Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 06:59 AM EDT

PDB ID	:	4EGX
Title	:	Crystal structure of KIF1A CC1-FHA tandem
Authors	:	Yu, J.; Huo, L.; Yue, Y.; Xu, T.; Zhang, M.; Feng, W.
Deposited on	:	2012-04-02
Resolution	:	2.51 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 (i) 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 (1)) were used in the production of this report:

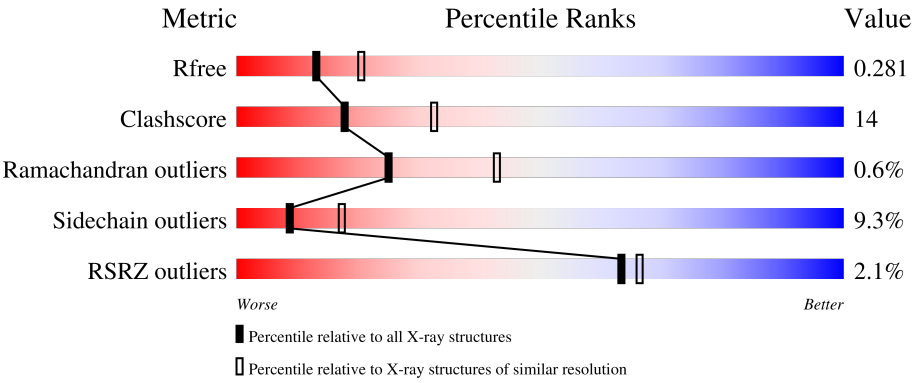
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	184	3% 68% 28%
1	B	184	2% 70% 26%
1	C	184	2% 64% 26% 5%
1	D	184	% 67% 24% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5591 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 Kinesin-like protein KIF1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1393	864	248	273	8			
1	B	180	Total	C	N	O	S	0	0	0
			1388	861	250	269	8			
1	C	174	Total	C	N	O	S	0	0	0
			1316	823	238	248	7			
1	D	173	Total	C	N	O	S	0	0	0
			1308	818	228	254	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	424	GLY	-	expression tag	UNP Q12756
A	425	PRO	-	expression tag	UNP Q12756
A	426	GLY	-	expression tag	UNP Q12756
A	427	SER	-	expression tag	UNP Q12756
A	428	GLU	-	expression tag	UNP Q12756
A	429	PHE	-	expression tag	UNP Q12756
B	424	GLY	-	expression tag	UNP Q12756
B	425	PRO	-	expression tag	UNP Q12756
B	426	GLY	-	expression tag	UNP Q12756
B	427	SER	-	expression tag	UNP Q12756
B	428	GLU	-	expression tag	UNP Q12756
B	429	PHE	-	expression tag	UNP Q12756
C	424	GLY	-	expression tag	UNP Q12756
C	425	PRO	-	expression tag	UNP Q12756
C	426	GLY	-	expression tag	UNP Q12756
C	427	SER	-	expression tag	UNP Q12756
C	428	GLU	-	expression tag	UNP Q12756
C	429	PHE	-	expression tag	UNP Q12756
D	424	GLY	-	expression tag	UNP Q12756
D	425	PRO	-	expression tag	UNP Q12756
D	426	GLY	-	expression tag	UNP Q12756

