Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:56 PM EDT

PDB ID	:	6Q3M
Title	:	Structure of CHD4 PHD2 - tandem chromodomains
Authors	:	Alt, A.; Mancini, E.J.
Deposited on	:	2018-12-04
Resolution	:	2.52 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:

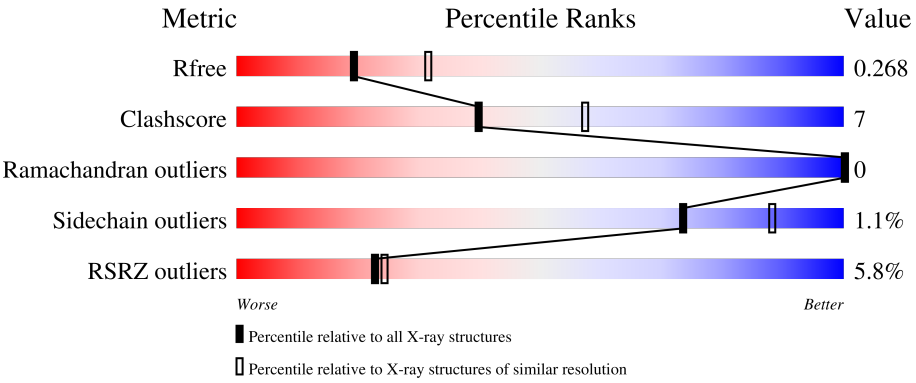
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	238	4% 78% 12% 9%
1	B	238	5% 77% 12% 10%
1	C	238	5% 76% 15% • 8%
1	D	238	8% 70% 13% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	705	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14178 atoms, of which 6721 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 Chromodomain-helicase-DNA-binding protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	H	N	O	S	0	0	0
			3493	1156	1684	315	320	18			
1	B	214	Total	C	H	N	O	S	0	0	0
			3433	1147	1641	313	314	18			
1	C	219	Total	C	H	N	O	S	0	0	0
			3505	1175	1667	319	325	19			
1	D	199	Total	C	H	N	O	S	0	0	0
			3188	1074	1507	292	297	18			

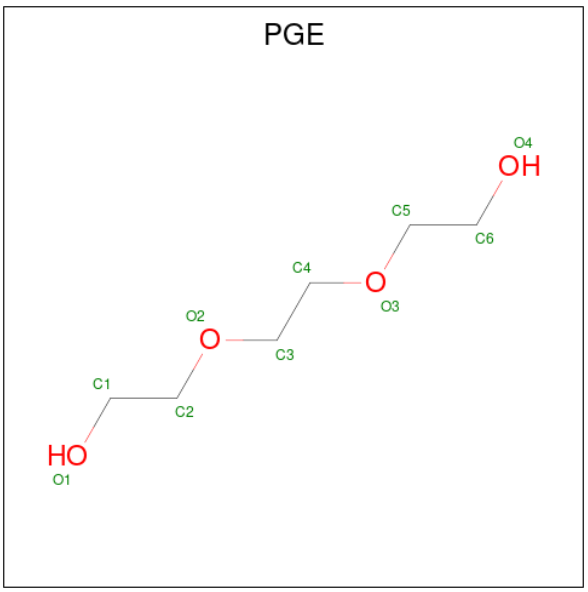
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	442	GLY	-	expression tag	UNP Q14839
A	443	PRO	-	expression tag	UNP Q14839
B	442	GLY	-	expression tag	UNP Q14839
B	443	PRO	-	expression tag	UNP Q14839
C	442	GLY	-	expression tag	UNP Q14839
C	443	PRO	-	expression tag	UNP Q14839
D	442	GLY	-	expression tag	UNP Q14839
D	443	PRO	-	expression tag	UNP Q14839

