Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

PDB ID	:	3G58
Title	:	Crystal structure of human phosphodiesterase 4d with d155988/pmnpq
Authors	:	Staker, B.L.
Deposited on	:	2009-02-04
Resolution	:	2.05 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
http://wwpdb.org/validation/2016/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:

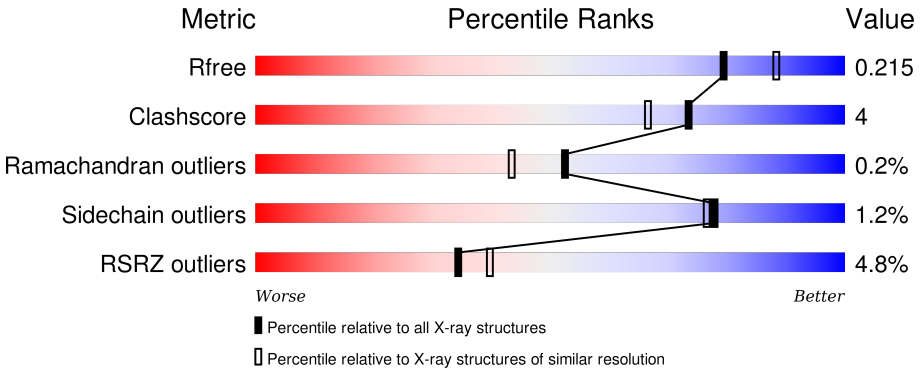
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.05 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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. 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	381	4% 81% 7% • 12%
1	B	381	3% 80% 6% 14%
1	C	381	5% 77% 8% 14%
1	D	381	5% 81% 8% • 9%

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
5	988	A	901	-	-	-	X
6	EDO	A	6	-	-	-	X
6	EDO	B	17	-	-	-	X
6	EDO	C	13	-	-	-	X
6	EDO	C	18	-	-	-	X
6	EDO	D	11	-	-	X	X
6	EDO	D	14	-	-	-	X
6	EDO	D	15	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12091 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2696	1706	461	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2633	1665	448	506	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	345	Total	C	N	O	S	0	0	0
			2786	1765	476	531	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	expression tag	UNP Q08499
A	579	ALA	SER	engineered	UNP Q08499
A	581	ALA	SER	engineered	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	expression tag	UNP Q08499
B	579	ALA	SER	engineered	UNP Q08499
B	581	ALA	SER	engineered	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	expression tag	UNP Q08499
C	579	ALA	SER	engineered	UNP Q08499
C	581	ALA	SER	engineered	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	expression tag	UNP Q08499
D	579	ALA	SER	engineered	UNP Q08499
D	581	ALA	SER	engineered	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

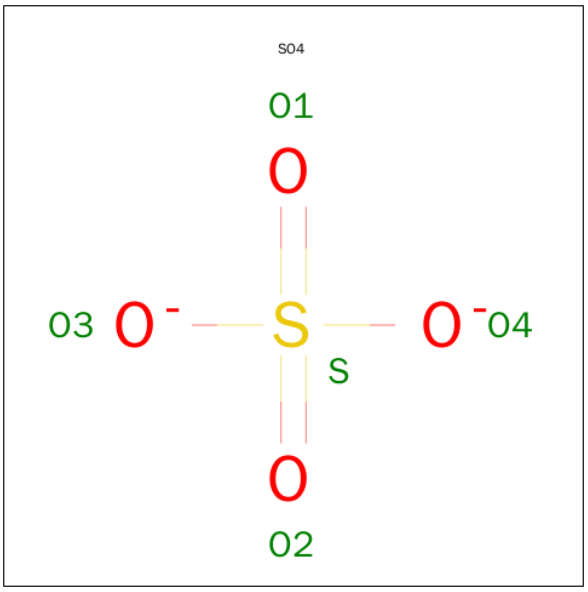
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

