



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 08:09 PM EDT

PDB ID : 4OT9
Title : crystal structure of the C-terminal domain of p100/NF-kB2
Authors : Tao, Z.H.; Huang, D.B.; Fusco, A.; Gupta, K.; Ware, C.F.; Duynne, G.V.
Deposited on : 2014-02-13
Resolution : 3.35 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

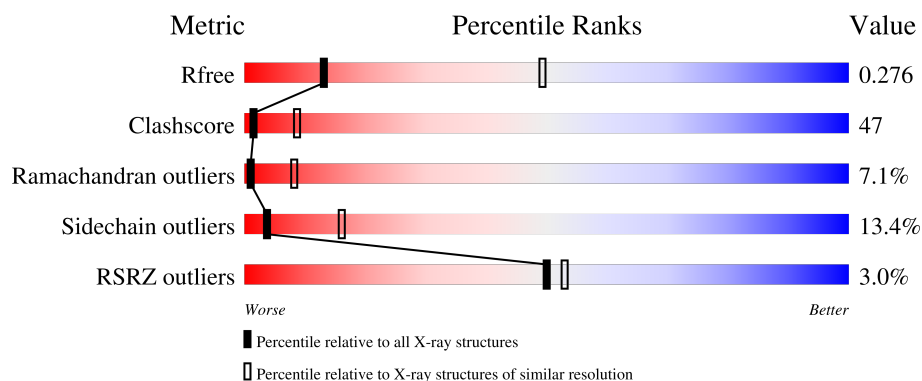
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	359	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2225 atoms, of which 1 is hydrogen 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 Nuclear factor NF-kappa-B p100 subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	H	N	O	S	0	0	0
			2215	1383	1	412	414	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	196.67Å 196.67Å 68.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.57 – 3.35 43.70 – 3.35	Depositor EDS
% Data completeness (in resolution range)	92.6 (29.57-3.35) 95.4 (43.70-3.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 3.32Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.233 , 0.272 0.238 , 0.276	Depositor DCC
R_{free} test set	594 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	113.4	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 106.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2225	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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	0.38	0/2253	0.56	0/3074