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

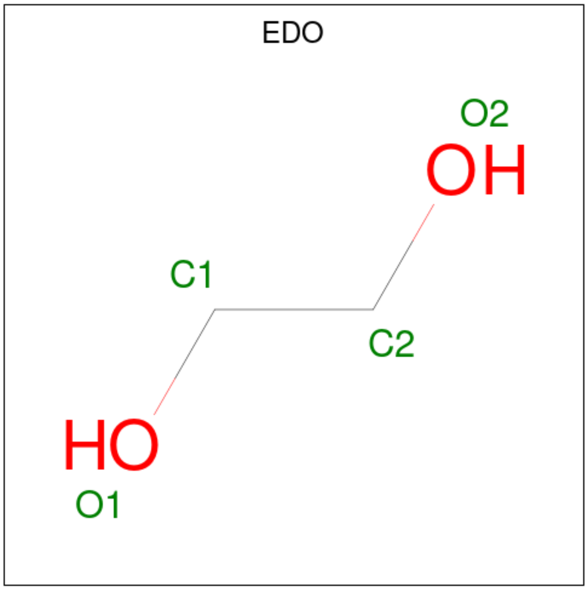
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	B	1	Total	C	H	O	0	0
			24	6	14	4		
3	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0

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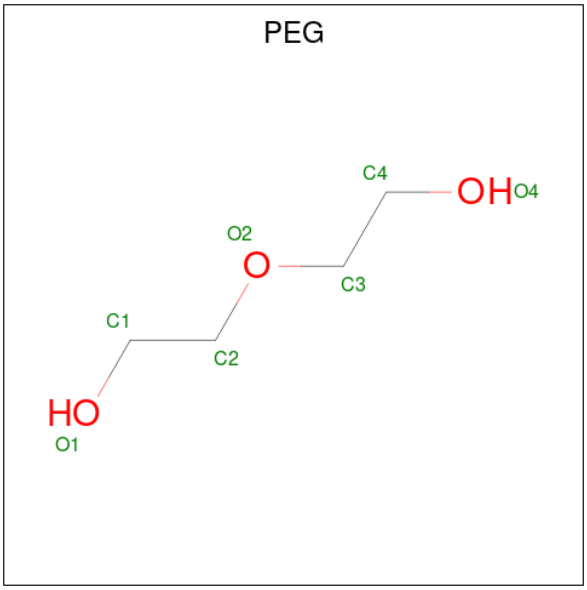
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	D	1	Total C H O 10 2 6 2	0	0
4	D	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 17 4 10 3	0	0
5	C	1	Total C H O 17 4 10 3	0	0

- Molecule 6 is water.

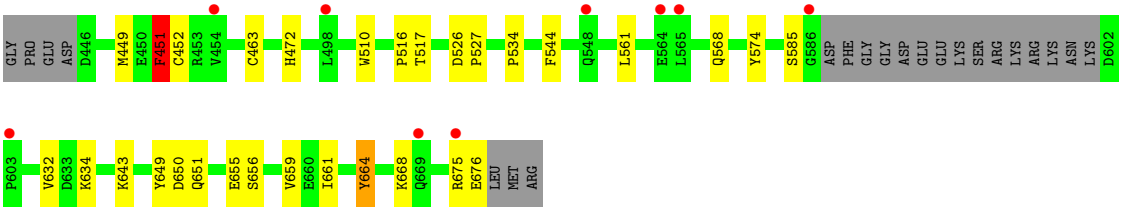
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	71	Total O 71 71	0	0
6	B	48	Total O 48 48	0	0
6	C	25	Total O 25 25	0	0
6	D	33	Total O 33 33	0	0

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.

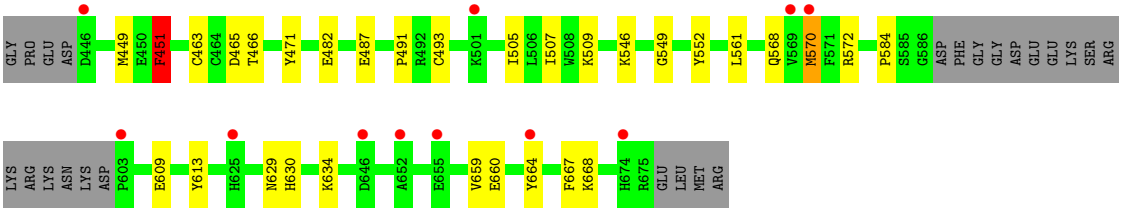
• Molecule 1: Chromodomain-helicase-DNA-binding protein 4

Chain A:



