



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 3V64 / pdb_00003v64
Title : Crystal Structure of agrin and LRP4
Authors : Zong, Y.; Zhang, B.; Gu, S.; Lee, K.; Zhou, J.; Yao, G.; Figueiredo, D.; Perry, K.; Mei, L.; Jin, R.
Deposited on : 2011-12-18
Resolution : 2.85 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

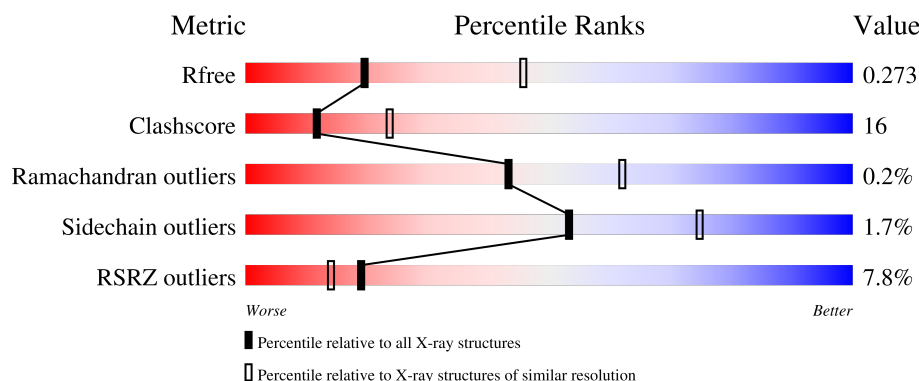
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	C	349	6% 67% 28% ..
1	D	349	7% 68% 27% ..
2	A	191	3% 79% 20% .
2	B	191	17% 61% 37% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8471 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 Low-density lipoprotein receptor-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	338	Total	C	N	O	S	0	0	0
			2700	1697	498	490	15			
1	D	334	Total	C	N	O	S	0	0	0
			2673	1683	492	483	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	738	LEU	-	expression tag	UNP Q9QYP1
C	739	GLU	-	expression tag	UNP Q9QYP1
C	740	VAL	-	expression tag	UNP Q9QYP1
C	741	LEU	-	expression tag	UNP Q9QYP1
C	742	PHE	-	expression tag	UNP Q9QYP1
C	743	GLN	-	expression tag	UNP Q9QYP1
C	744	GLY	-	expression tag	UNP Q9QYP1
D	738	LEU	-	expression tag	UNP Q9QYP1
D	739	GLU	-	expression tag	UNP Q9QYP1
D	740	VAL	-	expression tag	UNP Q9QYP1
D	741	LEU	-	expression tag	UNP Q9QYP1
D	742	PHE	-	expression tag	UNP Q9QYP1
D	743	GLN	-	expression tag	UNP Q9QYP1
D	744	GLY	-	expression tag	UNP Q9QYP1

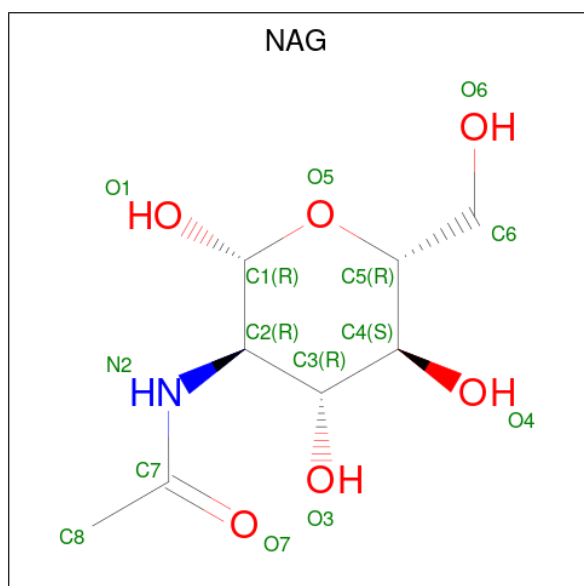
- Molecule 2 is a protein called Isoform 4 of Agrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	191	Total	C	N	O	S	0	0	0
			1470	927	263	277	3			
2	B	190	Total	C	N	O	S	0	0	0
			1465	924	262	276	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1758	ALA	-	expression tag	UNP P25304
B	1758	ALA	-	expression tag	UNP P25304

