



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:51 pm BST

PDB ID : 1OD5
Title : Crystal structure of glycinin A3B4 subunit homoheptamer
Authors : Adachi, M.; Kanamori, J.; Masuda, T.; Yagasaki, K.; Kitamura, K.; Mikami, B.; Utsumi, S.
Deposited on : 2003-02-13
Resolution : 2.10 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 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

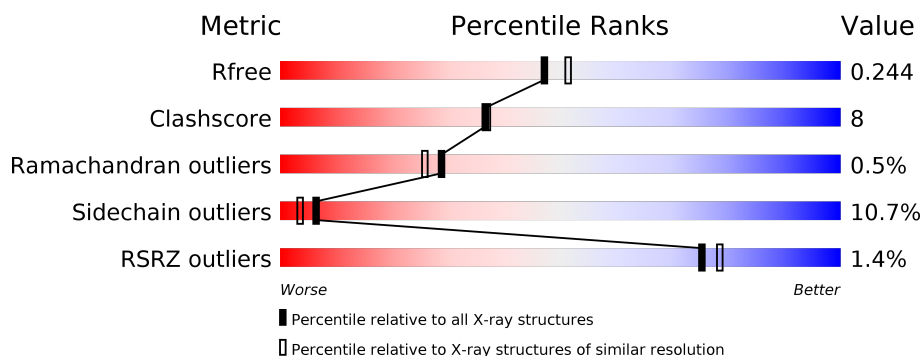
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	492	 % 59% 14% • • 22%
1	B	492	 % 59% 15% • • 22%

2 Entry composition [i](#)

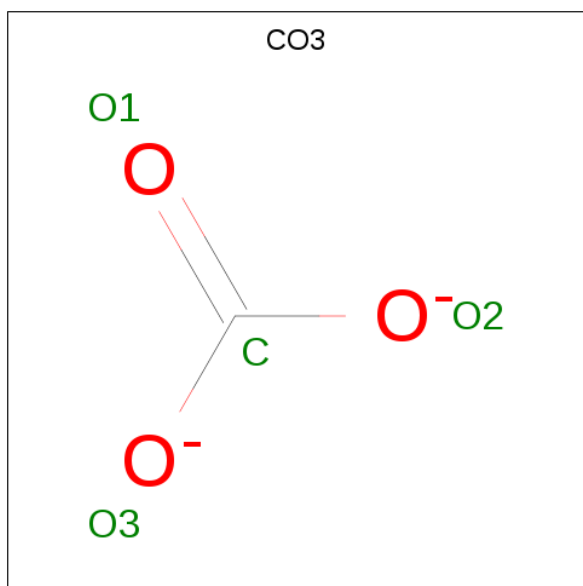
There are 4 unique types of molecules in this entry. The entry contains 6220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2998	1885	534	571	8			
1	B	382	Total	C	N	O	S	0	0	0
			2998	1885	534	571	8			

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total 102	O 102	0	0
4	B	112	Total 112	O 112	0	0

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.

[illegible]

Chain B:

59% 15% 22%

THR SER SER LYS PRE 37 L14 D20 421 422 433 434 435 436 437 446 447 454 457 464 475 476 487 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	114.84Å 114.84Å 191.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10 9.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.3 (10.00-2.10) 88.4 (9.98-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.09Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.254 0.194 , 0.244	Depositor DCC
R_{free} test set	4894 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6220	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO3