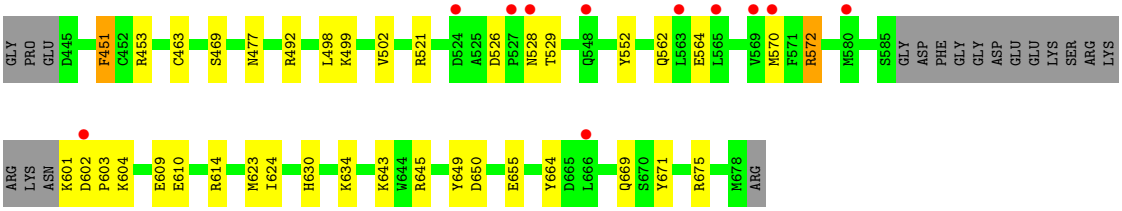
• Molecule 1: Chromodomain-helicase-DNA-binding protein 4

Chain B:



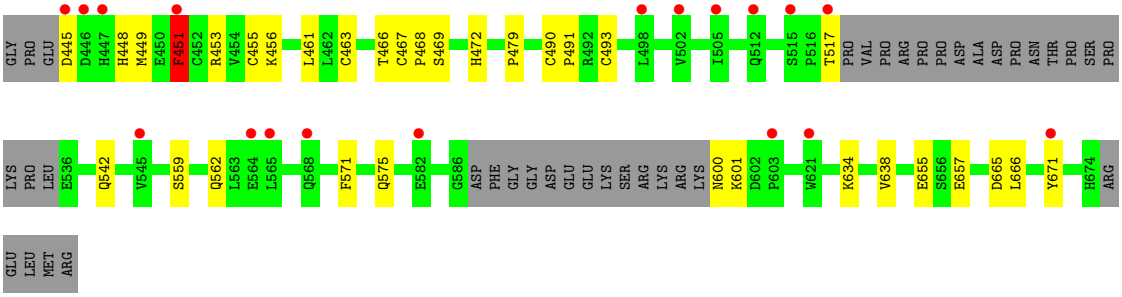
• Molecule 1: Chromodomain-helicase-DNA-binding protein 4

Chain C:



• Molecule 1: Chromodomain-helicase-DNA-binding protein 4

Chain D:


GLY PRO GLU D445 D446 H447 H448 M449 E450 F451 C452 R453 V454 C455 K456 L461 L462 C463 T466 C467 P468 S469 H472 P479 C490 P491 R492 C493 L498 V502 I505 Q512 S515 P516 T517 PRO VAL PRO ARG PRO PRO ASP ALA ASP PRO ASN THR PRO SER PRO
LYS PRO LEU E536 Q542 V545 S559 Q562 L563 E564 L565 Q568 F571 Q575 E582 G586 ASP PHE GLY GLY ASP GLU GLU LYS SER ARG LYS ARG LYS N600 K601 D602 P603 W621 K634 V638 E655 S656 E657 D665 L666 Y671 H674 ARG
GLU LEU MET ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.73Å 87.68Å 129.26Å 90.00° 93.57° 90.00°	Depositor
Resolution (Å)	64.50 – 2.52 72.52 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.3 (64.50-2.52) 99.3 (72.52-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.230 , 0.263 0.234 , 0.268	Depositor DCC
R_{free} test set	2574 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14178	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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: PGE, ZN, PEG, EDO

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	0.28	0/1878	0.54	2/2554 (0.1%)
1	B	0.28	0/1861	0.52	2/2530 (0.1%)
1	C	0.27	0/1907	0.50	0/2592
1	D	0.26	0/1741	0.52	2/2358 (0.1%)
All	All	0.27	0/7387	0.52	6/10034 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	PHE	CB-CG-CD2	-7.67	115.43	120.80
1	A	451	PHE	CB-CG-CD1	7.66	126.16	120.80
1	B	451	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	B	451	PHE	CB-CG-CD1	6.29	125.20	120.80
1	D	451	PHE	CB-CG-CD1	6.28	125.19	120.80
1	D	451	PHE	CB-CG-CD2	-6.26	116.42	120.80

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	1809	1684	1699	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1792	1641	1690	25	0
1	C	1838	1667	1733	32	0
1	D	1681	1507	1569	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	30	42	42	2	0
3	B	10	14	14	3	0
3	C	10	14	14	2	0
4	A	36	54	54	4	0
4	B	24	36	36	2	0
4	C	20	30	30	2	0
4	D	8	12	12	0	0
5	A	7	10	10	0	0
5	C	7	10	10	0	0
6	A	71	0	0	4	0
6	B	48	0	0	4	0
6	C	25	0	0	5	0
6	D	33	0	0	3	0
All	All	7457	6721	6913	104	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 7.