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

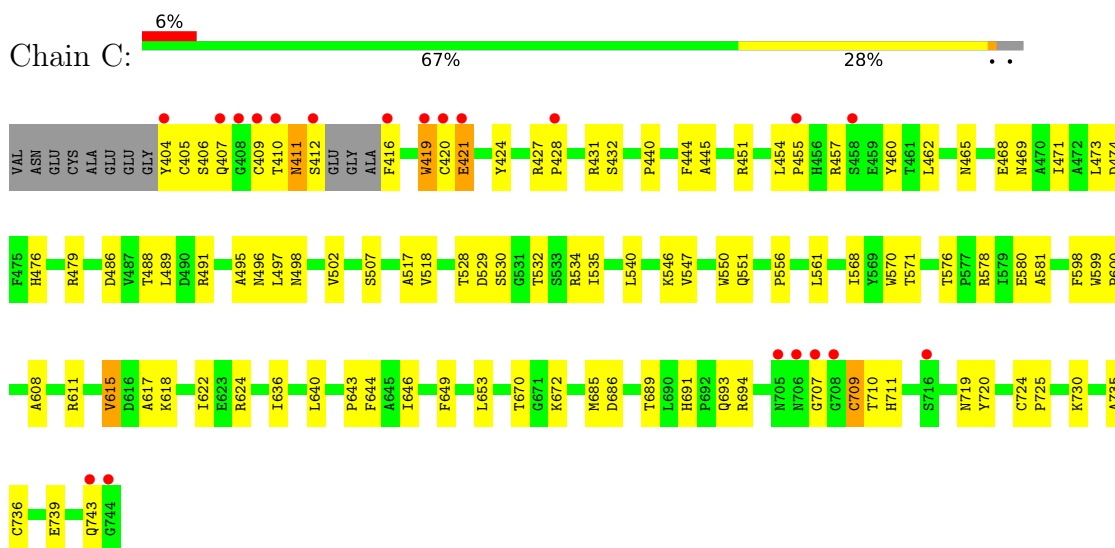
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	39	Total	O	0	0
			39	39		
6	A	25	Total	O	0	0
			25	25		
6	B	18	Total	O	0	0
			18	18		
6	D	28	Total	O	0	0
			28	28		

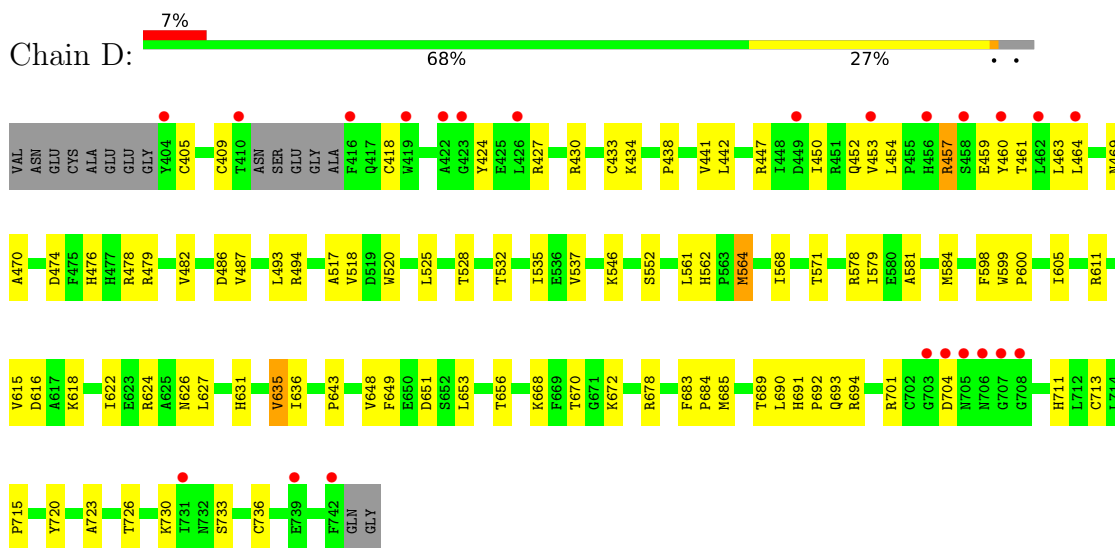
3 Residue-property plots

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.

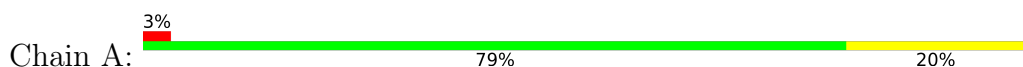
- Molecule 1: Low-density lipoprotein receptor-related protein 4

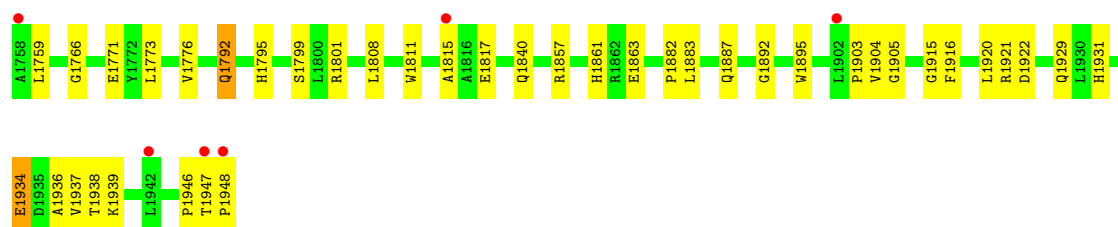


- Molecule 1: Low-density lipoprotein receptor-related protein 4

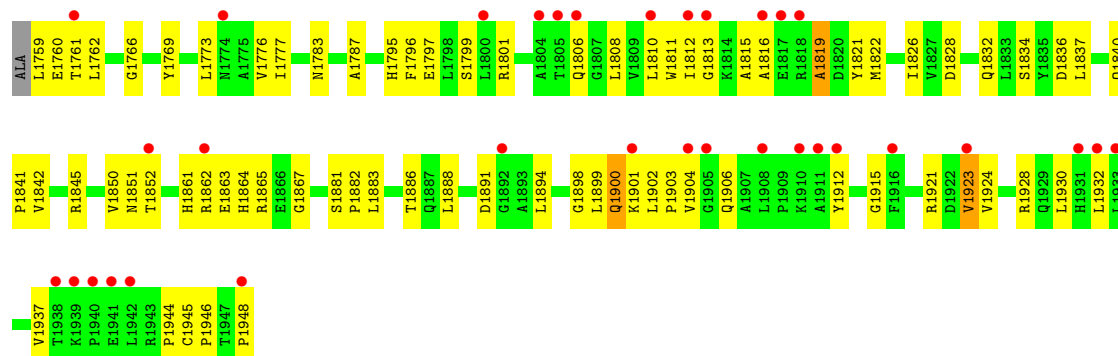


- Molecule 2: Isoform 4 of Agrin





• Molecule 2: Isoform 4 of Agrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.46Å 106.07Å 112.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.85) 98.2 (50.00-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.273 0.226 , 0.273	Depositor DCC
R_{free} test set	2034 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8471	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: PO4, NAG, CA