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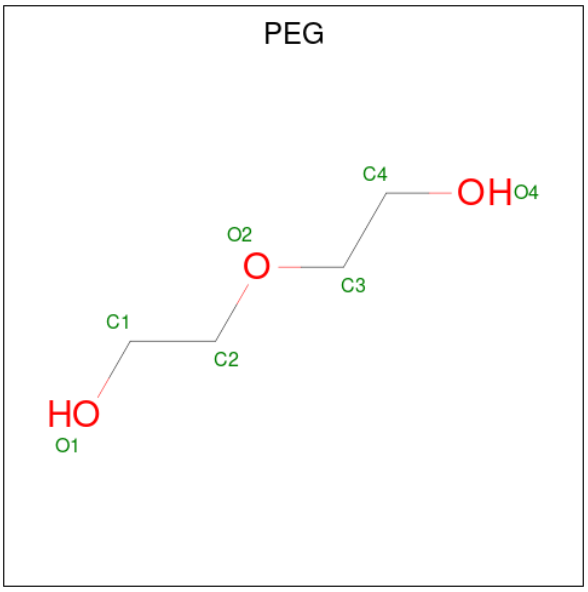
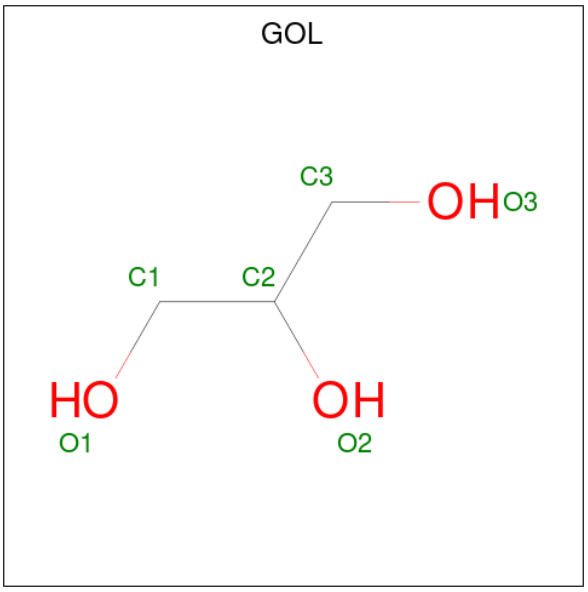
Chain	Residue	Modelled	Actual	Comment	Reference
D	427	SER	-	expression tag	UNP Q12756
D	428	GLU	-	expression tag	UNP Q12756
D	429	PHE	-	expression tag	UNP Q12756

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

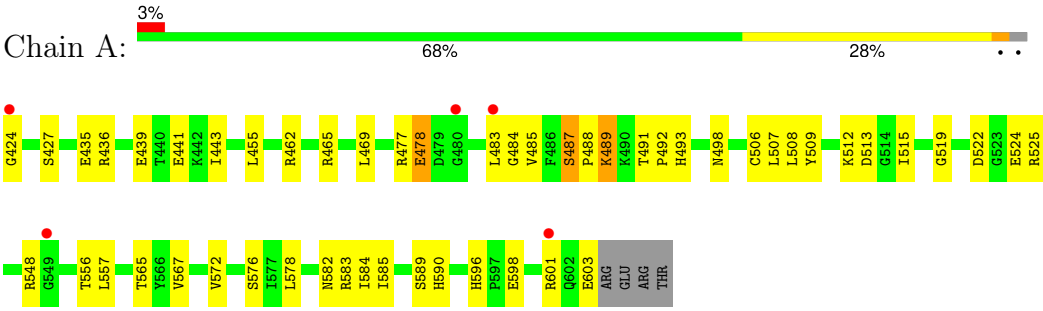
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	41	Total O 41 41	0	0
4	C	31	Total O 31 31	0	0
4	D	39	Total O 39 39	0	0

3 Residue-property plots (i)

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.

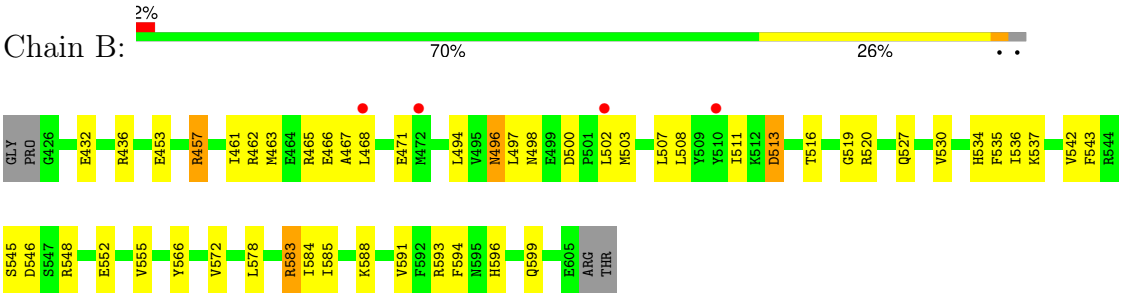
• Molecule 1: Kinesin-like protein KIF1A

Chain A:



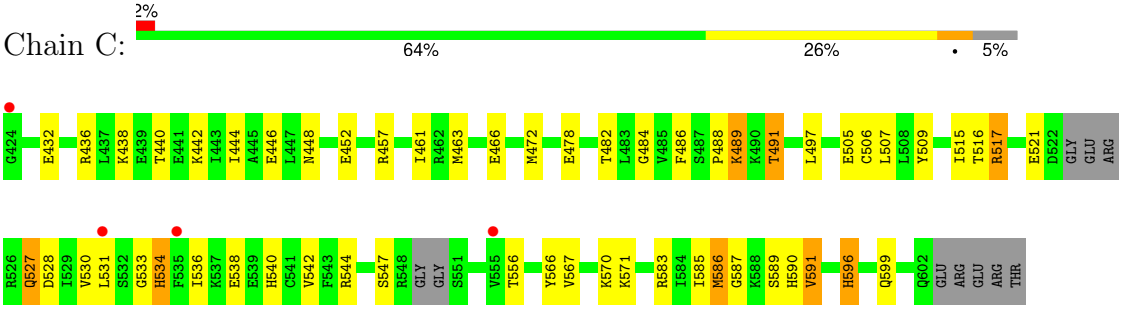
• Molecule 1: Kinesin-like protein KIF1A

Chain B:



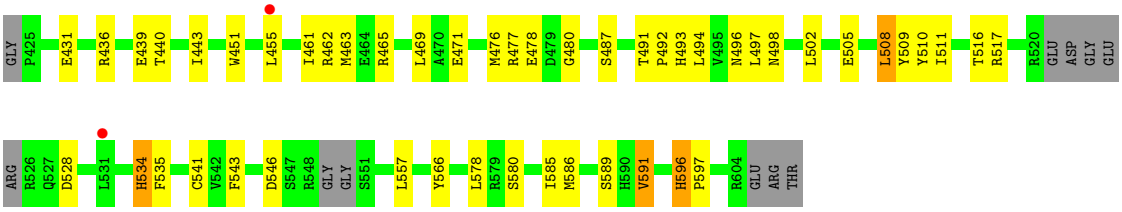
• Molecule 1: Kinesin-like protein KIF1A

Chain C:



• Molecule 1: Kinesin-like protein KIF1A

Chain D:


GLY P425 E431 R436 E439 T440 I443 W451 L455 I461 R462 M463 E464 R465 L469 A470 E471 M476 R477 E478 D479 G480 S487 T491 P492 H493 L494 V495 N496 L497 N498 L502 E505 L508 Y509 Y510 I511 T516 R517 R520 GLU ASP GLY GLU
ARG R526 Q527 D528 L531 H534 F535 C541 V542 F543 D546 S547 R548 GLY GLY S551 L557 Y566 L578 H579 S580 I585 M586 S589 H590 V591 H596 P597 R604 GLU ARG THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.94Å 87.86Å 101.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 38.98 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.51) 87.1 (38.98-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.283 0.252 , 0.281	Depositor DCC
R_{free} test set	1286 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 23.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.128 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PEG

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	0.51	0/1415	0.65	0/1905
1	B	0.50	0/1409	0.67	0/1896
1	C	0.54	0/1336	0.63	0/1802
1	D	0.50	0/1328	0.63	0/1793
All	All	0.51	0/5488	0.65	0/7396

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

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	1393	0	1344	36	0
1	B	1388	0	1344	38	0
1	C	1316	0	1269	48	0
1	D	1308	0	1242	40	0
2	A	7	0	10	1	0
2	C	7	0	10	0	0
3	A	6	0	8	0	0
3	D	6	0	8	3	0
4	A	49	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	41	0	0	3	0
4	C	31	0	0	0	0
4	D	39	0	0	1	0
All	All	5591	0	5235	145	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 14.