All (104) 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:B:463:CYS:SG	1:C:634:LYS:NZ	2.29	1.05
1:B:634:LYS:NZ	1:C:463:CYS:SG	2.35	0.98
1:A:463:CYS:SG	1:D:634:LYS:NZ	2.38	0.96
1:A:634:LYS:NZ	1:D:463:CYS:SG	2.43	0.92
1:A:585:SER:OG	6:A:801:HOH:O	1.92	0.88
1:C:601:LYS:HB2	1:C:604:LYS:HB2	1.59	0.85
1:C:499:LYS:O	6:C:801:HOH:O	1.95	0.84
1:C:602:ASP:HB3	1:C:603:PRO:HD3	1.59	0.82
1:C:564:GLU:OE1	1:C:572:ARG:NH1	2.14	0.80
1:D:655:GLU:OE2	6:D:801:HOH:O	1.99	0.79
1:C:655:GLU:OE2	6:C:802:HOH:O	1.99	0.78
4:B:706:EDO:O2	6:B:801:HOH:O	2.05	0.74
1:C:552:TYR:OH	4:C:705:EDO:O1	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ARG:NH2	6:C:803:HOH:O	2.23	0.72
1:D:479:PRO:O	1:D:517:THR:OG1	2.09	0.71
1:C:602:ASP:HB3	1:C:603:PRO:CD	2.21	0.70
1:A:651:GLN:OE1	6:A:802:HOH:O	2.10	0.68
1:C:526:ASP:O	6:C:803:HOH:O	2.11	0.68
1:A:517:THR:OG1	6:A:803:HOH:O	2.11	0.68
1:A:632:VAL:O	6:A:804:HOH:O	2.14	0.65
1:B:505:ILE:HG13	1:B:570:MET:HE1	1.81	0.63
1:D:600:ASN:OD1	1:D:601:LYS:N	2.31	0.62
1:C:502:VAL:HG12	1:C:570:MET:HE1	1.81	0.62
1:D:542:GLN:NE2	6:D:805:HOH:O	2.33	0.61
1:A:634:LYS:HD2	1:D:445:ASP:HB2	1.83	0.60
1:C:610:GLU:OE2	1:C:614:ARG:NH1	2.34	0.60
1:C:623:MET:SD	1:C:645:ARG:NH1	2.75	0.60
1:B:449:MET:HE3	1:B:451:PHE:CE1	2.36	0.60
1:C:528:ASN:OD1	1:C:529:THR:N	2.35	0.60
1:A:675:ARG:C	1:A:676:GLU:HG2	2.22	0.59
1:B:491:PRO:HG2	3:B:703:PGE:H1	1.86	0.57
1:A:451:PHE:O	1:A:451:PHE:HD1	1.87	0.57
1:C:502:VAL:HG12	1:C:570:MET:CE	2.34	0.56
1:D:448:HIS:ND1	6:D:806:HOH:O	2.33	0.56
1:C:601:LYS:O	1:C:601:LYS:HG3	2.05	0.56
1:A:451:PHE:HD1	1:A:451:PHE:C	2.10	0.55
1:B:449:MET:HE3	1:B:451:PHE:HE1	1.71	0.55
1:B:572:ARG:NH2	6:B:807:HOH:O	2.40	0.54
1:C:451:PHE:N	1:C:451:PHE:CD2	2.76	0.54
1:B:451:PHE:O	1:B:451:PHE:HD1	1.91	0.54
