:O	1:C:224:LEU:CD1	2.34	0.67
1:D:149:ASP:CA	1:D:181:ILE:HD11	2.24	0.66
1:B:203:PHE:HZ	1:B:227:LEU:CA	2.09	0.66
1:D:81:LYS:HZ2	1:D:105:GLU:HB3	1.59	0.65
1:D:182:TYR:HE1	1:D:206:GLU:HB2	1.61	0.65
1:A:57:GLY:H	1:A:59:GLN:HE22	1.42	0.65
1:B:44:GLN:NE2	1:D:227:LEU:HB2	2.11	0.64
1:D:6:THR:O	1:D:33:ALA:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ASN:OD1	1:D:245:ASN:CG	2.42	0.63
1:D:2:ILE:N	1:D:36:GLN:OE1	2.30	0.63
1:A:206:GLU:HA	1:A:206:GLU:OE1	2.00	0.61
1:B:203:PHE:CE1	1:B:227:LEU:HD23	2.35	0.61
1:A:198:ASN:O	1:A:222:ASN:OD1	2.18	0.61
1:B:203:PHE:HZ	1:B:227:LEU:CB	2.14	0.61
1:A:172:TRP:CZ2	1:A:207:VAL:HG21	2.37	0.60
1:A:149:ASP:N	1:A:149:ASP:OD1	2.34	0.59
1:B:222:ASN:HB2	1:B:246:ASN:HD21	1.68	0.58
1:D:2:ILE:HD11	1:D:6:THR:OG1	2.02	0.58
1:B:203:PHE:CZ	1:B:227:LEU:CA	2.79	0.58
1:C:225:THR:O	1:C:251:LEU:HD22	2.04	0.57
1:C:149:ASP:OD1	1:C:149:ASP:N	2.36	0.57
1:A:171:LEU:CD2	1:A:181:ILE:HD12	2.35	0.57
1:D:7:PRO:HA	1:D:33:ALA:HA	1.85	0.56
1:D:247:GLN:HE21	1:D:247:GLN:N	2.03	0.56
1:D:162:ASN:OD1	1:D:164:SER:OG	2.23	0.56
1:B:165:ASN:OD1	1:B:197:ASN:ND2	2.37	0.56
1:D:11:ILE:CG2	1:D:60:TYR:CE1	2.88	0.56
1:D:94:ASN:CB	1:D:96:LEU:CD1	2.84	0.56
1:B:65:ARG:CG	1:B:65:ARG:HH11	2.19	0.56
1:C:204:PRO:O	1:C:207:VAL:HG22	2.07	0.55
1:D:203:PHE:HD1	1:D:204:PRO:O	1.90	0.55
1:C:172:TRP:C	1:C:173:LYS:HG2	2.31	0.55
1:D:55:VAL:CG1	1:D:58:ILE:CD1	2.85	0.55
1:B:204:PRO:O	1:B:207:VAL:HG22	2.07	0.55
1:D:55:VAL:HG12	1:D:55:VAL:O	2.06	0.55
1:D:55:VAL:HG12	1:D:58:ILE:CB	2.31	0.55
1:B:2:ILE:CD1	1:B:60:TYR:CE2	2.90	0.54
1:D:99:LEU:CD1	1:D:120:LEU:HD21	2.36	0.54
1:D:99:LEU:HD13	1:D:120:LEU:HD21	1.89	0.54
1:D:182:TYR:CE1	1:D:206:GLU:HB2	2.40	0.54
1:B:203:PHE:HE1	1:B:226:SER:O	1.91	0.53
1:D:248:LEU:C	1:D:248:LEU:HD12	2.32	0.53
1:D:2:ILE:HG23	1:D:36:GLN:HB2	1.90	0.53
1:A:80:LEU:CD1	1:A:80:LEU:N	2.71	0.53
1:B:129:GLU:HG3	1:B:130:ARG:N	2.23	0.53
1:D:96:LEU:N	1:D:96:LEU:HD12	2.23	0.53
1:D:104:PHE:CD1	1:D:107:LEU:HD12	2.39	0.53
1:D:98:THR:C	1:D:99:LEU:CA	2.73	0.53
1:D:81:LYS:HZ1	1:D:105:GLU:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ILE:CG2	1:D:60:TYR:CD1	2.92	0.52
1:D:170:ARG:HA	1:D:173:LYS:HD2	1.92	0.52
1:D:129:GLU:HG3	1:D:130:ARG:CD	2.39	0.51
1:D:74:LEU:C	1:D:75:HIS:CA	2.74	0.51
1:C:105:GLU:O	1:C:130:ARG:HG3	2.11	0.51