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	0.82	1/3067 (0.0%)	1.48	32/4168 (0.8%)
1	B	0.83	0/3067	1.46	37/4168 (0.9%)
All	All	0.82	1/6134 (0.0%)	1.47	69/8336 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	VAL	CA-CB	5.19	1.65	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	B	132	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	A	322	VAL	CA-C-N	8.89	136.75	117.20
1	A	322	VAL	O-C-N	-8.76	108.69	122.70
1	A	485	GLY	CA-C-N	8.57	136.06	117.20
1	A	350	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	485	GLY	O-C-N	-8.53	109.06	122.70
1	A	132	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	B	323	GLU	CA-C-N	-8.07	99.43	117.20
1	B	418	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	132	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	A	430	VAL	CB-CA-C	-7.67	96.82	111.40
1	A	33	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	322	VAL	CG1-CB-CG2	-7.56	98.81	110.90
1	B	421	LEU	CA-CB-CG	7.54	132.65	115.30
1	A	384	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	A	384	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	A	33	TRP	CE2-CD2-CG	-7.36	101.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	132	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	A	421	LEU	CA-CB-CG	7.21	131.89	115.30
1	A	221	GLU	CA-CB-CG	-7.20	97.56	113.40
1	B	33	TRP	CD1-CG-CD2	7.18	112.05	106.30
1	B	380	TYR	N-CA-C	-7.14	91.72	111.00
1	A	350	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	A	251	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	B	402	ARG	NE-CZ-NH2	6.99	123.79	120.30
1	B	251	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	B	33	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	251	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	B	371	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	B	46	THR	CA-CB-CG2	6.61	121.66	112.40
1	B	340	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	367	LEU	CA-CB-CG	6.37	129.94	115.30
1	B	430	VAL	CB-CA-C	-6.31	99.42	111.40
1	B	363	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	A	380	TYR	N-CA-C	-6.19	94.29	111.00
1	B	251	TRP	CG-CD1-NE1	-6.12	103.98	110.10
1	B	384	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	337	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	132	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	400	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	54	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	33	TRP	CB-CG-CD1	-5.79	119.47	127.00
1	B	33	TRP	CB-CG-CD1	-5.68	119.61	127.00
1	B	132	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	B	376	ARG	CB-CG-CD	5.58	126.09	111.60
1	B	145	SER	N-CA-CB	-5.55	102.18	110.50
1	B	33	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	B	146	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	14	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	146	LEU	CA-CB-CG	5.39	127.70	115.30
1	B	132	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	B	350	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	54	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	177	MET	CG-SD-CE	-5.24	91.81	100.20
1	A	454	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	54	ARG	CA-CB-CG	5.23	124.91	113.40
1	B	57	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	22	ARG	NE-CZ-NH2	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	A	485	GLY	C-N-CA	5.18	134.66	121.70
1	B	329	MET	CA-CB-CG	5.16	122.07	113.30
1	B	485	GLY	O-C-N	-5.14	114.47	122.70
1	B	437	GLN	CA-CB-CG	5.11	124.65	113.40
1	B	22	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	54	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	62	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	439	LEU	CA-CB-CG	5.00	126.80	115.30

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	2998	0	2907	51	0
1	B	2998	0	2907	50	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	102	0	0	1	0
4	B	112	0	0	7	0
All	All	6220	0	5814	93	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 8.