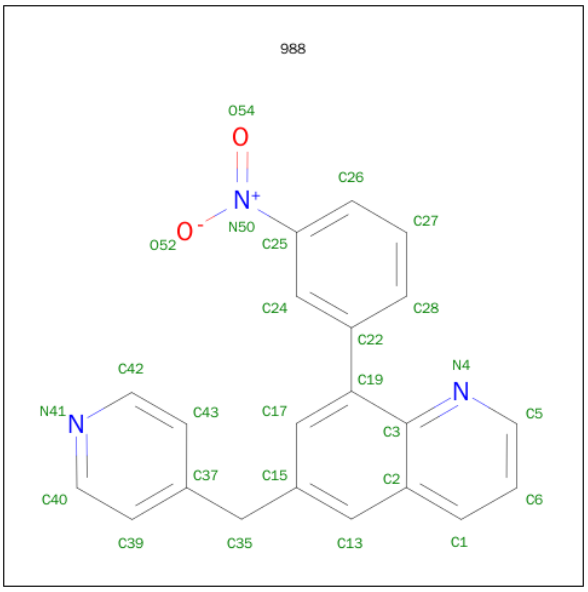
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is 8-(3-NITROPHENYL)-6-(PYRIDIN-4-YLMETHYL)QUINOLINE (three-letter code: 988) (formula: $C_{21}H_{15}N_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 26 21 3 2	0	0
5	B	1	Total C N O 26 21 3 2	0	0

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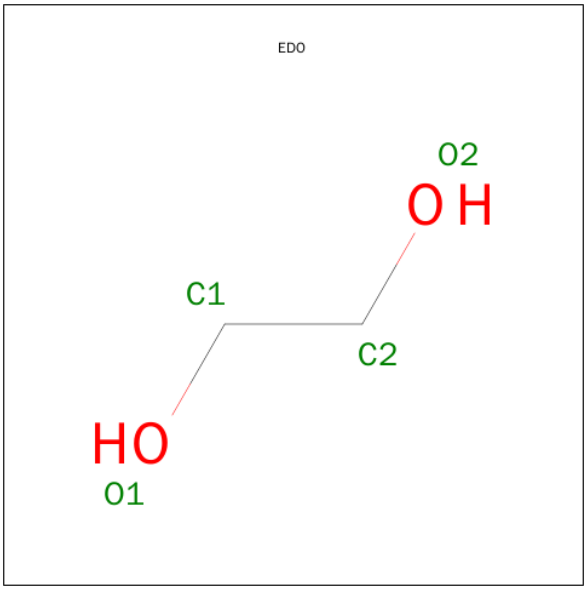
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 26 21 3 2	0	0
5	D	1	Total C N O 26 21 3 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 7 is water.

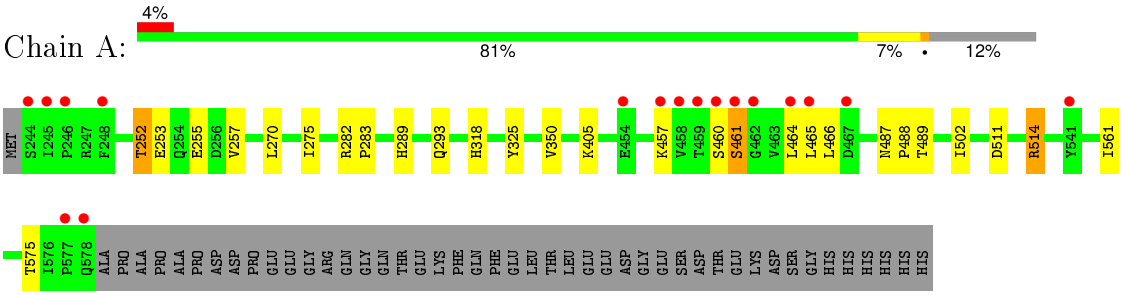
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	294	Total O 294 294	0	0
7	B	284	Total O 284 284	0	0
7	C	259	Total O 259 259	0	0
7	D	307	Total O 307 307	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