All (145) 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:C:505:GLU:HG2	1:C:531:LEU:HD23	1.43	1.00
1:C:505:GLU:CG	1:C:531:LEU:HD23	1.96	0.96
1:A:556:THR:HG23	4:A:833:HOH:O	1.64	0.94
1:C:517:ARG:HH11	1:C:517:ARG:HG2	1.29	0.94
1:B:497:LEU:HB2	1:B:591:VAL:HG23	1.48	0.94
1:B:457:ARG:HG3	1:B:457:ARG:HH11	1.38	0.89
1:D:436:ARG:HH21	3:D:701:GOL:H32	1.38	0.89
1:C:505:GLU:HG2	1:C:531:LEU:CD2	2.08	0.83
1:C:517:ARG:HG2	1:C:517:ARG:NH1	1.88	0.78
1:C:484:GLY:HA2	1:D:510:TYR:CE2	2.20	0.76
1:B:457:ARG:HH11	1:B:457:ARG:CG	1.99	0.75
1:B:591:VAL:HG21	1:D:480:GLY:HA2	1.69	0.75
1:D:436:ARG:HH21	3:D:701:GOL:C3	1.99	0.75
1:D:493:HIS:HB2	1:D:508:LEU:HD11	1.67	0.75
1:C:497:LEU:HB2	1:C:591:VAL:CG2	2.16	0.74
1:D:557:LEU:HB2	1:D:578:LEU:HD11	1.70	0.74
1:D:436:ARG:HE	3:D:701:GOL:H2	1.51	0.73
1:A:424:GLY:N	1:A:427:SER:HG	1.87	0.73
1:A:515:ILE:HG23	1:A:542:VAL:HG13	1.71	0.72
1:C:442:LYS:O	1:C:446:GLU:HG3	1.89	0.72
1:C:488:PRO:HB3	1:C:491:THR:HG23	1.71	0.72
1:D:535:PHE:CZ	1:D:589:SER:HB2	2.23	0.71
1:C:521:GLU:HA	1:C:530:VAL:HB	1.71	0.70
1:B:513:ASP:HA	1:B:545:SER:HB3	1.72	0.70
1:D:585:ILE:HG12	1:D:591:VAL:HG13	1.73	0.70
1:D:494:LEU:HG	1:D:511:ILE:HD11	1.73	0.69
1:D:493:HIS:HB2	1:D:508:LEU:CD1	2.23	0.69
1:D:440:THR:HA	1:D:443:ILE:HD12	1.75	0.68
1:D:534:HIS:CG	1:D:534:HIS:O	2.47	0.67
1:C:461:ILE:HD13	1:D:462:ARG:HH21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ILE:HG23	1:C:542:VAL:HG13	1.78	0.66
1:C:540:HIS:HD2	1:C:586:MET:HG2	1.60	0.65
1:C:517:ARG:HH11	1:C:517:ARG:CG	2.07	0.64
1:B:432:GLU:HG3	1:B:436:ARG:HH12	1.62	0.63
1:C:497:LEU:HB2	1:C:591:VAL:HG23	1.79	0.63
1:A:487:SER:O	1:A:489:LYS:HE2	1.98	0.63
1:B:463:MET:HB3	4:B:735:HOH:O	1.98	0.62
1:C:540:HIS:HE2	1:C:587:GLY:H	1.46	0.62
1:A:596:HIS:CE1	1:A:598:GLU:HG3	2.34	0.61
1:B:432:GLU:HG3	1:B:436:ARG:NH1	2.16	0.61
1:B:519:GLY:O	1:B:530:VAL:HA	2.01	0.60
1:C:463:MET:O	1:C:466:GLU:HG2	2.01	0.60
1:A:567:VAL:HG22	1:A:584:ILE:HG12	1.84	0.60
1:B:457:ARG:HG3	1:B:457:ARG:NH1	2.09	0.60
1:A:493:HIS:CD2	1:A:508:LEU:HD11	2.38	0.59
1:C:527:GLN:NE2	1:C:538:GLU:O	2.35	0.59
1:A:488:PRO:HD3	1:A:508:LEU:HD21	1.85	0.59
1:C:540:HIS:CD2	1:C:586:MET:HG2	2.37	0.59
1:D:463:MET:HB2	4:D:823:HOH:O	2.02	0.59
1:B:453:GLU:HG2	1:B:457:ARG:HH12	1.68	0.58
1:C:505:GLU:HG3	1:C:531:LEU:HD23	1.83	0.58
1:B:494:LEU:HG	1:B:511:ILE:HD11	1.87	0.57
1:C:585:ILE:HG23	1:C:590:HIS:O	2.05	0.57
1:C:432:GLU:O	1:C:436:ARG:HD2	2.06	0.56
1:B:467:ALA:O	1:B:471:GLU:HB2	2.06	0.56
1:A:441:GLU:HB3	2:A:701:PEG:H31	1.87	0.56
1:A:507:LEU:HD22	1:B:508:LEU:HD12	1.88	0.56
1:A:477:ARG:NE	1:A:483:LEU:HD21	2.21	0.55
1:B:546:ASP:OD1	1:B:548:ARG:HG3	2.07	0.54
1:C:472:MET:O	1:C:472:MET:HG2	2.07	0.54
1:B:503:MET:HA	1:B:503:MET:CE	2.37	0.54
1:A:485:VAL:O	1:B:507:LEU:N	2.41	0.53
1:A:507:LEU:HD23	1:B:507:LEU:HD21	1.91	0.53
1:B:527:GLN:HB2	1:B:530:VAL:HG12	1.90	0.53
1:C:567:VAL:O	1:C:570:LYS:HG2	2.08	0.53
1:A:488:PRO:HD2	1:A:493:HIS:CE1	2.44	0.53
1:D:541:CYS:SG	1:D:557:LEU:HD11	2.50	0.52
1:D:493:HIS:CB	1:D:508:LEU:HD11	2.37	0.52
1:A:507:LEU:CD2	1:B:507:LEU:HD21	2.40	0.52
1:D:517:ARG:HG3	1:D:528:ASP:OD2	2.09	0.51
1:B:453:GLU:HG2	1:B:457:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:GLY:HA3	1:C:536:ILE:HD13	1.92	0.51
1:A:522:ASP:HA	4:A:840:HOH:O	2.09	0.50
1:C:517:ARG:HB3	1:C:527:GLN:HG3	1.94	0.50
1:C:531:LEU:HD22	1:C:590:HIS:CE1	2.47	0.49