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	C	0.63	0/2773	0.71	1/3768 (0.0%)
1	D	0.61	0/2746	0.73	1/3732 (0.0%)
2	A	0.53	0/1499	0.71	0/2041
2	B	0.53	0/1494	0.81	4/2034 (0.2%)
All	All	0.59	0/8512	0.73	6/11575 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1819	ALA	N-CA-C	6.48	119.27	108.20
2	B	1852	THR	N-CA-C	-6.46	103.39	113.02
1	D	457	ARG	N-CA-C	-5.80	99.32	108.14
2	B	1816	ALA	N-CA-C	-5.61	100.74	109.72
1	C	709	CYS	CB-CA-C	-5.24	110.56	116.63
2	B	1851	ASN	N-CA-C	5.11	117.69	107.62

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	C	2700	0	2595	88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2673	0	2574	71	0
2	A	1470	0	1474	34	0
2	B	1465	0	1469	73	0
3	C	28	0	26	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
6	A	25	0	0	0	0
6	B	18	0	0	2	0
6	C	39	0	0	0	0
6	D	28	0	0	0	0
All	All	8471	0	8138	262	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 16.

All (262) 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)
2:A:1817:GLU:HG2	2:A:1904:VAL:HB	1.29	1.09
1:C:498:ASN:HB3	3:C:801:NAG:HN2	1.24	1.00
1:D:711:HIS:CD2	1:D:736:CYS:HB2	1.97	1.00
1:D:454:LEU:HD12	1:D:457:ARG:HH21	1.29	0.96
1:D:611:ARG:HD3	1:D:624:ARG:HD2	1.50	0.93
1:C:719:ASN:HD21	3:C:802:NAG:C1	1.83	0.92
2:B:1777:ILE:HG23	6:B:2101:HOH:O	1.70	0.91
2:B:1812:ILE:HD11	2:B:1894:LEU:HD13	1.53	0.91
1:C:719:ASN:ND2	3:C:802:NAG:C1	2.34	0.90
1:C:561:LEU:HD22	1:C:568:ILE:HD13	1.53	0.90
1:C:410:THR:O	1:C:411:ASN:HB2	1.69	0.90
1:C:498:ASN:CB	3:C:801:NAG:HN2	1.89	0.86
1:C:711:HIS:CD2	1:C:736:CYS:HB2	2.10	0.86
1:C:561:LEU:HD22	1:C:568:ILE:CD1	2.09	0.82
2:A:1946:PRO:O	2:A:1948:PRO:HD3	1.79	0.81
2:A:1773:LEU:HG	2:A:1937:VAL:HG21	1.62	0.80
1:C:498:ASN:HB3	3:C:801:NAG:N2	1.95	0.80
1:D:405:CYS:SG	1:D:409:CYS:HB3	2.23	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1861:HIS:HE1	2:B:1863:GLU:HG3	1.48	0.78
1:C:404:TYR:O	1:C:431:ARG:HB3	1.85	0.76
2:B:1822:MET:HE1	2:B:1862:ARG:HD3	1.68	0.76
1:C:615:VAL:HG11	1:C:643:PRO:HB2	1.66	0.76
2:B:1812:ILE:CD1	2:B:1894:LEU:HD13	2.15	0.75
1:D:520:TRP:HZ2	1:D:564:MET:HE1	1.50	0.75
2:B:1761:THR:O	2:B:1944:PRO:HA	1.88	0.74
1:C:622:ILE:HD12	1:C:640:LEU:HD11	1.68	0.74
1:D:450:ILE:O	1:D:463:LEU:HB2	1.91	0.71
2:B:1797:GLU:HB2	2:B:1924:VAL:HB	1.73	0.71
2:B:1901:LYS:C	2:B:1903:PRO:HD3	2.16	0.70
1:D:615:VAL:HG11	1:D:643:PRO:HB2	1.74	0.69
2:B:1773:LEU:HD12	2:B:1937:VAL:CG2	2.21	0.69
2:B:1946:PRO:C	2:B:1948:PRO:HD3	2.19	0.67
1:D:615:VAL:HG22	1:D:622:ILE:HG12	1.74	0.67
1:D:648:VAL:HG22	1:D:653:LEU:HD23	1.75	0.67
2:A:1922:ASP:HA	2:A:1929:GLN:HE22	1.58	0.67
2:B:1769:TYR:CD2	2:B:1900:GLN:HA	2.30	0.67
2:B:1904:VAL:HG23	2:B:1906:GLN:HG2	1.76	0.67
1:D:442:LEU:HB2	1:D:453:VAL:HG23	1.77	0.67
2:A:1795:HIS:N	5:A:2002:PO4:O4	2.22	0.67