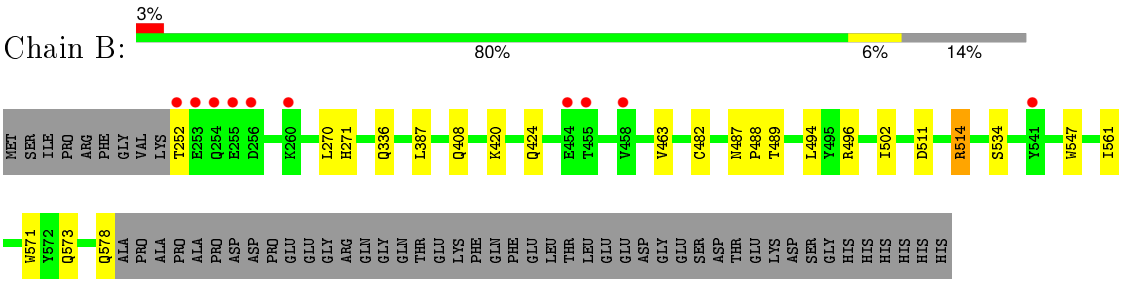
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



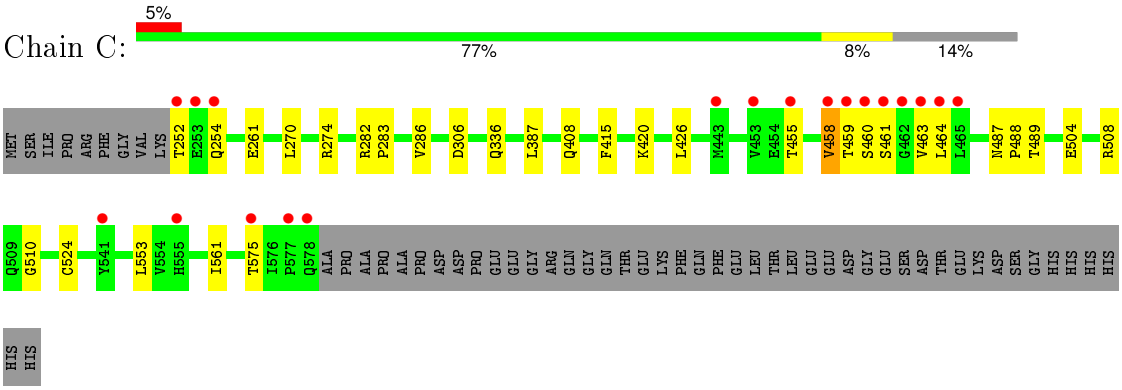
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



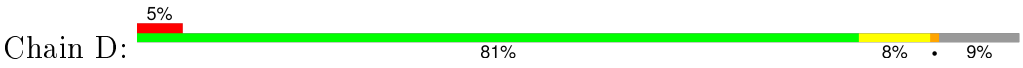
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

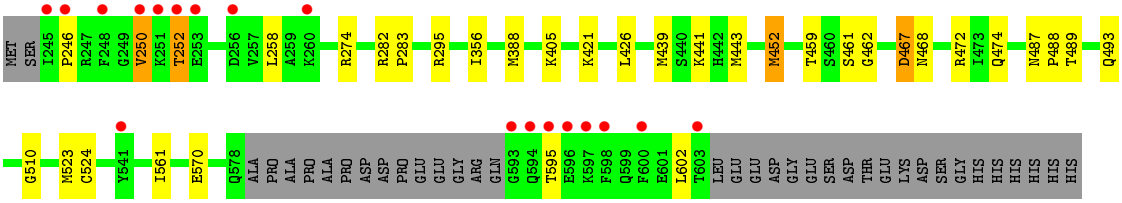
Chain C:



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain D:




MET SER T245 P246 R247 P248 G249 V250 K251 T252 E253 D256 V257 L258 A259 K260 R274 R282 P283 R295 I356 M388 K405 K421 L426 M439 S440 K441 H442 M443 M452 T459 S460 S461 G462 D467 N468 R472 I473 Q474 N487 P488 T489 Q493
G510 M523 C524 Y541 I561 E570 Q578 ALA PRO ALA PRO ALA PRO ASP ASP PRO GLU GLU GLY ARG GLN G593 Q594 T595 E596 K597 F598 Q599 P600 E601 L602 T603 LEU GLU GLU ASP GLY GLU SER ASP THR GLU LYS ASP SER GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.39Å 113.57Å 161.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.05 47.04 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.21-2.05) 89.6 (47.04-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.171 , 0.213 0.174 , 0.215	Depositor DCC
R_{free} test set	5153 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 102527 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12091	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, MG, ZN, 988, 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	0.50	0/2751	0.59	1/3739 (0.0%)
1	B	0.50	0/2687	0.61	2/3654 (0.1%)
1	C	0.50	0/2701	0.59	0/3670
1	D	0.53	0/2843	0.60	0/3859
All	All	0.51	0/10982	0.60	3/14922 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	514	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	514	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	514	ARG	NE-CZ-NH1	6.29	123.45	120.30