1:C:515:ILE:HG23	1:C:542:VAL:CG1	2.42	0.49
1:D:496:ASN:HD21	1:D:498:ASN:HB2	1.77	0.49
1:B:498:ASN:HB3	4:B:736:HOH:O	2.12	0.49
1:A:469:LEU:HA	1:A:469:LEU:HD23	1.65	0.48
1:A:491:THR:HG22	1:A:492:PRO:O	2.13	0.48
1:C:534:HIS:HE1	1:C:589:SER:HB3	1.78	0.48
1:C:484:GLY:HA3	1:D:508:LEU:O	2.12	0.48
1:D:535:PHE:HZ	1:D:589:SER:HB2	1.78	0.48
1:C:448:ASN:O	1:C:452:GLU:HG3	2.14	0.48
1:B:555:VAL:HG12	1:B:578:LEU:HD12	1.96	0.47
1:C:488:PRO:CB	1:C:491:THR:HG23	2.41	0.47
1:A:522:ASP:OD1	1:A:522:ASP:N	2.46	0.46
1:B:520:ARG:HD3	1:B:536:ILE:O	2.15	0.46
1:B:583:ARG:HG3	4:B:732:HOH:O	2.14	0.46
1:D:461:ILE:O	1:D:465:ARG:HG2	2.15	0.46
1:A:424:GLY:N	1:A:427:SER:OG	2.47	0.46
1:C:438:LYS:NZ	1:C:438:LYS:HB3	2.30	0.46
1:C:484:GLY:HA2	1:D:510:TYR:CD2	2.50	0.46
1:C:440:THR:O	1:C:444:ILE:HG13	2.16	0.46
1:C:515:ILE:N	1:C:515:ILE:HD12	2.31	0.46
1:C:540:HIS:HE2	1:C:587:GLY:N	2.12	0.46
1:D:462:ARG:HD3	1:D:463:MET:HE3	1.97	0.46
1:A:498:ASN:HD21	1:A:590:HIS:HA	1.81	0.45
1:C:544:ARG:HB3	1:C:556:THR:HG22	1.99	0.45
1:C:517:ARG:H	1:C:528:ASP:HB2	1.81	0.45
1:C:516:THR:OG1	1:D:477:ARG:NH1	2.48	0.44
1:C:517:ARG:CB	1:C:527:GLN:HG3	2.47	0.44
1:B:566:TYR:O	1:B:584:ILE:HA	2.17	0.44
1:A:601:ARG:HG2	1:A:601:ARG:HH11	1.80	0.44
1:A:439:GLU:O	1:A:443:ILE:HG13	2.17	0.44
1:D:471:GLU:OE1	1:D:491:THR:HG23	2.17	0.44
1:D:497:LEU:HB2	1:D:591:VAL:HB	1.99	0.44
1:A:596:HIS:HE1	1:A:598:GLU:HG3	1.83	0.43
1:D:596:HIS:HA	1:D:597:PRO:HD2	1.79	0.43
1:C:566:TYR:CE1	1:C:571:LYS:HB2	2.54	0.43
1:A:557:LEU:HB2	1:A:578:LEU:HD11	2.01	0.43
1:A:462:ARG:HD3	1:B:461:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ILE:HG12	1:B:591:VAL:HG12	2.02	0.42
1:C:438:LYS:NZ	1:C:438:LYS:CB	2.82	0.42
1:C:596:HIS:CG	1:C:599:GLN:HB2	2.54	0.42
1:D:508:LEU:HD12	1:D:509:TYR:N	2.34	0.42
1:B:585:ILE:HD11	1:D:478:GLU:HA	2.00	0.42
1:B:496:ASN:HD22	1:B:497:LEU:N	2.18	0.42
1:D:566:TYR:CD2	1:D:566:TYR:N	2.87	0.42
1:A:484:GLY:HA3	1:B:508:LEU:O	2.20	0.42
1:A:506:CYS:HB2	1:A:509:TYR:CZ	2.54	0.42
1:A:465:ARG:HD3	4:A:816:HOH:O	2.19	0.42
1:D:492:PRO:HB2	1:D:511:ILE:HB	2.02	0.42
1:A:583:ARG:HH11	1:A:585:ILE:HD11	1.85	0.41
1:B:591:VAL:HG21	1:D:480:GLY:CA	2.46	0.41
1:B:516:THR:HB	1:B:543:PHE:HB2	2.02	0.41
1:A:465:ARG:HH12	1:B:466:GLU:HB2	1.85	0.41
1:B:497:LEU:HD21	1:B:593:ARG:NH1	2.35	0.41
1:A:583:ARG:NH1	1:A:585:ILE:HD11	2.35	0.41
1:B:494:LEU:HD23	1:B:594:PHE:HA	2.02	0.41
1:B:596:HIS:ND1	1:B:599:GLN:HB2	2.36	0.41
1:C:506:CYS:HB2	1:C:509:TYR:CZ	2.55	0.41
1:D:516:THR:HB	1:D:543:PHE:HB2	2.02	0.41
1:A:478:GLU:H	1:A:478:GLU:HG3	1.59	0.41
1:A:557:LEU:HD21	1:A:565:THR:HG21	2.03	0.41
1:A:585:ILE:HA	1:A:590:HIS:O	2.21	0.41
1:C:484:GLY:HA2	1:D:510:TYR:HE2	1.76	0.41
1:D:469:LEU:C	1:D:471:GLU:H	2.24	0.41
1:C:452:GLU:HG2	1:D:451:TRP:CH2	2.56	0.40
1:D:469:LEU:HD23	1:D:469:LEU:HA	1.88	0.40
1:B:534:HIS:HB3	1:B:535:PHE:CE2	2.57	0.40
1:D:439:GLU:O	1:D:443:ILE:HG13	2.21	0.40
1:C:489:LYS:H	1:C:489:LYS:HG2	1.76	0.40
1:A:519:GLY:HA3	1:A:538:GLU:O	2.21	0.40
1:D:502:LEU:HG	1:D:505:GLU:OE2	2.22	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	178/184 (97%)	167 (94%)	8 (4%)	3 (2%)	9 16
1	B	178/184 (97%)	167 (94%)	10 (6%)	1 (1%)	25 43
1	C	168/184 (91%)	162 (96%)	6 (4%)	0	100 100
1	D	167/184 (91%)	160 (96%)	7 (4%)	0	100 100
All	All	691/736 (94%)	656 (95%)	31 (4%)	4 (1%)	25 43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	LEU
1	A	478	GLU
1	A	548	ARG
1	A	513	ASP