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	2214	1	2197	206	1
2	A	10	0	0	0	0
All	All	2224	1	2197	206	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 47.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ASN:HD21	1:A:693:ASP:H	1.12	0.97
1:A:442:ARG:HH11	1:A:442:ARG:HA	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:GLU:HB3	1:A:632:GLN:HB2	1.50	0.92
1:A:449:ARG:HH11	1:A:449:ARG:HB3	1.34	0.90
1:A:456:ARG:HH21	1:A:479:HIS:HD2	1.22	0.88
1:A:736:LEU:HD13	1:A:736:LEU:H	1.42	0.85
1:A:568:LEU:HD23	1:A:606:LEU:HB2	1.58	0.83
1:A:471:ARG:HD2	1:A:509:TYR:HD1	1.46	0.81
1:A:446:TYR:CE1	1:A:450:LEU:HD13	2.15	0.81
1:A:456:ARG:NH1	1:A:478:ARG:HH12	1.80	0.79
1:A:674:LEU:H	1:A:674:LEU:HD12	1.47	0.79
1:A:524:ASN:HD21	1:A:528:GLN:HB2	1.47	0.79
1:A:620:VAL:HA	1:A:624:ALA:HB3	1.66	0.77
1:A:664:ARG:NH2	1:A:697:GLU:H	1.84	0.76
1:A:517:LEU:HD11	1:A:549:VAL:HB	1.68	0.75
1:A:638:LEU:HD12	1:A:638:LEU:H	1.51	0.74
1:A:446:TYR:CZ	1:A:450:LEU:HD13	2.21	0.74
1:A:449:ARG:HB3	1:A:449:ARG:NH1	2.04	0.73
1:A:474:LEU:HD12	1:A:510:VAL:HG21	1.71	0.73
1:A:511:ILE:HD12	1:A:519:VAL:HG11	1.71	0.72
1:A:537:THR:OG1	1:A:539:GLN:HG3	1.89	0.71
1:A:670:THR:H	1:A:673:HIS:HD2	1.39	0.71
1:A:488:GLY:O	1:A:524:ASN:HA	1.90	0.70
1:A:592:LEU:HA	1:A:603:PRO:HG3	1.74	0.70
1:A:519:VAL:HA	1:A:522:LEU:HD13	1.74	0.69
1:A:670:THR:HB	1:A:671:PRO:HD2	1.74	0.68
1:A:636:THR:HG22	1:A:639:HIS:ND1	2.07	0.68
1:A:664:ARG:HH22	1:A:697:GLU:H	1.42	0.68
1:A:450:LEU:HD23	1:A:451:PHE:N	2.10	0.66
1:A:650:VAL:O	1:A:654:VAL:HG23	1.95	0.66
1:A:529:THR:HG22	1:A:532:HIS:ND1	2.10	0.66
1:A:490:THR:HG23	1:A:493:HIS:HB2	1.78	0.66
1:A:497:ILE:HD11	1:A:533:LEU:HD13	1.76	0.66
1:A:492:LEU:HB2	1:A:507:ILE:HG21	1.79	0.65
1:A:501:THR:O	1:A:505:GLU:HG2	1.97	0.64
1:A:519:VAL:HG23	1:A:522:LEU:HD22	1.79	0.64
1:A:556:LEU:HD23	1:A:560:GLY:O	1.97	0.64
1:A:524:ASN:ND2	1:A:528:GLN:HB2	2.13	0.64
1:A:570:ALA:HB3	1:A:573:GLY:HA2	1.81	0.63
1:A:442:ARG:HA	1:A:442:ARG:NH1	2.10	0.62
1:A:654:VAL:HG11	1:A:690:ALA:HB1	1.81	0.62
1:A:599:GLU:CB	1:A:632:GLN:HB2	2.27	0.62
1:A:479:HIS:O	1:A:480:LEU:HD22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ASN:ND2	1:A:693:ASP:H	1.90	0.62
1:A:650:VAL:HG21	1:A:683:LEU:HD11	1.79	0.62
1:A:436:ALA:C	1:A:438:GLU:H	2.04	0.61
1:A:698:ASN:OD1	1:A:731:HIS:HB2	2.00	0.61
1:A:662:ASN:HD21	1:A:693:ASP:N	1.94	0.61
1:A:620:VAL:HG11	1:A:657:LEU:HD11	1.83	0.61
1:A:599:GLU:HG2	1:A:632:GLN:NE2	2.17	0.60
1:A:526:LEU:HD22	1:A:558:ARG:HD2	1.85	0.59
1:A:450:LEU:O	1:A:453:LEU:HB2	2.02	0.59
1:A:466:VAL:HG23	1:A:467:THR:HG23	1.85	0.59
1:A:567:ALA:C	1:A:569:ARG:H	2.06	0.59
1:A:552:ASP:HB3	1:A:555:LEU:CD2	2.32	0.59
1:A:616:LEU:O	1:A:620:VAL:HG12	2.03	0.58
1:A:645:GLU:HB3	1:A:680:TYR:CZ	2.38	0.58
1:A:567:ALA:O	1:A:569:ARG:N	2.36	0.58
1:A:470:ALA:HB3	1:A:506:GLN:NE2	2.19	0.58
1:A:627:GLU:OE2	1:A:660:ASN:HB3	2.03	0.58
1:A:589:VAL:N	1:A:590:PRO:HD2	2.18	0.58
1:A:503:VAL:HA	1:A:506:GLN:OE1	2.04	0.57
1:A:674:LEU:O	1:A:678:LEU:HD23	2.04	0.57
1:A:436:ALA:O	1:A:438:GLU:N	2.38	0.57
1:A:643:GLU:C	1:A:645:GLU:H	2.07	0.57