1:A:451:PHE:C	1:A:451:PHE:CD1	2.82	0.53
1:A:561:LEU:HD13	4:A:712:EDO:H11	1.89	0.53
1:A:544:PHE:HE1	3:A:705:PGE:H32	1.74	0.53
1:D:451:PHE:C	1:D:451:PHE:HD1	2.13	0.52
1:B:561:LEU:HD13	3:B:703:PGE:H4	1.92	0.52
1:D:451:PHE:C	1:D:451:PHE:CD1	2.83	0.52
1:A:449:MET:HE3	1:A:451:PHE:CE1	2.45	0.52
1:A:568:GLN:OE1	4:A:707:EDO:H12	2.10	0.52
1:C:453:ARG:NH2	1:C:469:SER:OG	2.43	0.51
1:A:574:TYR:OH	4:A:714:EDO:O2	2.28	0.51
1:D:461:LEU:HD23	1:D:472:HIS:CD2	2.46	0.50
1:A:661:ILE:HD12	1:A:664:TYR:CE1	2.47	0.50
1:C:601:LYS:HB2	1:C:604:LYS:CB	2.39	0.49
1:C:675:ARG:NH1	4:C:706:EDO:O1	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ARG:O	1:A:676:GLU:HG2	2.12	0.48
1:B:466:THR:OG1	1:B:493:CYS:SG	2.68	0.48
1:B:507:ILE:HG13	1:B:584:PRO:HG2	1.96	0.48
1:D:665:ASP:OD1	1:D:666:LEU:N	2.47	0.48
1:A:650:ASP:N	1:A:650:ASP:OD1	2.46	0.47
1:B:568:GLN:O	1:B:572:ARG:HG2	2.13	0.47
1:C:650:ASP:OD1	1:C:650:ASP:N	2.46	0.47
1:A:655:GLU:HG2	1:A:661:ILE:HD11	1.97	0.47
1:B:509:LYS:HB3	4:B:705:EDO:H21	1.97	0.46
1:D:490:CYS:HB2	1:D:491:PRO:HD2	1.98	0.46
1:B:451:PHE:HD1	1:B:451:PHE:C	2.19	0.45
1:B:482:GLU:N	1:B:482:GLU:OE1	2.49	0.45
1:B:451:PHE:C	1:B:451:PHE:CD1	2.90	0.45
1:B:659:VAL:HG12	1:B:660:GLU:N	2.31	0.45
1:D:461:LEU:HD23	1:D:472:HIS:HD2	1.81	0.45
1:B:629:ASN:OD1	1:B:630:HIS:N	2.47	0.45
1:D:466:THR:OG1	1:D:493:CYS:SG	2.70	0.44
1:C:451:PHE:N	1:C:451:PHE:HD2	2.13	0.44
1:C:624:ILE:HD11	1:C:664:TYR:CD1	2.52	0.44
1:C:669:GLN:NE2	6:C:806:HOH:O	2.49	0.44
1:A:452:CYS:HB2	1:A:472:HIS:CE1	2.52	0.44
1:B:471:TYR:OH	3:B:703:PGE:H5	2.18	0.44
1:D:453:ARG:NH2	1:D:469:SER:OG	2.50	0.44
1:D:467:CYS:HB2	1:D:468:PRO:HD2	2.00	0.43
1:D:638:VAL:HB	1:D:657:GLU:OE2	2.18	0.43
1:C:630:HIS:HB3	1:C:671:TYR:HE1	1.84	0.43
1:C:624:ILE:HD11	1:C:664:TYR:HD1	1.84	0.43
1:A:451:PHE:O	1:A:451:PHE:CD1	2.68	0.43