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	146/159 (92%)	133 (91%)	13 (9%)	9 19
1	B	145/159 (91%)	132 (91%)	13 (9%)	9 19
1	C	135/159 (85%)	120 (89%)	15 (11%)	6 11
1	D	135/159 (85%)	124 (92%)	11 (8%)	11 23
All	All	561/636 (88%)	509 (91%)	52 (9%)	9 17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	GLU
1	A	436	ARG
1	A	455	LEU
1	A	487	SER
1	A	489	LYS
1	A	512	LYS
1	A	524	GLU
1	A	525	ARG
1	A	572	VAL
1	A	576	SER
1	A	582	ASN
1	A	589	SER
1	A	603	GLU
1	B	457	ARG
1	B	462	ARG
1	B	465	ARG
1	B	468	LEU
1	B	496	ASN
1	B	500	ASP
1	B	513	ASP
1	B	537	LYS
1	B	542	VAL
1	B	552	GLU
1	B	572	VAL
1	B	583	ARG
1	B	588	LYS
1	C	457	ARG
1	C	478	GLU
1	C	482	THR
1	C	486	PHE
1	C	489	LYS
1	C	491	THR
1	C	507	LEU
1	C	517	ARG
1	C	527	GLN
1	C	534	HIS
1	C	547	SER
1	C	583	ARG
1	C	586	MET
1	C	591	VAL
1	C	596	HIS
1	D	431	GLU