1:A:609:ARG:HA	1:A:644:MET:HE1	1.86	0.56
1:A:444:ARG:HH11	1:A:445:GLU:HA	1.69	0.56
1:A:679:GLY:HA2	1:A:742:VAL:HG21	1.87	0.56
1:A:547:LEU:HD11	1:A:581:LEU:HD23	1.87	0.56
1:A:697:GLU:HA	1:A:731:HIS:O	2.05	0.56
1:A:471:ARG:HD2	1:A:509:TYR:CD1	2.35	0.56
1:A:497:ILE:CD1	1:A:533:LEU:HD13	2.36	0.56
1:A:578:LEU:HG	1:A:582:LEU:CD2	2.36	0.55
1:A:588:ALA:C	1:A:590:PRO:HD2	2.27	0.55
1:A:456:ARG:HH12	1:A:478:ARG:HH12	1.54	0.55
1:A:602:TYR:HB3	1:A:603:PRO:HD2	1.88	0.55
1:A:700:GLU:HA	1:A:730:GLY:HA2	1.90	0.54
1:A:436:ALA:HB1	1:A:437:PRO:CD	2.38	0.53
1:A:679:GLY:O	1:A:681:PRO:HD3	2.08	0.53
1:A:595:MET:SD	1:A:595:MET:N	2.82	0.53
1:A:447:ASN:N	1:A:447:ASN:ND2	2.55	0.53
1:A:450:LEU:HD23	1:A:450:LEU:C	2.29	0.53
1:A:630:GLU:OE1	1:A:632:GLN:HB3	2.08	0.53
1:A:440:LEU:HD23	1:A:441:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ARG:NH1	1:A:445:GLU:HA	2.24	0.52
1:A:516:ASP:C	1:A:518:GLY:H	2.13	0.52
1:A:588:ALA:HA	1:A:591:GLN:NE2	2.25	0.52
1:A:446:TYR:CZ	1:A:450:LEU:CD1	2.90	0.52
1:A:631:ARG:HH21	1:A:631:ARG:HG3	1.74	0.52
1:A:694:ILE:HD13	1:A:694:ILE:O	2.10	0.51
1:A:444:ARG:HE	1:A:444:ARG:C	2.14	0.51
1:A:511:ILE:CD1	1:A:519:VAL:HG11	2.40	0.51
1:A:456:ARG:HH21	1:A:479:HIS:CD2	2.14	0.51
1:A:569:ARG:O	1:A:570:ALA:HB2	2.11	0.51
1:A:508:VAL:HG13	1:A:549:VAL:HG21	1.93	0.50
1:A:531:LEU:HD23	1:A:563:ALA:HB2	1.93	0.50
1:A:570:ALA:HB3	1:A:573:GLY:CA	2.40	0.50
1:A:551:ALA:O	1:A:553:PRO:HD3	2.12	0.50
1:A:700:GLU:H	1:A:700:GLU:CD	2.14	0.50
1:A:442:ARG:HH12	1:A:445:GLU:CD	2.14	0.50
1:A:556:LEU:N	1:A:556:LEU:HD12	2.25	0.50
1:A:664:ARG:HA	1:A:669:ASN:O	2.12	0.50
1:A:456:ARG:CZ	1:A:478:ARG:HH12	2.25	0.50
1:A:588:ALA:HA	1:A:591:GLN:HE22	1.76	0.50
1:A:736:LEU:H	1:A:736:LEU:CD1	2.19	0.50
1:A:552:ASP:HB3	1:A:555:LEU:HD23	1.93	0.50
1:A:446:TYR:O	1:A:450:LEU:HB3	2.12	0.49
1:A:640:LEU:O	1:A:644:MET:HG2	2.11	0.49
1:A:441:GLN:HA	1:A:441:GLN:OE1	2.12	0.49
1:A:444:ARG:NH1	1:A:448:ALA:HB2	2.27	0.49
1:A:701:PRO:HA	1:A:731:HIS:NE2	2.27	0.49
1:A:670:THR:O	1:A:673:HIS:HB2	2.12	0.49
1:A:478:ARG:HA	1:A:481:LEU:HD22	1.94	0.48
1:A:453:LEU:HG	1:A:479:HIS:CD2	2.48	0.48
1:A:595:MET:HB2	1:A:600:GLY:CA	2.43	0.48
1:A:602:TYR:HB2	1:A:605:HIS:HD2	1.77	0.48
1:A:515:GLN:C	1:A:517:LEU:H	2.17	0.48
1:A:589:VAL:N	1:A:590:PRO:CD	2.76	0.48
1:A:664:ARG:HH21	1:A:696:ALA:HA	1.78	0.48
1:A:463:ASP:O	1:A:466:VAL:HG22	2.12	0.48
1:A:633:GLY:O	1:A:665:THR:HB	2.14	0.48
1:A:684:THR:O	1:A:688:LEU:HD23	2.14	0.48
1:A:596:PRO:HD2	1:A:601:LEU:N	2.29	0.47
1:A:447:ASN:N	1:A:447:ASN:HD22	2.11	0.47
1:A:640:LEU:O	1:A:643:GLU:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:VAL:HA	1:A:522:LEU:CD1	2.44	0.47
1:A:444:ARG:HH11	1:A:448:ALA:HB2	1.80	0.47
1:A:456:ARG:HG2	1:A:457:SER:N	2.30	0.47
1:A:526:LEU:CD2	1:A:558:ARG:HD2	2.45	0.47
1:A:496:ILE:HG12	1:A:504:ILE:HD13	1.97	0.47
1:A:553:PRO:HB2	1:A:591:GLN:OE1	2.15	0.47
1:A:596:PRO:O	1:A:600:GLY:HA2	2.15	0.47
1:A:456:ARG:CG	1:A:457:SER:N	2.78	0.47
1:A:461:LEU:HD12	1:A:473:LEU:HD11	1.97	0.47
1:A:596:PRO:HG2	1:A:601:LEU:H	1.78	0.47
1:A:490:THR:HG23	1:A:493:HIS:CB	2.45	0.46
1:A:552:ASP:OD2	1:A:554:ALA:HB3	2.13	0.46