1:C:176:ASN:O	1:C:178:GLY:N	2.44	0.50
1:D:8:ILE:HB	1:D:30:VAL:O	2.11	0.50
1:B:2:ILE:HD11	1:B:60:TYR:CE2	2.46	0.50
1:B:65:ARG:NH1	1:B:85:ASN:HB3	2.27	0.50
1:B:149:ASP:N	1:B:149:ASP:OD1	2.44	0.50
1:D:35:THR:O	1:D:36:GLN:C	2.55	0.50
1:D:101:GLN:O	1:D:101:GLN:HG3	2.12	0.50
1:B:203:PHE:HZ	1:B:227:LEU:CD2	2.21	0.49
1:D:174:HIS:HD2	1:D:175:ALA:N	2.09	0.49
1:A:203:PHE:HD1	1:A:204:PRO:O	1.96	0.49
1:B:170:ARG:HA	1:B:173:LYS:HD2	1.94	0.49
1:D:206:GLU:O	1:D:209:LYS:N	2.40	0.49
1:B:201:ASP:OD1	1:B:202:GLU:HG2	2.13	0.49
1:D:242:ASN:OD1	1:D:244:SER:OG	2.29	0.48
1:B:2:ILE:HG12	1:B:60:TYR:CD2	2.48	0.48
1:D:96:LEU:HD13	1:D:118:ASN:OD1	2.13	0.48
1:B:65:ARG:HH11	1:B:65:ARG:HG3	1.78	0.48
1:D:149:ASP:N	1:D:149:ASP:OD1	2.46	0.48
1:D:173:LYS:O	1:D:176:ASN:HB2	2.14	0.48
1:A:204:PRO:O	1:A:207:VAL:HG12	2.13	0.47
1:D:57:GLY:O	1:D:60:TYR:HD1	1.97	0.47
1:D:99:LEU:HD13	1:D:120:LEU:CD2	2.44	0.47
1:D:221:ASN:HA	1:D:245:ASN:HB3	1.97	0.47
1:A:172:TRP:CH2	1:A:207:VAL:HG21	2.50	0.46
1:B:203:PHE:CZ	1:B:227:LEU:HD22	2.50	0.46
1:D:58:ILE:N	1:D:59:GLN:OE1	2.48	0.46
1:D:2:ILE:CG2	1:D:36:GLN:HB2	2.46	0.46
1:B:8:ILE:CG1	1:B:34:VAL:HG21	2.46	0.46
1:D:111:THR:HG22	1:D:133:SER:O	2.15	0.46
1:D:206:GLU:O	1:D:207:VAL:C	2.58	0.46
1:A:82:GLU:HB2	3:A:404:HOH:O	2.15	0.46
1:B:224:LEU:H	1:B:246:ASN:HD22	1.63	0.46
1:D:111:THR:HA	1:D:134:LEU:HA	1.97	0.46
1:B:127:VAL:HG13	1:B:128:PHE:CD2	2.50	0.46
1:D:174:HIS:CD2	1:D:175:ALA:N	2.83	0.46
1:A:57:GLY:H	1:A:59:GLN:NE2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ASP:HA	1:D:223:GLN:O	2.16	0.45
1:D:246:ASN:O	1:D:249:GLN:HB2	2.17	0.45
1:B:211:LEU:HD23	1:B:211:LEU:N	2.31	0.45
1:B:11:ILE:CG2	1:B:60:TYR:CE1	3.00	0.45
1:C:65:ARG:HG3	1:C:65:ARG:HH11	1.82	0.45
1:D:174:HIS:HD2	1:D:175:ALA:H	1.65	0.45
1:C:127:VAL:HG13	1:C:128:PHE:CD2	2.52	0.45
1:D:127:VAL:HG13	1:D:128:PHE:CD2	2.51	0.45
1:A:171:LEU:HD22	1:A:181:ILE:CD1	2.43	0.44
1:C:82:GLU:OE1	1:C:106:LYS:CE	2.65	0.44
1:B:115:LEU:HB2	1:B:139:LEU:HD23	2.00	0.44
1:D:182:TYR:CD2	1:D:182:TYR:N	2.86	0.43
1:D:246:ASN:O	1:D:249:GLN:CB	2.66	0.43
1:C:127:VAL:HG13	1:C:128:PHE:CG	2.52	0.43
1:D:180:PRO:O	1:D:182:TYR:CE2	2.71	0.43
1:C:201:ASP:HA	1:C:223:GLN:O	2.19	0.43
1:D:174:HIS:C	1:D:176:ASN:H	2.25	0.43
1:D:17:PHE:CZ	1:D:55:VAL:HG13	2.53	0.43
1:D:77:ILE:HD12	1:D:103:VAL:CG2	2.38	0.43