1:D:571:PHE:CE2	1:D:575:GLN:NE2	2.87	0.43
1:A:510:TRP:CZ3	3:A:704:PGE:H22	2.53	0.43
1:C:498:LEU:HD21	1:C:562:GLN:HB3	2.00	0.43
1:B:465:ASP:OD2	1:B:487:GLU:HA	2.19	0.42
1:A:516:PRO:HB2	1:A:534:PRO:HB2	2.02	0.42
1:B:609:GLU:HA	1:B:613:TYR:HB2	2.01	0.42
1:C:643:LYS:HE3	1:C:649:TYR:CE1	2.55	0.42
1:A:568:GLN:OE1	4:A:707:EDO:C1	2.68	0.41
1:A:526:ASP:OD1	1:A:527:PRO:HD2	2.20	0.41
1:D:449:MET:CE	1:D:451:PHE:HE1	2.34	0.41
1:A:643:LYS:HE3	1:A:649:TYR:CE1	2.56	0.41
1:D:559:SER:OG	1:D:562:GLN:HB2	2.21	0.41
1:C:492:ARG:NH1	3:C:703:PGE:O1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:CYS:O	1:D:456:LYS:HB2	2.21	0.41
1:B:549:GLY:N	6:B:802:HOH:O	2.27	0.41
1:B:572:ARG:CZ	6:B:807:HOH:O	2.68	0.41
1:B:664:TYR:O	1:B:668:LYS:HG3	2.21	0.41
1:C:477:ASN:H	3:C:703:PGE:H62	1.86	0.41
1:A:656:SER:HB3	1:A:659:VAL:HG23	2.03	0.40
1:A:664:TYR:CE2	1:A:668:LYS:HE3	2.57	0.40
1:C:609:GLU:O	1:C:614:ARG:HG3	2.22	0.40
1:B:546:LYS:HD2	1:B:552:TYR:CZ	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	212/238 (89%)	208 (98%)	4 (2%)	0	100	100
1	B	210/238 (88%)	207 (99%)	3 (1%)	0	100	100
1	C	215/238 (90%)	205 (95%)	10 (5%)	0	100	100
1	D	193/238 (81%)	187 (97%)	6 (3%)	0	100	100
All	All	830/952 (87%)	807 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	202/221 (91%)	200 (99%)	2 (1%)	76 89
1	B	200/221 (90%)	197 (98%)	3 (2%)	65 83
1	C	206/221 (93%)	204 (99%)	2 (1%)	76 89
1	D	186/221 (84%)	184 (99%)	2 (1%)	73 88
All	All	794/884 (90%)	785 (99%)	9 (1%)	73 88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	PHE
1	A	664	TYR
1	B	451	PHE
1	B	570	MET
1	B	667	PHE
1	C	451	PHE
1	C	572	ARG
1	D	451	PHE
1	D	671	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	GLN
1	D	472	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)