All (93) 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:175:GLU:HG2	1:A:176:THR:HG23	1.64	0.78
1:B:334:ASN:HD21	1:B:337:ARG:H	1.31	0.78
1:B:76:GLY:HA2	1:B:136:THR:HB	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG22	4:B:2105:HOH:O	1.87	0.74
1:A:322:VAL:HB	1:A:323:GLU:HA	1.72	0.72
1:B:170:ASP:H	1:B:236:GLN:HE22	1.39	0.71
1:A:236:GLN:H	1:A:236:GLN:HE21	1.42	0.68
1:A:34:ASN:HD22	1:A:36:GLN:H	1.41	0.68
1:B:236:GLN:H	1:B:236:GLN:HE21	1.42	0.67
1:A:246:VAL:HG22	1:A:251:TRP:HZ3	1.59	0.66
1:B:47:VAL:HG21	1:B:421:LEU:HD21	1.78	0.64
1:A:334:ASN:HD21	1:A:337:ARG:H	1.43	0.64
1:B:34:ASN:HD22	1:B:36:GLN:H	1.45	0.64
1:A:387:ASN:HD21	1:A:451:VAL:H	1.44	0.63
1:A:170:ASP:H	1:A:236:GLN:HE22	1.45	0.62
1:B:323:GLU:HB3	1:B:327:CYS:HB2	1.83	0.60
1:A:480:GLN:O	1:A:484:GLN:HB2	2.01	0.60
1:B:376:ARG:H	1:B:376:ARG:HE	1.50	0.60
1:A:64:PRO:HG3	1:A:156:LEU:HD12	1.83	0.59
1:A:159:ASN:HD22	1:A:176:THR:HB	1.68	0.58
1:B:75:LYS:HG3	1:B:136:THR:HG22	1.85	0.57
1:B:387:ASN:HD21	1:B:451:VAL:H	1.52	0.57
1:A:467:LEU:HD23	1:A:478:VAL:HG13	1.86	0.57
1:B:387:ASN:H	1:B:387:ASN:HD22	1.53	0.57
1:A:358:THR:HG23	1:B:330:LYS:HD2	1.85	0.57
1:B:323:GLU:HA	4:B:2064:HOH:O	2.05	0.56
1:A:322:VAL:HG12	1:A:324:GLU:HG3	1.86	0.56
1:A:387:ASN:H	1:A:387:ASN:HD22	1.52	0.56
1:A:330:LYS:HD2	1:B:358:THR:HG23	1.88	0.56
1:A:250:LYS:HD2	1:B:339:SER:HB3	1.87	0.56
1:B:417:ARG:HG2	4:B:2099:HOH:O	2.06	0.55
1:A:328:THR:HG23	4:B:2071:HOH:O	2.07	0.55
1:A:246:VAL:HG22	1:A:251:TRP:CZ3	2.39	0.54
1:A:90:GLU:O	1:B:346:PRO:HD2	2.07	0.54
1:A:373:VAL:HG22	1:A:440:GLU:HG2	1.89	0.54
4:A:2097:HOH:O	1:B:322:VAL:HB	2.06	0.54
1:A:401:VAL:HG21	1:A:416:LEU:HD12	1.89	0.54
1:A:321:GLY:HA3	4:B:2107:HOH:O	2.06	0.54
1:B:467:LEU:HD23	1:B:478:VAL:HG13	1.91	0.53
1:A:50:ARG:HH22	1:A:67:GLN:HE22	1.54	0.53
1:A:220:ASN:ND2	1:A:223:THR:H	2.06	0.53
1:B:173:HIS:HD2	4:B:2054:HOH:O	1.93	0.52
1:B:37:HIS:HD2	4:B:2011:HOH:O	1.93	0.51
1:A:323:GLU:HB2	1:A:327:CYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:ND2	1:A:36:GLN:H	2.08	0.51
1:A:220:ASN:HD22	1:A:223:THR:H	1.59	0.50
1:A:321:GLY:N	1:B:454:TYR:HH	2.09	0.50
1:B:462:ILE:CG2	1:B:466:VAL:HG22	2.42	0.50
1:B:385:ASN:HD21	1:B:445:LYS:NZ	2.11	0.49
1:A:376:ARG:H	1:A:376:ARG:NE	2.11	0.49
1:A:387:ASN:ND2	1:A:451:VAL:H	2.11	0.49
1:A:50:ARG:HH12	1:A:67:GLN:NE2	2.11	0.49
1:A:34:ASN:O	1:A:37:HIS:HD2	1.96	0.48
1:A:322:VAL:CB	1:A:323:GLU:HA	2.40	0.48
1:B:220:ASN:HD22	1:B:223:THR:H	1.60	0.48
1:B:206:SER:HA	1:B:228:ARG:HB2	1.96	0.48
1:B:462:ILE:CG2	1:B:467:LEU:HD13	2.45	0.47
1:B:376:ARG:N	1:B:376:ARG:HE	2.12	0.47
1:B:376:ARG:NE	1:B:376:ARG:H	2.12	0.46
1:B:387:ASN:HD22	1:B:387:ASN:N	2.13	0.46
1:A:351:ILE:HG12	1:A:372:VAL:HB	1.97	0.46
1:B:225:GLU:O	1:B:228:ARG:HG2	2.15	0.46
1:B:334:ASN:ND2	1:B:337:ARG:HB2	2.31	0.45
1:B:20:ASP:OD1	1:B:37:HIS:HE1	1.99	0.45
1:A:454:TYR:CE2	1:B:322:VAL:HG22	2.51	0.45
1:B:250:LYS:O	1:B:251:TRP:HB2	2.16	0.45
1:A:334:ASN:ND2	1:A:337:ARG:HG3	2.33	0.44
1:B:170:ASP:H	1:B:236:GLN:NE2	2.12	0.44
1:A:70:ILE:HG21	1:A:442:VAL:HG11	2.00	0.44
1:A:14:LEU:HD22	1:A:411:VAL:HG23	2.00	0.44
1:B:14:LEU:HD22	1:B:411:VAL:HG23	1.99	0.44
1:A:324:GLU:HB3	1:B:353:THR:HG21	2.00	0.43
1:A:376:ARG:HH21	1:A:438:GLY:HA3	1.83	0.43
1:B:345:ASN:HD21	1:B:492:ASN:ND2	2.17	0.43
1:B:424:VAL:HG11	1:B:430:VAL:HG22	2.00	0.43
1:A:424:VAL:HG11	1:A:430:VAL:HG22	2.01	0.43
1:A:82:PHE:HZ	1:A:331:LEU:HD21	1.83	0.43
1:A:462:ILE:CG2	1:A:466:VAL:HG22	2.48	0.43
1:B:235:LYS:HB3	1:B:236:GLN:HE21	1.84	0.43
1:B:492:ASN:H	1:B:492:ASN:ND2	2.17	0.42
1:B:64:PRO:HG3	1:B:156:LEU:HD12	2.01	0.42
1:B:91:LYS:O	1:B:108:GLN:HA	2.19	0.42
1:B:386:LEU:HD11	1:B:453:SER:HB2	2.01	0.42
1:A:454:TYR:CZ	1:A:457:ASP:HB2	2.55	0.42
1:A:403:VAL:HG22	1:A:430:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:HD21	1:B:337:ARG:HB2	1.85	0.41
1:B:322:VAL:HB	1:B:323:GLU:H	1.71	0.41
1:A:376:ARG:HG3	1:A:436:GLU:O	2.20	0.41
1:B:385:ASN:HD21	1:B:445:LYS:HZ3	1.67	0.41
1:A:344:TYR:CD2	1:B:249:PRO:HG3	2.56	0.40
1:A:170:ASP:HA	1:A:200:GLU:HA	2.04	0.40
1:A:175:GLU:HG2	1:A:176:THR:N	2.37	0.40
1:B:245:SER:HA	1:B:251:TRP:CZ3	2.56	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	A	374/492 (76%)	352 (94%)	20 (5%)	2 (0%)	29	26
1	B	374/492 (76%)	351 (94%)	21 (6%)	2 (0%)	29	26
All	All	748/984 (76%)	703 (94%)	41 (6%)	4 (0%)	29	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	VAL
1	B	323	GLU
1	B	484	GLN
1	A	158	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	A	332/435 (76%)	294 (89%)	38 (11%)	5	3
1	B	332/435 (76%)	299 (90%)	33 (10%)	8	5
All	All	664/870 (76%)	593 (89%)	71 (11%)	6	3