2:B:1796:PHE:CZ	2:B:1812:ILE:HG13	2.30	0.67
1:D:528:THR:HG22	1:D:535:ILE:HG12	1.78	0.66
1:C:416:PHE:O	1:C:416:PHE:CD2	2.49	0.66
2:B:1776:VAL:HG12	2:B:1777:ILE:N	2.12	0.65
1:C:419:TRP:CD1	1:C:419:TRP:C	2.75	0.64
2:A:1936:ALA:HB3	2:A:1939:LYS:HD3	1.79	0.63
1:C:410:THR:O	1:C:411:ASN:CB	2.43	0.63
2:A:1817:GLU:CG	2:A:1904:VAL:HB	2.18	0.63
2:B:1822:MET:CE	2:B:1862:ARG:HD3	2.28	0.63
1:C:404:TYR:HB3	1:C:431:ARG:HD2	1.80	0.63
1:C:710:THR:OG1	1:C:735:ALA:HA	1.98	0.62
2:B:1932:LEU:HD12	2:B:1932:LEU:H	1.63	0.62
1:C:454:LEU:HD13	1:C:457:ARG:HH21	1.64	0.62
1:C:528:THR:HG22	1:C:535:ILE:HG12	1.81	0.62
1:D:626:ASN:OD1	1:D:631:HIS:HB2	1.99	0.61
1:C:576:THR:O	1:C:578:ARG:NE	2.33	0.61
2:B:1861:HIS:CE1	2:B:1863:GLU:HG3	2.33	0.61
1:C:534:ARG:HD2	1:C:547:VAL:HG11	1.83	0.61
1:D:424:TYR:HB3	1:D:433:CYS:HB3	1.83	0.61
2:B:1766:GLY:O	2:B:1915:GLY:HA3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:HIS:HD2	1:D:736:CYS:HB2	1.62	0.60
2:A:1934:GLU:H	2:A:1934:GLU:CD	2.10	0.60
1:C:407:GLN:OE1	1:C:608:ALA:HB1	2.02	0.60
1:C:689:THR:HB	1:C:694:ARG:HD3	1.82	0.60
1:D:454:LEU:CD1	1:D:457:ARG:HH21	2.09	0.60
1:C:404:TYR:CB	1:C:431:ARG:HD2	2.32	0.60
2:A:1931:HIS:HB3	2:A:1934:GLU:HG2	1.83	0.60
1:D:520:TRP:CZ2	1:D:564:MET:HE1	2.35	0.60
2:A:1776:VAL:HG12	2:A:1892:GLY:HA3	1.84	0.59
1:D:571:THR:HG22	1:D:579:ILE:HG12	1.84	0.59
2:A:1801:ARG:NH1	2:A:1947:THR:OG1	2.34	0.59
1:C:404:TYR:HB2	1:C:431:ARG:CZ	2.32	0.59
1:C:615:VAL:HG22	1:C:622:ILE:HG13	1.84	0.59
1:C:469:ASN:O	1:C:486:ASP:HA	2.03	0.58
2:B:1832:GLN:HG2	2:B:1845:ARG:HG3	1.84	0.58
1:C:530:SER:HA	1:C:556:PRO:HD2	1.84	0.58
2:B:1801:ARG:NH1	2:B:1948:PRO:HD2	2.19	0.58
1:D:452:GLN:HE21	1:D:463:LEU:HD21	1.68	0.58
2:B:1899:LEU:C	2:B:1901:LYS:H	2.12	0.58
2:B:1773:LEU:CD1	2:B:1937:VAL:CG2	2.82	0.57
1:D:635:VAL:HG23	1:D:636:ILE:HG13	1.85	0.57
2:A:1771:GLU:HB3	2:A:1938:THR:HB	1.88	0.56
1:C:462:LEU:HD21	1:C:465:ASN:HB2	1.87	0.56
2:B:1795:HIS:ND1	2:B:1861:HIS:HD2	2.03	0.56
2:B:1862:ARG:NH1	2:B:1864:HIS:O	2.38	0.56
2:B:1761:THR:HG22	2:B:1921:ARG:HB3	1.88	0.56
2:B:1795:HIS:ND1	2:B:1861:HIS:CD2	2.74	0.56
2:B:1808:LEU:HB2	2:B:1912:TYR:HA	1.87	0.56
2:B:1773:LEU:HD12	2:B:1937:VAL:HG22	1.87	0.55
2:B:1806:GLN:HG2	2:B:1828:ASP:H	1.72	0.55
2:B:1902:LEU:O	2:B:1902:LEU:HD12	2.06	0.55
2:B:1923:VAL:HB	2:B:1930:LEU:HB3	1.89	0.55
2:A:1857:ARG:HH12	2:A:1922:ASP:HB2	1.72	0.54
1:C:416:PHE:O	1:C:416:PHE:CG	2.59	0.54
2:B:1812:ILE:HB	2:B:1822:MET:HB3	1.89	0.54
1:C:469:ASN:HB2	1:C:488:THR:HG23	1.88	0.54
1:C:528:THR:HB	1:C:556:PRO:HB2	1.88	0.54
1:C:517:ALA:HB1	1:C:561:LEU:HG	1.90	0.54
1:C:405:CYS:SG	1:C:409:CYS:HB3	2.47	0.54
2:B:1759:LEU:HD13	2:B:1760:GLU:N	2.23	0.53
2:B:1801:ARG:HH12	2:B:1948:PRO:HD2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:ILE:HD13	1:C:636:ILE:HD13	1.90	0.53