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Mol	Chain	Res	Type
1	D	455	LEU
1	D	476	MET
1	D	487	SER
1	D	508	LEU
1	D	534	HIS
1	D	546	ASP
1	D	580	SER
1	D	586	MET
1	D	591	VAL
1	D	596	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	582	ASN
1	B	496	ASN
1	B	568	ASN
1	B	595	ASN
1	C	527	GLN
1	C	534	HIS
1	D	496	ASN

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)

4 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	$\#\|Z\| > 2$
3	GOL	A	702	-	5,5,5	0.33	0	5,5,5	0.78	0
2	PEG	C	701	-	6,6,6	0.70	0	5,5,5	0.37	0
3	GOL	D	701	-	5,5,5	0.42	0	5,5,5	0.55	0
2	PEG	A	701	-	6,6,6	1.02	0	5,5,5	0.97	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	GOL	A	702	-	-	2/4/4/4	-
2	PEG	C	701	-	-	3/4/4/4	-
3	GOL	D	701	-	-	4/4/4/4	-
2	PEG	A	701	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GOL	O1-C1-C2-O2
3	A	702	GOL	O1-C1-C2-C3
3	D	701	GOL	O1-C1-C2-O2
3	D	701	GOL	O1-C1-C2-C3
3	D	701	GOL	C1-C2-C3-O3
2	A	701	PEG	O1-C1-C2-O2
3	D	701	GOL	O2-C2-C3-O3
2	C	701	PEG	O2-C3-C4-O4
2	C	701	PEG	C4-C3-O2-C2
2	C	701	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	GOL	3	0
2	A	701	PEG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	180/184 (97%)	-0.14	5 (2%)	53	56	32, 45, 69, 85	0
1	B	180/184 (97%)	-0.04	4 (2%)	62	65	31, 48, 75, 85	0
1	C	174/184 (94%)	0.00	4 (2%)	60	63	35, 53, 75, 100	0
1	D	173/184 (94%)	0.00	2 (1%)	79	80	35, 54, 72, 92	0
All	All	707/736 (96%)	-0.04	15 (2%)	63	66	31, 50, 74, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	MET	4.8
1	B	468	LEU	3.6
1	B	502	LEU	3.4
1	A	424	GLY	3.0
1	A	549	GLY	3.0
1	D	455	LEU	2.7
1	C	555	VAL	2.7
1	D	531	LEU	2.4
1	C	531	LEU	2.2
1	C	535	PHE	2.1
1	A	480	GLY	2.1
1	A	483	LEU	2.0
1	C	424	GLY	2.0
1	A	601	ARG	2.0
1	B	510	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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	PEG	C	701	7/7	0.78	0.20	42,42,44,45	0
3	GOL	D	701	6/6	0.80	0.22	40,42,43,43	0
3	GOL	A	702	6/6	0.86	0.22	43,44,45,46	0
2	PEG	A	701	7/7	0.89	0.41	43,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.