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	34	ASN
1	A	54	ARG
1	A	57	LEU
1	A	87	GLU
1	A	108	GLN
1	A	118	ASN
1	A	135	ASN
1	A	144	ILE
1	A	158	GLN
1	A	177	MET
1	A	213	LEU
1	A	218	ASN
1	A	220	ASN
1	A	236	GLN
1	A	322	VAL
1	A	323	GLU
1	A	328	THR
1	A	331	LEU
1	A	364	GLN
1	A	367	LEU
1	A	372	VAL
1	A	376	ARG
1	A	380	TYR
1	A	387	ASN
1	A	390	SER
1	A	417	ARG
1	A	418	ARG
1	A	427	ASN
1	A	430	VAL
1	A	458	VAL
1	A	466	VAL
1	A	467	LEU

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Mol	Chain	Res	Type
1	A	468	SER
1	A	480	GLN
1	A	484	GLN
1	A	487	SER
1	A	492	ASN
1	B	34	ASN
1	B	54	ARG
1	B	57	LEU
1	B	87	GLU
1	B	108	GLN
1	B	118	ASN
1	B	135	ASN
1	B	136	THR
1	B	138	ASP
1	B	144	ILE
1	B	213	LEU
1	B	220	ASN
1	B	231	ASP
1	B	236	GLN
1	B	241	GLU
1	B	251	TRP
1	B	322	VAL
1	B	323	GLU
1	B	328	THR
1	B	331	LEU
1	B	367	LEU
1	B	376	ARG
1	B	380	TYR
1	B	382	PRO
1	B	387	ASN
1	B	402	ARG
1	B	415	GLU
1	B	430	VAL
1	B	436	GLU
1	B	439	LEU
1	B	464	SER
1	B	480	GLN
1	B	492	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	67	GLN
1	A	135	ASN
1	A	159	ASN
1	A	168	ASN
1	A	220	ASN
1	A	236	GLN
1	A	325	ASN
1	A	334	ASN
1	A	385	ASN
1	A	387	ASN
1	A	484	GLN
1	A	492	ASN
1	B	34	ASN
1	B	37	HIS
1	B	53	ASN
1	B	55	ASN
1	B	135	ASN
1	B	168	ASN
1	B	173	HIS
1	B	220	ASN
1	B	236	GLN
1	B	325	ASN
1	B	334	ASN
1	B	385	ASN
1	B	387	ASN
1	B	449	ASN
1	B	480	GLN
1	B	484	GLN
1	B	492	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are 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	CO3	A	496	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	B	497	-	0,3,3	0.00	-	0,3,3	0.00	-

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	382/492 (77%)	-0.39	6 (1%) 72 75	8, 20, 41, 60	0
1	B	382/492 (77%)	-0.41	5 (1%) 77 80	7, 19, 41, 58	0
All	All	764/984 (77%)	-0.40	11 (1%) 75 78	7, 20, 41, 60	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	GLY	4.0
1	B	178	GLN	3.9
1	B	322	VAL	3.8
1	A	178	GLN	3.4
1	A	251	TRP	3.4
1	B	251	TRP	2.9
1	A	176	THR	2.7
1	A	484	GLN	2.6
1	A	321	GLY	2.3
1	A	54	ARG	2.2
1	B	200	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	CO3	B	497	4/4	0.91	0.09	25,25,30,33	0
2	CO3	A	496	4/4	0.97	0.06	20,22,25,31	0
3	MG	A	498	1/1	0.98	0.05	6,6,6,6	0
3	MG	B	499	1/1	1.00	0.08	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.