1:D:447:ARG:HA	1:D:470:ALA:O	2.09	0.53
1:C:646:ILE:HD11	1:C:653:LEU:HD22	1.90	0.53
2:B:1795:HIS:HB2	2:B:1861:HIS:HD2	1.72	0.53
2:A:1946:PRO:C	2:A:1948:PRO:HD3	2.32	0.52
1:D:730:LYS:HE2	1:D:733:SER:HA	1.92	0.52
2:B:1799:SER:HB2	2:B:1921:ARG:HG2	1.91	0.52
2:B:1811:TRP:NE1	2:B:1813:GLY:HA3	2.25	0.52
2:B:1819:ALA:HB2	2:B:1906:GLN:CD	2.35	0.52
1:D:476:HIS:ND1	1:D:478:ARG:O	2.24	0.52
1:D:546:LYS:HE3	1:D:723:ALA:HB1	1.92	0.52
1:D:568:ILE:O	1:D:581:ALA:HA	2.10	0.52
2:B:1862:ARG:NH2	2:B:1888:LEU:HB2	2.25	0.52
1:D:454:LEU:HD12	1:D:457:ARG:NH2	2.12	0.52
1:C:719:ASN:HD21	3:C:802:NAG:C2	2.22	0.52
1:C:719:ASN:CG	3:C:802:NAG:C1	2.83	0.51
1:C:561:LEU:CD2	1:C:568:ILE:HD13	2.35	0.51
2:B:1773:LEU:CD1	2:B:1937:VAL:HG21	2.40	0.51
1:C:529:ASP:HB3	1:C:532:THR:HB	1.91	0.51
1:C:404:TYR:HB3	1:C:431:ARG:CD	2.41	0.51
1:D:454:LEU:N	1:D:459:GLU:OE1	2.43	0.51
1:C:495:ALA:HB2	1:C:502:VAL:HG12	1.93	0.51
1:C:724:CYS:SG	1:C:730:LYS:HD2	2.51	0.51
2:A:1771:GLU:HG2	2:A:1937:VAL:HB	1.91	0.51
1:D:452:GLN:HB2	1:D:461:THR:HB	1.93	0.51
2:A:1808:LEU:O	2:A:1916:PHE:HB2	2.11	0.51
1:D:453:VAL:CG1	1:D:678:ARG:HH11	2.24	0.50
1:D:651:ASP:HA	1:D:668:LYS:HE2	1.93	0.50
1:D:450:ILE:HD12	1:D:464:LEU:HD12	1.94	0.50
1:D:598:PHE:HB3	1:D:618:LYS:HB3	1.92	0.50
1:C:498:ASN:CB	3:C:801:NAG:N2	2.65	0.50
2:B:1840:GLN:HB3	2:B:1841:PRO:HD2	1.93	0.50
2:A:1801:ARG:HH12	2:A:1947:THR:HG1	1.55	0.50
2:B:1795:HIS:HB2	2:B:1861:HIS:CD2	2.46	0.50
2:B:1840:GLN:O	2:B:1882:PRO:HD2	2.11	0.50
2:B:1842:VAL:HB	2:B:1881:SER:HA	1.94	0.50
2:B:1862:ARG:HH21	2:B:1888:LEU:HB2	1.76	0.50
1:D:713:CYS:SG	1:D:720:TYR:CD1	3.05	0.50
2:A:1795:HIS:HB2	2:A:1861:HIS:CD2	2.47	0.49
1:D:474:ASP:HB3	1:D:518:VAL:HG23	1.94	0.49
1:C:615:VAL:HG13	1:C:643:PRO:HG2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:TRP:CZ3	1:C:551:GLN:HG2	2.48	0.49
1:D:459:GLU:HG2	1:D:460:TYR:N	2.27	0.49
1:C:495:ALA:CB	1:C:502:VAL:HG12	2.42	0.49
1:D:469:ASN:O	1:D:486:ASP:HA	2.13	0.49
1:D:683:PHE:CD2	1:D:685:MET:HE2	2.48	0.49
1:C:476:HIS:CE1	1:C:479:ARG:HG3	2.48	0.48
2:B:1902:LEU:N	2:B:1903:PRO:HD3	2.27	0.48
1:D:691:HIS:HD2	1:D:693:GLN:HB2	1.77	0.48
2:B:1946:PRO:O	2:B:1948:PRO:HD3	2.14	0.48
1:D:615:VAL:CG1	1:D:643:PRO:HG2	2.43	0.48
2:A:1817:GLU:HA	2:A:1905:GLY:H	1.77	0.48
2:B:1821:TYR:CE2	2:B:1836:ASP:HB2	2.48	0.48
2:B:1865:ARG:HG3	2:B:1886:THR:HG22	1.95	0.48
1:C:571:THR:HB	1:C:600:PRO:HB2	1.96	0.48
1:C:615:VAL:CG1	1:C:643:PRO:HG2	2.43	0.48
1:C:468:GLU:HG3	1:C:489:LEU:HD21	1.95	0.48
2:A:1840:GLN:HB2	2:A:1882:PRO:HG2	1.95	0.48
1:C:406:SER:OG	1:C:432:SER:HA	2.14	0.48
2:B:1776:VAL:CG1	2:B:1777:ILE:N	2.76	0.47
2:B:1832:GLN:HG2	2:B:1845:ARG:CG	2.44	0.47
2:B:1773:LEU:CD1	2:B:1937:VAL:HG22	2.45	0.47
1:C:496:ASN:OD1	1:C:497:LEU:N	2.48	0.47