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	2696	0	2645	19	0
1	B	2633	0	2573	16	0
1	C	2647	0	2599	22	0
1	D	2786	0	2731	34	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
5	A	26	0	15	0	0
5	B	26	0	15	1	0
5	C	26	0	15	0	0
5	D	26	0	15	0	0
6	A	16	0	24	1	0
6	B	16	0	24	3	0
6	C	16	0	24	0	0
6	D	20	0	30	7	0
7	A	294	0	0	1	1
7	B	284	0	0	4	0
7	C	259	0	0	2	0
7	D	307	0	0	5	0
All	All	12091	0	10710	89	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (89) 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:D:439:MET:HE2	1:D:602:LEU:HD13	1.36	1.07
1:D:439:MET:HE2	1:D:602:LEU:CD1	1.90	1.01
1:D:439:MET:CE	1:D:602:LEU:CD1	2.51	0.89
1:A:575:THR:HG21	7:A:774:HOH:O	1.76	0.85
1:D:356:ILE:HD13	6:D:14:EDO:H22	1.61	0.81
1:D:439:MET:CE	1:D:602:LEU:HD13	2.08	0.80
1:D:493:GLN:HE22	6:D:11:EDO:C1	1.95	0.80
1:C:464:LEU:HD21	1:C:553:LEU:HD11	1.65	0.78
1:D:493:GLN:HE22	6:D:11:EDO:H12	1.46	0.77
1:A:252:THR:HG22	1:A:255:GLU:H	1.51	0.75
1:C:306:ASP:OD2	7:C:1059:HOH:O	2.04	0.75
1:B:271:HIS:HA	6:B:10:EDO:H11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:THR:O	1:D:461:SER:O	2.05	0.73
1:D:472:ARG:CZ	7:D:931:HOH:O	2.39	0.71
1:B:489:THR:HB	1:B:561:ILE:HG23	1.73	0.69
1:D:439:MET:HE2	1:D:602:LEU:HD11	1.77	0.67
1:C:387:LEU:O	1:C:387:LEU:HD23	1.95	0.67
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.27	0.66
1:B:496:ARG:HD3	1:B:571:TRP:CZ3	2.30	0.66
1:D:439:MET:CE	1:D:602:LEU:HD11	2.26	0.65
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.30	0.65
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.31	0.63
1:D:472:ARG:NE	7:D:931:HOH:O	2.31	0.62
1:A:457:LYS:HG2	1:A:465:LEU:HD23	1.84	0.58
1:B:387:LEU:HG	7:B:698:HOH:O	2.04	0.58
1:D:570:GLU:OE1	7:D:849:HOH:O	2.17	0.57
1:A:252:THR:CG2	1:A:255:GLU:H	2.17	0.57
1:A:575:THR:O	1:A:575:THR:HG22	2.07	0.55
1:A:489:THR:HB	1:A:561:ILE:HG23	1.88	0.55
1:B:271:HIS:CA	6:B:10:EDO:H11	2.38	0.54
1:C:489:THR:HB	1:C:561:ILE:HG23	1.90	0.54
1:A:460:SER:O	1:A:461:SER:CB	2.55	0.54
1:D:493:GLN:NE2	6:D:11:EDO:H12	2.18	0.53
1:C:252:THR:N	7:C:1085:HOH:O	2.40	0.53
1:D:523:MET:HE1	1:D:595:THR:HA	1.89	0.53
1:C:387:LEU:HD23	1:C:387:LEU:C	2.29	0.53
1:A:405:LYS:NZ	1:D:405:LYS:NZ	2.57	0.53
1:C:487:ASN:HB2	1:C:488:PRO:HD3	1.92	0.52
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.91	0.52