1:A:478:ARG:C	1:A:480:LEU:H	2.19	0.46
1:A:456:ARG:HA	1:A:459:ARG:NH2	2.30	0.46
1:A:511:ILE:HD12	1:A:519:VAL:CG1	2.43	0.46
1:A:446:TYR:HD1	1:A:447:ASN:HD22	1.64	0.45
1:A:436:ALA:HB1	1:A:437:PRO:HD2	1.96	0.45
1:A:499:GLY:O	1:A:501:THR:N	2.44	0.45
1:A:556:LEU:HD23	1:A:560:GLY:C	2.36	0.45
1:A:562:SER:H	1:A:565:HIS:HD2	1.63	0.45
1:A:646:GLU:HB3	1:A:649:LEU:HB2	1.98	0.45
1:A:500:GLN:HA	1:A:500:GLN:OE1	2.15	0.45
1:A:562:SER:H	1:A:565:HIS:CD2	2.35	0.45
1:A:620:VAL:HG21	1:A:657:LEU:HD11	1.99	0.45
1:A:592:LEU:O	1:A:593:LEU:HG	2.16	0.45
1:A:632:GLN:HG3	1:A:633:GLY:N	2.32	0.45
1:A:638:LEU:HD11	1:A:659:ALA:HB1	1.98	0.45
1:A:436:ALA:C	1:A:438:GLU:N	2.70	0.45
1:A:567:ALA:C	1:A:569:ARG:N	2.71	0.44
1:A:516:ASP:O	1:A:518:GLY:N	2.49	0.44
1:A:591:GLN:NE2	1:A:591:GLN:H	2.15	0.44
1:A:480:LEU:HD13	1:A:480:LEU:HA	1.82	0.44
1:A:477:GLN:O	1:A:480:LEU:HB2	2.16	0.44
1:A:490:THR:HG22	1:A:493:HIS:ND1	2.33	0.44
1:A:620:VAL:HG21	1:A:657:LEU:CD1	2.47	0.44
1:A:532:HIS:O	1:A:536:ILE:HG13	2.18	0.44
1:A:442:ARG:HH11	1:A:442:ARG:CA	2.17	0.43
1:A:556:LEU:HB3	1:A:560:GLY:HA2	2.00	0.43
1:A:655:THR:OG1	1:A:656:LYS:N	2.51	0.43
1:A:554:ALA:O	1:A:556:LEU:HD12	2.17	0.43
1:A:470:ALA:HB3	1:A:506:GLN:HE21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASP:OD2	1:A:488:GLY:N	2.51	0.43
1:A:575:PRO:HB3	1:A:615:CYS:SG	2.59	0.43
1:A:741:LYS:CE	1:A:745:LEU:HD11	2.49	0.43
1:A:441:GLN:HG3	1:A:445:GLU:OE2	2.18	0.43
1:A:490:THR:CG2	1:A:493:HIS:ND1	2.82	0.43
1:A:539:GLN:HE21	1:A:539:GLN:HB3	1.59	0.43
1:A:609:ARG:HH21	1:A:609:ARG:HG3	1.84	0.43
1:A:631:ARG:HG3	1:A:631:ARG:NH2	2.34	0.43
1:A:674:LEU:H	1:A:674:LEU:CD1	2.24	0.43
1:A:588:ALA:O	1:A:591:GLN:NE2	2.51	0.42
1:A:739:SER:HB3	1:A:742:VAL:HG23	2.01	0.42
1:A:511:ILE:HG21	1:A:520:VAL:HG13	2.01	0.42
1:A:670:THR:H	1:A:673:HIS:CD2	2.28	0.42
1:A:481:LEU:O	1:A:491:PRO:HD2	2.20	0.42
1:A:508:VAL:CG1	1:A:549:VAL:HG21	2.50	0.42
1:A:698:ASN:CG	1:A:699:GLU:H	2.22	0.42
1:A:516:ASP:O	1:A:519:VAL:HG12	2.18	0.42
1:A:602:TYR:HD1	1:A:602:TYR:H	1.66	0.42
1:A:737:THR:HG21	1:A:742:VAL:HB	2.01	0.42
1:A:591:GLN:C	1:A:593:LEU:H	2.24	0.41
1:A:669:ASN:OD1	1:A:698:ASN:HB3	2.20	0.41
1:A:493:HIS:O	1:A:497:ILE:HG12	2.21	0.41
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.84	0.41
1:A:555:LEU:HD13	1:A:555:LEU:HA	1.85	0.41
1:A:737:THR:CG2	1:A:742:VAL:HB	2.50	0.41
1:A:474:LEU:O	1:A:474:LEU:HD13	2.20	0.41
1:A:589:VAL:HG22	1:A:590:PRO:HD3	2.03	0.41
1:A:453:LEU:O	1:A:456:ARG:HG2	2.19	0.41
1:A:586:ALA:N	1:A:587:PRO:HD2	2.36	0.41
1:A:596:PRO:CG	1:A:601:LEU:H	2.33	0.41
1:A:529:THR:OG1	1:A:530:PRO:HD2	2.21	0.41
1:A:664:ARG:NH2	1:A:696:ALA:HA	2.35	0.41
1:A:456:ARG:NH2	1:A:479:HIS:HD2	2.04	0.41
1:A:550:GLY:O	1:A:551:ALA:HB3	2.21	0.40
1:A:680:TYR:HB3	1:A:683:LEU:HB3	2.03	0.40
1:A:452:GLY:O	1:A:456:ARG:N	2.54	0.40
1:A:526:LEU:HD22	1:A:558:ARG:CD	2.51	0.40
1:A:665:THR:H	1:A:669:ASN:H	1.68	0.40
1:A:529:THR:HG22	1:A:532:HIS:CE1	2.56	0.40
1:A:638:LEU:HD12	1:A:638:LEU:N	2.28	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:ND2	1:A:447:ASN:ND2[10_665]	1.81	0.39