1:D:615:VAL:HG11	1:D:643:PRO:CB	2.43	0.47
1:C:534:ARG:HD2	1:C:547:VAL:CG1	2.44	0.47
1:C:546:LYS:HB2	1:C:725:PRO:HA	1.97	0.47
2:B:1796:PHE:HZ	2:B:1812:ILE:HG13	1.77	0.47
2:B:1883:LEU:HD22	1:D:532:THR:HG23	1.96	0.47
1:D:701:ARG:HD2	1:D:715:PRO:HB3	1.95	0.47
1:C:689:THR:HB	1:C:694:ARG:CD	2.44	0.47
2:B:1777:ILE:CG2	6:B:2101:HOH:O	2.46	0.47
2:B:1826:ILE:HG21	2:B:1850:VAL:HG21	1.96	0.47
2:B:1808:LEU:HD22	2:B:1912:TYR:O	2.16	0.46
1:D:720:TYR:CD1	1:D:720:TYR:C	2.93	0.46
1:D:711:HIS:NE2	1:D:736:CYS:HB2	2.26	0.46
1:D:704:ASP:CG	1:D:704:ASP:O	2.58	0.46
1:C:488:THR:HG22	2:B:1787:ALA:HB1	1.98	0.46
2:B:1834:SER:HA	2:B:1842:VAL:O	2.16	0.46
1:C:707:GLY:C	1:C:709:CYS:H	2.24	0.46
2:A:1811:TRP:HB3	2:A:1895:TRP:HB2	1.96	0.46
1:D:453:VAL:HG11	1:D:678:ARG:HH11	1.80	0.46
2:A:1840:GLN:O	2:A:1882:PRO:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:TRP:CZ2	1:D:564:MET:CE	2.99	0.46
1:C:469:ASN:ND2	1:C:471:ILE:HD11	2.31	0.45
1:D:552:SER:O	1:D:578:ARG:NH2	2.49	0.45
2:A:1861:HIS:HE1	2:A:1863:GLU:HG2	1.80	0.45
2:B:1810:LEU:HD11	2:B:1894:LEU:CD1	2.46	0.45
1:C:474:ASP:HB3	1:C:518:VAL:HG23	1.99	0.45
2:A:1766:GLY:O	2:A:1915:GLY:HA3	2.17	0.45
1:C:611:ARG:HD3	1:C:624:ARG:HD2	1.96	0.45
1:C:711:HIS:NE2	1:C:736:CYS:HB2	2.29	0.45
2:A:1861:HIS:CE1	2:A:1863:GLU:HG2	2.52	0.45
1:D:525:LEU:O	1:D:537:VAL:HA	2.16	0.45
1:D:571:THR:HB	1:D:600:PRO:HB2	1.98	0.45
1:D:605:ILE:HG23	1:D:627:LEU:HD11	1.98	0.45
2:B:1796:PHE:HE2	2:B:1822:MET:SD	2.39	0.45
1:C:570:TRP:CZ2	1:C:580:GLU:HB2	2.53	0.44
2:B:1761:THR:HB	2:B:1945:CYS:HB2	1.99	0.44
2:B:1862:ARG:HA	2:B:1867:GLY:HA2	1.99	0.44
1:C:617:ALA:HA	1:C:643:PRO:HD2	2.00	0.44
1:D:649:PHE:HB2	1:D:689:THR:HG21	2.00	0.44
1:D:562:HIS:CE1	1:D:564:MET:HG3	2.53	0.43
1:C:444:PHE:HA	1:C:686:ASP:O	2.18	0.43
2:B:1837:LEU:HD21	2:B:1862:ARG:CZ	2.48	0.43
1:C:691:HIS:HE1	1:C:693:GLN:HG2	1.83	0.43
2:A:1815:ALA:HA	2:A:1903:PRO:HG3	2.00	0.43
1:C:568:ILE:O	1:C:581:ALA:HA	2.18	0.43
1:C:451:ARG:NH1	1:C:460:TYR:OH	2.50	0.43
1:C:644:PHE:HD2	1:C:685:MET:O	2.01	0.43
2:A:1792:GLN:NE2	2:A:1887:GLN:HG2	2.33	0.43
1:D:418:CYS:HB2	1:D:430:ARG:O	2.18	0.43
2:A:1792:GLN:NE2	2:A:1887:GLN:HE21	2.17	0.43
1:C:427:ARG:HB3	1:C:428:PRO:HD2	2.00	0.43
2:B:1899:LEU:O	2:B:1901:LYS:N	2.48	0.43
2:B:1904:VAL:HG23	2:B:1906:GLN:CG	2.46	0.43
1:D:518:VAL:HG22	1:D:525:LEU:HD12	2.00	0.43
1:C:445:ALA:HB2	1:C:473:LEU:HD23	2.01	0.43
1:D:517:ALA:HB1	1:D:561:LEU:HG	2.00	0.43
1:C:561:LEU:CD2	1:C:568:ILE:CD1	2.90	0.42
1:D:561:LEU:HB3	1:D:584:MET:HE2	2.01	0.42
1:D:469:ASN:HD22	1:D:487:VAL:HG22	1.85	0.42
1:D:649:PHE:CD1	1:D:694:ARG:HG2	2.55	0.42
2:A:1936:ALA:CB	2:A:1939:LYS:HD3	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:691:HIS:CG	1:D:692:PRO:HD2	2.54	0.42
1:C:410:THR:HG1	1:C:419:TRP:HZ3	1.66	0.42