1:B:496:ARG:HD2	7:B:854:HOH:O	2.09	0.52
1:D:493:GLN:NE2	6:D:11:EDO:C1	2.72	0.49
1:B:494:LEU:HD21	6:B:10:EDO:H12	1.95	0.49
1:C:282:ARG:N	1:C:283:PRO:CD	2.76	0.49
1:C:459:THR:HG23	1:C:461:SER:N	2.27	0.49
1:C:282:ARG:O	1:C:286:VAL:HG22	2.13	0.49
1:D:489:THR:HB	1:D:561:ILE:HG23	1.95	0.48
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.46	0.48
1:C:575:THR:O	1:C:575:THR:HG22	2.14	0.48
1:B:420:LYS:HE2	1:B:424:GLN:HE22	1.79	0.47
1:D:282:ARG:N	1:D:283:PRO:CD	2.78	0.47
1:D:295:ARG:HB3	6:D:14:EDO:H21	1.96	0.47
1:A:487:ASN:HB2	1:A:488:PRO:HD3	1.97	0.46
1:C:459:THR:HG23	1:C:461:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:THR:HG22	1:C:455:THR:O	2.16	0.46
1:A:464:LEU:HD21	1:A:466:LEU:HD21	1.96	0.46
1:C:261:GLU:OE2	1:C:274:ARG:NH1	2.48	0.46
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.98	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.98	0.46
1:D:443:MET:HG2	7:D:767:HOH:O	2.15	0.45
1:C:510:GLY:HA3	1:C:524:CYS:O	2.16	0.45
1:D:510:GLY:HA3	1:D:524:CYS:O	2.16	0.45
1:D:441:LYS:HE2	7:D:741:HOH:O	2.17	0.45
1:A:253:GLU:O	1:A:257:VAL:HG23	2.17	0.44
1:B:482:CYS:HB3	1:B:547:TRP:CZ2	2.52	0.44
1:A:289:HIS:CE1	1:A:293:GLN:HE21	2.36	0.44
1:C:420:LYS:HE2	1:C:420:LYS:HB2	1.87	0.44
1:D:439:MET:HE1	1:D:602:LEU:HD11	1.99	0.44
1:D:523:MET:CE	1:D:595:THR:HA	2.48	0.44
1:B:408:GLN:OE1	1:C:408:GLN:OE1	2.35	0.44
1:A:270:LEU:HD11	1:A:275:ILE:CD1	2.48	0.43
1:B:534:SER:HB3	5:B:902:988:H26	2.01	0.43
1:A:325:TYR:CG	1:A:502:ILE:HD13	2.54	0.43
1:B:487:ASN:HB2	1:B:488:PRO:HD3	2.00	0.43
1:A:350:VAL:HG11	1:A:466:LEU:HD12	2.01	0.43
1:D:252:THR:HG21	1:D:258:LEU:HD23	2.01	0.42
1:A:318:HIS:HE1	6:A:6:EDO:C1	2.32	0.42
1:D:467:ASP:HB3	1:D:468:ASN:HD22	1.83	0.42
1:C:459:THR:HG22	1:C:463:VAL:H	1.84	0.42
1:D:459:THR:C	1:D:461:SER:O	2.58	0.42
1:C:415:PHE:CE1	1:C:426:LEU:HD21	2.54	0.42
1:D:388:MET:HE2	1:D:388:MET:HA	2.02	0.42
1:D:452:MET:HE3	1:D:474:GLN:NE2	2.35	0.41
1:C:458:VAL:HG13	1:C:459:THR:O	2.20	0.41
1:A:282:ARG:N	1:A:283:PRO:CD	2.83	0.41
1:D:295:ARG:HH11	6:D:14:EDO:H11	1.86	0.41
1:D:487:ASN:HB2	1:D:488:PRO:HD3	2.01	0.41
1:B:252:THR:HG22	7:B:951:HOH:O	2.21	0.40
1:D:467:ASP:CB	1:D:468:ASN:HD22	2.34	0.40
7:B:134:HOH:O	1:D:250:VAL:HG22	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:GLY:N	7:A:695:HOH:O[4_455]	2.02	0.18