Of 37 ligands modelled in this entry, 8 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
4	EDO	A	711	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	B	708	-	3,3,3	0.43	0	2,2,2	0.43	0
3	PGE	A	703	-	9,9,9	0.50	0	8,8,8	0.57	0
4	EDO	C	708	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	B	704	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	C	705	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	C	707	-	3,3,3	0.44	0	2,2,2	0.34	0
3	PGE	A	705	-	9,9,9	0.49	0	8,8,8	0.49	0
4	EDO	D	703	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	B	705	-	3,3,3	0.43	0	2,2,2	0.43	0
4	EDO	A	707	-	3,3,3	0.41	0	2,2,2	0.36	0
5	PEG	A	715	-	6,6,6	0.48	0	5,5,5	0.49	0
3	PGE	C	703	-	9,9,9	0.51	0	8,8,8	0.35	0
4	EDO	C	704	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.39	0
3	PGE	A	704	-	9,9,9	0.50	0	8,8,8	0.30	0
4	EDO	B	706	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	A	713	-	3,3,3	0.45	0	2,2,2	0.45	0
4	EDO	B	707	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	A	710	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	B	709	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	A	709	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	A	714	-	3,3,3	0.45	0	2,2,2	0.39	0
5	PEG	C	709	-	6,6,6	0.49	0	5,5,5	0.42	0
4	EDO	C	706	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	D	704	-	3,3,3	0.43	0	2,2,2	0.39	0
3	PGE	B	703	-	9,9,9	0.50	0	8,8,8	0.34	0
4	EDO	A	712	-	3,3,3	0.42	0	2,2,2	0.44	0
4	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.35	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
4	EDO	A	711	-	-	0/1/1/1	-
4	EDO	B	708	-	-	0/1/1/1	-
3	PGE	A	703	-	-	2/7/7/7	-
4	EDO	C	708	-	-	0/1/1/1	-
4	EDO	B	704	-	-	1/1/1/1	-
4	EDO	C	705	-	-	1/1/1/1	-
4	EDO	C	707	-	-	0/1/1/1	-
3	PGE	A	705	-	-	5/7/7/7	-
4	EDO	D	703	-	-	0/1/1/1	-
4	EDO	B	705	-	-	1/1/1/1	-
4	EDO	A	707	-	-	1/1/1/1	-
5	PEG	A	715	-	-	3/4/4/4	-
3	PGE	C	703	-	-	4/7/7/7	-
4	EDO	C	704	-	-	1/1/1/1	-
4	EDO	A	708	-	-	0/1/1/1	-
3	PGE	A	704	-	-	1/7/7/7	-
4	EDO	B	706	-	-	0/1/1/1	-
4	EDO	A	713	-	-	0/1/1/1	-
4	EDO	B	707	-	-	1/1/1/1	-
4	EDO	A	710	-	-	1/1/1/1	-
4	EDO	B	709	-	-	0/1/1/1	-
4	EDO	A	709	-	-	0/1/1/1	-
4	EDO	A	714	-	-	1/1/1/1	-
5	PEG	C	709	-	-	0/4/4/4	-
4	EDO	C	706	-	-	0/1/1/1	-
4	EDO	D	704	-	-	0/1/1/1	-
3	PGE	B	703	-	-	5/7/7/7	-
4	EDO	A	712	-	-	0/1/1/1	-
4	EDO	A	706	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	PGE	O2-C3-C4-O3
3	A	705	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	703	PGE	C1-C2-O2-C3
3	B	703	PGE	O3-C5-C6-O4
3	C	703	PGE	O3-C5-C6-O4
3	C	703	PGE	O2-C3-C4-O3
4	A	714	EDO	O1-C1-C2-O2
3	B	703	PGE	O1-C1-C2-O2
3	C	703	PGE	O1-C1-C2-O2
4	B	704	EDO	O1-C1-C2-O2
3	A	704	PGE	O3-C5-C6-O4
3	B	703	PGE	C4-C3-O2-C2
5	A	715	PEG	C4-C3-O2-C2
3	A	705	PGE	O1-C1-C2-O2
5	A	715	PEG	O1-C1-C2-O2
3	A	705	PGE	O3-C5-C6-O4
3	B	703	PGE	C6-C5-O3-C4
5	A	715	PEG	O2-C3-C4-O4
4	A	710	EDO	O1-C1-C2-O2
4	B	705	EDO	O1-C1-C2-O2
4	B	707	EDO	O1-C1-C2-O2
4	C	704	EDO	O1-C1-C2-O2
4	A	706	EDO	O1-C1-C2-O2
3	C	703	PGE	C1-C2-O2-C3
3	A	705	PGE	C3-C4-O3-C5
3	A	705	PGE	C6-C5-O3-C4
4	C	705	EDO	O1-C1-C2-O2
4	A	707	EDO	O1-C1-C2-O2
3	B	703	PGE	C1-C2-O2-C3