1:C:534:ARG:NH1	2:A:1883:LEU:HD23	2.35	0.42
1:C:622:ILE:HD12	1:C:640:LEU:CD1	2.45	0.42
1:D:670:THR:HB	1:D:672:LYS:HD2	2.01	0.42
2:A:1811:TRP:CZ2	2:A:1903:PRO:HG2	2.54	0.42
1:D:478:ARG:O	1:D:479:ARG:HB3	2.19	0.42
1:C:670:THR:HG22	1:C:672:LYS:H	1.84	0.42
2:A:1840:GLN:OE1	2:A:1840:GLN:HA	2.20	0.42
2:B:1899:LEU:C	2:B:1901:LYS:N	2.77	0.42
1:D:441:VAL:HB	1:D:690:LEU:HB3	2.01	0.42
1:C:454:LEU:HA	1:C:455:PRO:HD2	1.93	0.41
1:D:564:MET:H	1:D:564:MET:HG2	1.52	0.41
2:B:1808:LEU:HG	2:B:1898:GLY:HA2	2.02	0.41
1:D:656:THR:HB	1:D:684:PRO:HB2	2.02	0.41
1:D:599:TRP:O	1:D:616:ASP:HA	2.20	0.41
1:C:719:ASN:HB3	1:C:720:TYR:H	1.70	0.41
1:C:739:GLU:O	1:C:743:GLN:HG3	2.20	0.41
1:D:438:PRO:O	1:D:691:HIS:HE1	2.04	0.41
1:C:407:GLN:CD	1:C:608:ALA:HB1	2.46	0.41
1:C:598:PHE:HB3	1:C:618:LYS:HB3	2.02	0.41
1:C:599:TRP:CE2	2:B:1783:ASN:HB2	2.56	0.41
2:B:1762:LEU:CD1	2:B:1932:LEU:HB3	2.51	0.41
2:B:1815:ALA:HB3	2:B:1891:ASP:OD2	2.20	0.41
1:D:427:ARG:HD3	1:D:434:LYS:HD2	2.03	0.41
1:C:411:ASN:OD1	1:C:411:ASN:O	2.39	0.41
1:C:421:GLU:O	1:C:424:TYR:HB2	2.21	0.41
1:D:546:LYS:HA	1:D:726:THR:HG23	2.01	0.41
2:A:1795:HIS:ND1	2:A:1861:HIS:HD2	2.18	0.40
1:D:482:VAL:O	1:D:494:ARG:HA	2.21	0.40
1:D:615:VAL:HG11	1:D:643:PRO:CG	2.51	0.40
1:C:491:ARG:HD3	1:C:507:SER:HA	2.03	0.40
1:C:462:LEU:CD2	1:C:465:ASN:HB2	2.52	0.40
1:D:711:HIS:HD2	1:D:736:CYS:CB	2.32	0.40
2:B:1769:TYR:CE2	2:B:1900:GLN:HA	2.56	0.40
2:B:1806:GLN:NE2	2:B:1828:ASP:OD1	2.55	0.40
1:C:440:PRO:HG3	1:C:649:PHE:CE2	2.56	0.40
1:C:598:PHE:CD2	1:C:618:LYS:HG2	2.57	0.40
2:A:1799:SER:HB2	2:A:1921:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/349 (96%)	308 (92%)	25 (8%)	1 (0%)	36	54
1	D	330/349 (95%)	300 (91%)	30 (9%)	0	100	100
2	A	189/191 (99%)	179 (95%)	10 (5%)	0	100	100
2	B	188/191 (98%)	179 (95%)	8 (4%)	1 (0%)	24	42
All	All	1041/1080 (96%)	966 (93%)	73 (7%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	411	ASN
2	B	1900	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	290/297 (98%)	284 (98%)	6 (2%)	47	70
1	D	287/297 (97%)	284 (99%)	3 (1%)	68	83
2	A	156/156 (100%)	152 (97%)	4 (3%)	40	65
2	B	156/156 (100%)	154 (99%)	2 (1%)	61	79
All	All	889/906 (98%)	874 (98%)	15 (2%)	53	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	412	SER
1	C	419	TRP
1	C	420	CYS
1	C	421	GLU
1	C	540	LEU
1	C	615	VAL
2	A	1759	LEU
2	A	1792	GLN
2	A	1920	LEU
2	A	1934	GLU
2	B	1923	VAL
2	B	1928	ARG
1	D	493	LEU
1	D	564	MET
1	D	635	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	477	HIS
1	C	551	GLN
1	C	682	HIS
1	C	688	HIS
1	C	719	ASN
2	A	1792	GLN
2	A	1861	HIS
2	A	1864	HIS
2	A	1887	GLN
2	A	1929	GLN
2	B	1832	GLN
2	B	1840	GLN
2	B	1861	HIS
2	B	1864	HIS
2	B	1927	HIS
1	D	452	GLN
1	D	562	HIS
1	D	596	HIS
1	D	691	HIS
1	D	706	ASN
1	D	711	HIS