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	333/381 (87%)	325 (98%)	7 (2%)	1 (0%)	46 36
1	B	325/381 (85%)	319 (98%)	6 (2%)	0	100 100
1	C	325/381 (85%)	316 (97%)	9 (3%)	0	100 100
1	D	341/381 (90%)	326 (96%)	14 (4%)	1 (0%)	46 36
All	All	1324/1524 (87%)	1286 (97%)	36 (3%)	2 (0%)	52 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	246	PRO
1	A	461	SER

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	302/345 (88%)	301 (100%)	1 (0%)	94 95
1	B	296/345 (86%)	292 (99%)	4 (1%)	74 72
1	C	299/345 (87%)	296 (99%)	3 (1%)	82 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	312/345 (90%)	305 (98%)	7 (2%)	60 53
All	All	1209/1380 (88%)	1194 (99%)	15 (1%)	78 76

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

Mol	Chain	Res	Type
1	A	252	THR
1	B	463	VAL
1	B	502	ILE
1	B	573	GLN
1	B	578	GLN
1	C	254	GLN
1	C	458	VAL
1	C	460	SER
1	D	250	VAL
1	D	252	THR
1	D	274	ARG
1	D	421	LYS
1	D	426	LEU
1	D	452	MET
1	D	467	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	493	GLN
1	B	289	HIS
1	B	424	GLN
1	B	474	GLN
1	B	555	HIS
1	B	573	GLN
1	C	254	GLN
1	C	289	HIS
1	C	559	GLN
1	D	254	GLN
1	D	289	HIS
1	D	293	GLN
1	D	474	GLN
1	D	493	GLN
1	D	599	GLN

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

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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	SO4	A	1	-	4,4,4	0.48	0	6,6,6	0.61	0
6	EDO	A	12	-	3,3,3	0.49	0	2,2,2	0.21	0
6	EDO	A	6	-	3,3,3	0.39	0	2,2,2	0.38	0
6	EDO	A	7	-	3,3,3	0.48	0	2,2,2	0.34	0
6	EDO	A	9	-	3,3,3	0.46	0	2,2,2	0.44	0
5	988	A	901	-	27,29,29	2.11	3 (11%)	37,40,40	1.90	11 (29%)
6	EDO	B	10	-	3,3,3	0.28	0	2,2,2	0.63	0
6	EDO	B	17	-	3,3,3	0.51	0	2,2,2	0.42	0
6	EDO	B	3	-	3,3,3	0.45	0	2,2,2	0.50	0
6	EDO	B	8	-	3,3,3	0.42	0	2,2,2	0.39	0
5	988	B	902	-	27,29,29	2.11	3 (11%)	37,40,40	1.59	8 (21%)
6	EDO	C	13	-	3,3,3	0.31	0	2,2,2	0.65	0
6	EDO	C	16	-	3,3,3	0.52	0	2,2,2	0.32	0
6	EDO	C	18	-	3,3,3	0.40	0	2,2,2	0.38	0
6	EDO	C	5	-	3,3,3	0.46	0	2,2,2	0.28	0
5	988	C	903	-	27,29,29	1.98	3 (11%)	37,40,40	1.74	8 (21%)
6	EDO	D	11	-	3,3,3	0.22	0	2,2,2	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	D	14	-	3,3,3	0.55	0	2,2,2	0.21	0
6	EDO	D	15	-	3,3,3	0.43	0	2,2,2	0.58	0
6	EDO	D	2	-	3,3,3	0.49	0	2,2,2	0.24	0
6	EDO	D	4	-	3,3,3	0.44	0	2,2,2	0.59	0
5	988	D	904	-	27,29,29	2.15	3 (11%)	37,40,40	1.79	6 (16%)