1:D:94:ASN:HB2	1:D:96:LEU:HD13	2.00	0.43
1:D:65:ARG:HH11	1:D:65:ARG:HG3	1.84	0.43
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.83	0.42
1:B:127:VAL:HG13	1:B:128:PHE:CG	2.55	0.42
1:D:96:LEU:HD12	1:D:96:LEU:H	1.85	0.42
1:D:201:ASP:OD1	1:D:202:GLU:HG2	2.18	0.42
1:A:105:GLU:O	1:A:130:ARG:HG3	2.20	0.42
1:C:97:GLU:C	1:C:98:THR:CG2	2.93	0.42
1:A:203:PHE:CD1	1:A:204:PRO:O	2.73	0.42
1:D:211:LEU:N	1:D:211:LEU:CD1	2.82	0.42
1:A:59:GLN:NE2	1:A:59:GLN:H	2.18	0.42
1:A:46:ILE:HD11	1:B:227:LEU:HD12	2.01	0.41
1:A:80:LEU:N	1:A:80:LEU:HD12	2.33	0.41
1:D:81:LYS:NZ	1:D:105:GLU:HB2	2.18	0.41
1:D:81:LYS:NZ	1:D:105:GLU:H	2.17	0.41
1:A:27:LYS:HE3	1:A:34:VAL:HG12	2.02	0.41
1:B:132:ALA:O	1:B:157:ASN:ND2	2.52	0.41
1:B:182:TYR:CE1	1:B:206:GLU:HB3	2.55	0.41
1:D:180:PRO:HG2	1:D:182:TYR:CZ	2.55	0.41
1:B:182:TYR:CZ	1:B:206:GLU:HB3	2.56	0.41
1:C:60:TYR:O	1:C:62:PRO:HD3	2.20	0.41
1:D:55:VAL:HG23	1:D:74:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HB2	1:A:139:LEU:HD23	2.03	0.41
1:A:211:LEU:N	1:A:211:LEU:CD1	2.84	0.41
1:D:72:ASN:O	1:D:94:ASN:HA	2.20	0.41
1:D:115:LEU:HB2	1:D:139:LEU:HD23	2.03	0.41
1:D:127:VAL:HG13	1:D:128:PHE:CG	2.56	0.40
1:D:72:ASN:O	1:D:94:ASN:OD1	2.39	0.40
1:D:140:SER:OG	1:D:141:ASN:ND2	2.54	0.40
1:C:211:LEU:N	1:C:211:LEU:CD1	2.83	0.40
1:C:247:GLN:O	1:C:251:LEU:N	2.54	0.40
1:D:2:ILE:HG22	1:D:36:GLN:CD	2.45	0.40
1:B:145:ALA:HA	1:B:167:ASN:O	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:C:130:ARG:NH1	1:D:247:GLN:OE1[3_554]	1.53	0.67

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	251/254 (99%)	233 (93%)	16 (6%)	2 (1%)	16	44
1	B	251/254 (99%)	232 (92%)	18 (7%)	1 (0%)	30	59
1	C	251/254 (99%)	231 (92%)	16 (6%)	4 (2%)	7	27
1	D	250/254 (98%)	229 (92%)	17 (7%)	4 (2%)	7	27
All	All	1003/1016 (99%)	925 (92%)	67 (7%)	11 (1%)	11	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	LEU
1	A	131	LEU
1	B	61	LEU
1	C	131	LEU
1	C	252	PRO
1	D	131	LEU
1	D	101	GLN
1	C	177	PRO
1	D	102	GLY
1	C	61	LEU
1	A	61	LEU

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	230/230 (100%)	216 (94%)	14 (6%)	17	46
1	B	230/230 (100%)	219 (95%)	11 (5%)	23	55
1	C	230/230 (100%)	219 (95%)	11 (5%)	23	55
1	D	229/230 (100%)	215 (94%)	14 (6%)	17	46
All	All	919/920 (100%)	869 (95%)	50 (5%)	20	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	80	LEU