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	705	EDO	1	0
3	A	705	PGE	1	0
4	B	705	EDO	1	0
4	A	707	EDO	2	0
3	C	703	PGE	2	0
3	A	704	PGE	1	0
4	B	706	EDO	1	0
4	A	714	EDO	1	0
4	C	706	EDO	1	0
3	B	703	PGE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	712	EDO	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	216/238 (90%)	0.77	9 (4%)	36	40	31, 49, 85, 130	0
1	B	214/238 (89%)	0.76	11 (5%)	28	30	37, 57, 97, 142	0
1	C	219/238 (92%)	0.60	11 (5%)	28	31	37, 63, 104, 138	0
1	D	199/238 (83%)	1.02	18 (9%)	9	9	42, 66, 116, 153	0
All	All	848/952 (89%)	0.78	49 (5%)	23	24	31, 58, 102, 153	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	445	ASP	8.4
1	D	446	ASP	6.3
1	B	446	ASP	4.9
1	C	528	ASN	4.5
1	D	447	HIS	4.3
1	A	675	ARG	3.7
1	D	603	PRO	3.6
1	D	515	SER	3.3
1	D	451	PHE	3.3
1	B	674	HIS	3.3
1	D	498	LEU	3.2
1	D	517	THR	3.0
1	B	664	TYR	3.0
1	D	564	GLU	3.0
1	A	603	PRO	2.9
1	C	666	LEU	2.9
1	D	671	TYR	2.8
1	B	603	PRO	2.8
1	C	570	MET	2.7
1	C	602	ASP	2.7
1	D	512	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	655	GLU	2.6
1	C	524	ASP	2.6
1	A	586	GLY	2.5
1	B	569	VAL	2.5
1	C	565	LEU	2.4
1	B	646	ASP	2.4
1	C	569	VAL	2.4
1	C	580	MET	2.4
1	D	565	LEU	2.3
1	D	545	VAL	2.3
1	D	582	GLU	2.3
1	A	669	GLN	2.2
1	A	564	GLU	2.2
1	C	548	GLN	2.2
1	B	625	HIS	2.2
1	D	568	GLN	2.2
1	A	548	GLN	2.1
1	B	501	LYS	2.1
1	A	454	VAL	2.1
1	A	498	LEU	2.1
1	D	502	VAL	2.1
1	C	563	LEU	2.1
1	D	621	TRP	2.1
1	B	652	ALA	2.0
1	C	527	PRO	2.0
1	B	570	MET	2.0
1	A	565	LEU	2.0
1	D	505	ILE	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 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
4	EDO	B	705	4/4	0.58	0.62	59,70,75,76	0
4	EDO	A	713	4/4	0.69	0.40	57,68,69,73	0
4	EDO	A	708	4/4	0.71	0.27	60,72,74,76	0
4	EDO	C	707	4/4	0.71	0.35	58,70,73,77	0
4	EDO	A	710	4/4	0.74	0.35	56,67,72,72	0
5	PEG	C	709	7/7	0.74	0.32	59,70,76,77	0
3	PGE	A	704	10/10	0.79	0.28	57,69,73,78	0
3	PGE	C	703	10/10	0.80	0.38	55,66,75,75	0
4	EDO	B	707	4/4	0.80	0.18	58,69,72,73	0
4	EDO	C	708	4/4	0.82	0.42	58,70,76,77	0
3	PGE	B	703	10/10	0.83	0.39	57,68,72,72	0
3	PGE	A	705	10/10	0.83	0.34	53,65,71,71	0
4	EDO	D	704	4/4	0.83	0.54	58,69,74,76	0
4	EDO	A	712	4/4	0.83	0.36	59,71,72,73	0
4	EDO	D	703	4/4	0.84	0.32	55,66,70,74	0
4	EDO	A	709	4/4	0.84	0.42	55,66,72,73	0
4	EDO	C	704	4/4	0.84	0.29	58,69,73,75	0
4	EDO	C	705	4/4	0.85	0.41	50,63,74,76	0
4	EDO	B	706	4/4	0.86	0.27	58,70,72,72	0
3	PGE	A	703	10/10	0.87	0.24	55,68,72,72	0
4	EDO	B	704	4/4	0.87	0.39	54,65,69,69	0
4	EDO	A	707	4/4	0.87	0.29	56,67,70,72	0
5	PEG	A	715	7/7	0.88	0.24	55,66,71,75	0
4	EDO	A	711	4/4	0.89	0.32	56,67,69,70	0
4	EDO	A	706	4/4	0.90	0.27	53,64,68,68	0
4	EDO	B	709	4/4	0.90	0.36	55,66,71,72	0
4	EDO	B	708	4/4	0.91	0.19	60,72,74,80	0
4	EDO	C	706	4/4	0.91	0.55	59,71,73,77	0
4	EDO	A	714	4/4	0.93	0.25	50,60,69,70	0
2	ZN	C	702	1/1	0.98	0.22	58,58,58,58	0
2	ZN	A	701	1/1	0.98	0.24	50,50,50,50	0
2	ZN	A	702	1/1	0.98	0.26	52,52,52,52	0
2	ZN	D	702	1/1	0.99	0.18	75,75,75,75	0
2	ZN	B	702	1/1	0.99	0.29	50,50,50,50	0
2	ZN	C	701	1/1	0.99	0.24	50,50,50,50	0
2	ZN	B	701	1/1	0.99	0.26	50,50,50,50	0
2	ZN	D	701	1/1	0.99	0.17	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.