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
6	EDO	A	12	-	-	0/1/1/1	0/0/0/0
6	EDO	A	6	-	-	0/1/1/1	0/0/0/0
6	EDO	A	7	-	-	0/1/1/1	0/0/0/0
6	EDO	A	9	-	-	0/1/1/1	0/0/0/0
5	988	A	901	-	-	0/12/12/12	0/4/4/4
6	EDO	B	10	-	-	0/1/1/1	0/0/0/0
6	EDO	B	17	-	-	0/1/1/1	0/0/0/0
6	EDO	B	3	-	-	0/1/1/1	0/0/0/0
6	EDO	B	8	-	-	0/1/1/1	0/0/0/0
5	988	B	902	-	-	0/12/12/12	0/4/4/4
6	EDO	C	13	-	-	0/1/1/1	0/0/0/0
6	EDO	C	16	-	-	0/1/1/1	0/0/0/0
6	EDO	C	18	-	-	0/1/1/1	0/0/0/0
6	EDO	C	5	-	-	0/1/1/1	0/0/0/0
5	988	C	903	-	-	0/12/12/12	0/4/4/4
6	EDO	D	11	-	-	0/1/1/1	0/0/0/0
6	EDO	D	14	-	-	0/1/1/1	0/0/0/0
6	EDO	D	15	-	-	0/1/1/1	0/0/0/0
6	EDO	D	2	-	-	0/1/1/1	0/0/0/0
6	EDO	D	4	-	-	0/1/1/1	0/0/0/0
5	988	D	904	-	-	0/12/12/12	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	988	C2-C3	3.88	1.47	1.42
5	A	901	988	C2-C3	4.12	1.48	1.42
5	C	903	988	C19-C3	4.16	1.48	1.43
5	B	902	988	C2-C3	4.26	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	988	C19-C3	4.28	1.49	1.43
5	A	901	988	C19-C3	4.33	1.49	1.43
5	D	904	988	C19-C3	4.48	1.49	1.43
5	D	904	988	C2-C3	4.67	1.49	1.42
5	C	903	988	O54-N50	7.82	1.38	1.22
5	B	902	988	O54-N50	8.29	1.39	1.22
5	A	901	988	O54-N50	8.36	1.39	1.22
5	D	904	988	O54-N50	8.37	1.39	1.22