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 ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	802	-	14,14,15	0.54	0	17,19,21	0.84	0
5	PO4	B	2002	-	4,4,4	0.97	0	6,6,6	0.44	0
5	PO4	C	804	-	4,4,4	0.94	0	6,6,6	0.42	0
5	PO4	C	805	-	4,4,4	0.94	0	6,6,6	0.49	0
5	PO4	A	2002	-	4,4,4	1.08	0	6,6,6	0.45	0
3	NAG	C	801	1	14,14,15	0.59	0	17,19,21	0.83	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
3	NAG	C	801	1	-	2/6/23/26	0/1/1/1
3	NAG	C	802	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802	NAG	O5-C5-C6-O6
3	C	802	NAG	C4-C5-C6-O6
3	C	801	NAG	C4-C5-C6-O6
3	C	801	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	NAG	4	0
5	A	2002	PO4	1	0
3	C	801	NAG	4	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, 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	C	338/349 (96%)	0.18	20 (5%) 28 21	15, 37, 85, 157	0
1	D	334/349 (95%)	0.44	23 (6%) 23 17	18, 50, 109, 139	0
2	A	191/191 (100%)	0.12	6 (3%) 51 43	20, 39, 93, 137	0
2	B	190/191 (99%)	1.06	33 (17%) 4 3	19, 76, 123, 148	0
All	All	1053/1080 (97%)	0.41	82 (7%) 19 14	15, 47, 108, 157	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1818	ARG	5.6
1	C	407	GLN	5.3
2	B	1817	GLU	5.3
1	D	419	TRP	4.9
1	C	416	PHE	4.7
1	D	705	ASN	4.4
2	B	1816	ALA	4.3
1	D	704	ASP	3.9
1	D	462	LEU	3.8
1	C	708	GLY	3.6
1	D	708	GLY	3.6
1	D	706	ASN	3.5
2	B	1812	ILE	3.4
1	D	416	PHE	3.4
1	D	739	GLU	3.4
2	A	1758	ALA	3.3
1	C	419	TRP	3.3
1	D	707	GLY	3.2
2	B	1948	PRO	3.2
1	C	410	THR	3.1
1	D	453	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	742	PHE	3.1
2	B	1938	THR	3.0
2	B	1923	VAL	3.0
1	C	404	TYR	3.0
1	C	408	GLY	2.8
2	B	1892	GLY	2.8
2	A	1942	LEU	2.8
2	A	1948	PRO	2.8
1	D	404	TYR	2.7
2	B	1904	VAL	2.7
2	B	1805	THR	2.6
1	C	707	GLY	2.6
1	D	426	LEU	2.6
1	C	412	SER	2.6
1	D	410	THR	2.6
2	B	1933	LEU	2.5
1	C	706	ASN	2.5
2	B	1931	HIS	2.5
2	B	1901	LYS	2.5
2	B	1800	LEU	2.5
2	B	1940	PRO	2.5
2	B	1932	LEU	2.4
1	C	455	PRO	2.4
2	B	1911	ALA	2.4
2	B	1852	THR	2.4
1	C	705	ASN	2.4
1	C	421	GLU	2.4
1	C	743	GLN	2.4
1	D	731	ILE	2.4
1	D	458	SER	2.4
2	A	1947	THR	2.4
2	B	1862	ARG	2.3
2	B	1916	PHE	2.3
2	B	1810	LEU	2.3
2	B	1942	LEU	2.3
1	D	423	GLY	2.3
2	B	1813	GLY	2.3
2	B	1908	LEU	2.3
1	D	449	ASP	2.3
1	D	422	ALA	2.2
2	B	1804	ALA	2.2
2	B	1912	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1905	GLY	2.2
2	B	1774	ASN	2.2
1	C	409	CYS	2.2
1	C	420	CYS	2.2
1	C	458	SER	2.2
2	B	1910	LYS	2.2
2	B	1941	GLU	2.2
1	D	456	HIS	2.2
1	D	460	TYR	2.2
2	B	1761	THR	2.1
2	A	1902	LEU	2.1
2	B	1806	GLN	2.1
2	B	1939	LYS	2.1
1	D	464	LEU	2.1
1	C	716	SER	2.0
1	C	744	GLY	2.0
1	D	703	GLY	2.0
2	A	1815	ALA	2.0
1	C	428	PRO	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
3	NAG	C	802	14/15	0.53	0.18	120,139,147,148	0
3	NAG	C	801	14/15	0.60	0.15	90,97,100,100	0
4	CA	C	803	1/1	0.65	0.16	66,66,66,66	0
5	PO4	B	2002	5/5	0.75	0.21	96,106,114,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	C	805	5/5	0.78	0.22	79,88,110,111	0
4	CA	D	802	1/1	0.83	0.09	76,76,76,76	0
5	PO4	C	804	5/5	0.88	0.20	75,87,88,90	0
4	CA	D	801	1/1	0.91	0.08	85,85,85,85	0
4	CA	B	2001	1/1	0.93	0.07	77,77,77,77	0
5	PO4	A	2002	5/5	0.95	0.10	44,44,47,48	0
4	CA	A	2001	1/1	0.96	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.