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	294/359 (82%)	225 (76%)	48 (16%)	21 (7%)	1 8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	568	LEU
1	A	517	LEU
1	A	584	SER
1	A	598	PHE
1	A	632	GLN
1	A	736	LEU
1	A	479	HIS
1	A	643	GLU
1	A	681	PRO
1	A	753	THR
1	A	437	PRO
1	A	500	GLN
1	A	570	ALA
1	A	754	MET
1	A	551	ALA
1	A	593	LEU
1	A	599	GLU
1	A	728	PHE
1	A	644	MET
1	A	698	ASN
1	A	602	TYR

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	224/288 (78%)	194 (87%)	30 (13%)	4 16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	440	LEU
1	A	442	ARG
1	A	444	ARG
1	A	447	ASN
1	A	449	ARG
1	A	450	LEU
1	A	461	LEU
1	A	480	LEU
1	A	481	LEU
1	A	482	THR
1	A	484	GLN
1	A	490	THR
1	A	493	HIS
1	A	529	THR
1	A	552	ASP
1	A	582	LEU
1	A	589	VAL
1	A	591	GLN
1	A	595	MET
1	A	599	GLU
1	A	614	GLU
1	A	616	LEU
1	A	629	THR
1	A	630	GLU
1	A	645	GLU
1	A	657	LEU
1	A	658	ARG
1	A	694	ILE
1	A	735	ASP
1	A	736	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	A	455	GLN
1	A	479	HIS
1	A	484	GLN
1	A	521	ASN
1	A	525	HIS
1	A	539	GLN
1	A	565	HIS
1	A	583	GLN
1	A	591	GLN
1	A	605	HIS
1	A	662	ASN
1	A	673	HIS

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](#)

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	802	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	A	801	-	4,4,4	0.28	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	298/359 (83%)	0.19	9 (3%)	50 53	71, 120, 191, 236	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	PRO	9.3
1	A	571	GLY	7.9
1	A	726	SER	7.2
1	A	727	SER	5.3
1	A	572	ALA	3.8
1	A	753	THR	3.0
1	A	518	GLY	2.6
1	A	599	GLU	2.5
1	A	755	GLU	2.3

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, 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(\AA^2)	Q<0.9
2	SO4	A	802	5/5	0.83	0.22	93,152,201,215	0
2	SO4	A	801	5/5	0.88	0.23	102,128,160,188	0

6.5 Other polymers [i](#)

There are no such residues in this entry.