1	A	133	SER
1	A	164	SER
1	A	197	ASN
1	A	205	LYS
1	A	206	GLU
1	A	207	VAL
1	A	211	LEU
1	A	224	LEU
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	247	GLN
1	A	250	SER
1	B	65	ARG
1	B	123	LEU
1	B	125	GLN
1	B	133	SER
1	B	149	ASP
1	B	164	SER
1	B	233	GLU
1	B	247	GLN
1	B	248	LEU
1	B	249	GLN
1	B	250	SER
1	C	103	VAL
1	C	164	SER
1	C	173	LYS
1	C	197	ASN
1	C	211	LEU
1	C	233	GLU
1	C	244	SER
1	C	247	GLN
1	C	248	LEU
1	C	250	SER
1	C	251	LEU
1	D	2	ILE
1	D	51	ASP
1	D	58	ILE
1	D	81	LYS
1	D	82	GLU
1	D	99	LEU
1	D	108	THR
1	D	164	SER
1	D	211	LEU
1	D	223	GLN
1	D	233	GLU
1	D	244	SER
1	D	247	GLN
1	D	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	141	ASN
1	A	165	ASN
1	A	247	GLN
1	B	141	ASN
1	B	148	ASN
1	B	246	ASN
1	C	93	ASN
1	C	141	ASN
1	C	165	ASN
1	D	94	ASN
1	D	117	ASN
1	D	141	ASN
1	D	174	HIS
1	D	176	ASN
1	D	247	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	SO4	A	301	-	4,4,4	0.52	0	6,6,6	0.57	0
2	SO4	B	301	-	4,4,4	0.58	0	6,6,6	0.43	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	98:THR	C	99:LEU	N	1.70
1	D	74:LEU	C	75:HIS	N	1.69

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, 95th 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 ²)	Q<0.9
1	A	253/254 (99%)	-0.33	2 (0%) 82 77	33, 52, 82, 113	0
1	B	253/254 (99%)	-0.00	7 (2%) 55 46	38, 63, 105, 128	0
1	C	253/254 (99%)	0.02	11 (4%) 40 31	36, 67, 116, 173	0
1	D	252/254 (99%)	0.48	12 (4%) 35 28	52, 98, 162, 181	0
All	All	1011/1016 (99%)	0.04	32 (3%) 50 41	33, 67, 135, 181	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	GLN	3.6
1	D	1	THR	3.2
1	D	3	THR	3.2
1	B	250	SER	3.0
1	A	233	GLU	3.0
1	D	4	VAL	2.9
1	B	206	GLU	2.8
1	C	153	GLU	2.8
1	D	74	LEU	2.8
1	D	8	ILE	2.7
1	B	251	LEU	2.6
1	C	82	GLU	2.6
1	B	203	PHE	2.5
1	D	5	SER	2.5
1	C	201	ASP	2.5
1	C	250	SER	2.5
1	B	201	ASP	2.4
1	D	2	ILE	2.4
1	C	251	LEU	2.4
1	A	232	PHE	2.3
1	D	140	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	252	PRO	2.3
1	B	252	PRO	2.2
1	D	34	VAL	2.2
1	C	253	THR	2.2
1	D	250	SER	2.2
1	D	50	SER	2.1
1	B	253	THR	2.0
1	C	75	HIS	2.0
1	D	36	GLN	2.0
1	C	248	LEU	2.0
1	C	232	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
2	SO4	B	301	5/5	0.90	0.13	69,78,86,89	0
2	SO4	A	301	5/5	0.92	0.12	72,75,78,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.