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	901	988	C19-C3-C2	-5.70	116.57	119.28
5	C	903	988	C19-C3-C2	-5.18	116.82	119.28
5	D	904	988	C19-C3-C2	-5.14	116.84	119.28
5	B	902	988	C19-C3-C2	-4.23	117.27	119.28
5	D	904	988	C2-C3-N4	-2.67	119.39	122.50
5	C	903	988	C35-C15-C13	-2.51	117.52	123.46
5	A	901	988	C28-C22-C19	-2.25	117.22	120.87
5	B	902	988	C2-C3-N4	-2.20	119.94	122.50
5	C	903	988	C2-C3-N4	-2.14	120.02	122.50
5	A	901	988	C43-C42-N41	-2.13	119.94	123.64
5	C	903	988	C22-C19-C3	-2.09	119.36	122.68
5	B	902	988	C43-C42-N41	-2.08	120.02	123.64
5	A	901	988	C39-C40-N41	-2.08	120.03	123.64
5	A	901	988	C22-C19-C3	-2.05	119.43	122.68
5	B	902	988	C35-C15-C13	-2.02	118.66	123.46
5	B	902	988	C24-C25-N50	2.08	120.63	118.80
5	D	904	988	C13-C15-C17	2.09	120.74	118.55
5	C	903	988	C13-C15-C17	2.15	120.80	118.55
5	A	901	988	C13-C15-C17	2.19	120.84	118.55
5	A	901	988	C42-N41-C40	2.22	122.19	116.83
5	D	904	988	C26-C25-N50	2.50	121.50	119.48
5	B	902	988	C13-C15-C17	2.50	121.17	118.55
5	C	903	988	C5-N4-C3	2.60	120.45	117.37
5	A	901	988	C28-C22-C24	2.71	121.77	118.17
5	B	902	988	C5-N4-C3	2.77	120.65	117.37
5	A	901	988	C5-N4-C3	2.92	120.83	117.37
5	C	903	988	C24-C25-N50	3.18	121.59	118.80
5	D	904	988	C5-N4-C3	3.63	121.68	117.37
5	A	901	988	C24-C25-N50	3.97	122.29	118.80
5	B	902	988	C19-C3-N4	4.27	122.79	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	903	988	C19-C3-N4	4.66	123.16	118.76
5	A	901	988	C19-C3-N4	4.70	123.20	118.76
5	D	904	988	C19-C3-N4	5.30	123.76	118.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6	EDO	1	0
6	B	10	EDO	3	0
5	B	902	988	1	0
6	D	11	EDO	4	0
6	D	14	EDO	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	335/381 (87%)	0.25	17 (5%)	32	36	15, 24, 57, 67	0
1	B	327/381 (85%)	0.05	10 (3%)	52	60	16, 27, 43, 75	0
1	C	327/381 (85%)	0.14	19 (5%)	26	30	15, 26, 58, 69	0
1	D	345/381 (90%)	0.09	18 (5%)	31	36	15, 25, 60, 66	0
All	All	1334/1524 (87%)	0.13	64 (4%)	34	40	15, 26, 54, 75	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	600	PHE	8.4
1	B	252	THR	8.2
1	A	578	GLN	6.9
1	A	461	SER	6.5
1	C	462	GLY	5.9
1	B	253	GLU	5.8
1	D	245	ILE	5.7
1	C	460	SER	5.6
1	D	593	GLY	5.4
1	A	458	VAL	5.4
1	C	461	SER	5.1
1	A	462	GLY	4.9
1	A	577	PRO	4.9
1	C	458	VAL	4.8
1	D	595	THR	4.7
1	D	250	VAL	4.6
1	D	252	THR	4.5
1	B	254	GLN	4.4
1	A	460	SER	4.4
1	A	459	THR	4.2
1	D	246	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	253	GLU	4.1
1	C	541	TYR	4.1
1	A	465	LEU	4.1
1	A	244	SER	4.0
1	D	541	TYR	4.0
1	D	597	LYS	3.8
1	D	251	LYS	3.7
1	C	463	VAL	3.6
1	C	459	THR	3.6
1	A	467	ASP	3.5
1	A	541	TYR	3.5
1	C	253	GLU	3.5
1	A	457	LYS	3.4
1	C	578	GLN	3.3
1	A	246	PRO	3.3
1	C	254	GLN	3.3
1	D	248	PHE	3.2
1	C	577	PRO	3.2
1	D	256	ASP	3.1
1	D	594	GLN	3.1
1	B	255	GLU	3.1
1	C	453	VAL	3.0
1	D	598	PHE	3.0
1	D	260	LYS	2.9
1	B	541	TYR	2.9
1	B	256	ASP	2.8
1	D	603	THR	2.8
1	C	464	LEU	2.7
1	B	455	THR	2.7
1	C	575	THR	2.7
1	C	455	THR	2.6
1	C	465	LEU	2.5
1	C	555	HIS	2.4
1	A	454	GLU	2.4
1	A	464	LEU	2.4
1	B	454	GLU	2.3
1	B	458	VAL	2.2
1	D	596	GLU	2.2
1	B	260	LYS	2.1
1	C	252	THR	2.1
1	A	248	PHE	2.1
1	A	245	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	443	MET	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	EDO	A	6	4/4	0.88	0.30	19.70	44,44,44,46	0
6	EDO	D	14	4/4	0.81	0.33	8.85	38,38,40,42	0
6	EDO	D	15	4/4	0.92	0.14	4.53	40,41,41,42	0
6	EDO	C	13	4/4	0.90	0.22	3.47	19,29,32,37	0
6	EDO	C	18	4/4	0.93	0.19	2.74	49,49,50,50	0
5	988	A	901	26/26	0.92	0.18	2.31	30,35,40,40	0
6	EDO	D	11	4/4	0.89	0.22	2.28	23,30,35,40	0
6	EDO	B	17	4/4	0.89	0.18	2.27	40,40,41,41	0
6	EDO	B	3	4/4	0.96	0.19	1.96	32,33,33,35	0
4	SO4	A	1	5/5	0.96	0.17	1.90	38,43,47,48	0
6	EDO	D	2	4/4	0.97	0.13	1.84	24,24,25,25	0
5	988	C	903	26/26	0.93	0.17	1.73	25,31,35,37	0
6	EDO	A	7	4/4	0.97	0.17	1.72	28,32,33,35	0
6	EDO	B	10	4/4	0.89	0.22	1.32	31,34,38,41	0
5	988	B	902	26/26	0.92	0.14	1.21	33,36,39,41	0
6	EDO	D	4	4/4	0.87	0.22	1.17	42,43,44,44	0
6	EDO	C	5	4/4	0.95	0.16	0.63	27,29,29,30	0
6	EDO	A	9	4/4	0.96	0.13	0.55	37,37,37,39	0
6	EDO	B	8	4/4	0.96	0.11	0.08	25,26,27,28	0
6	EDO	C	16	4/4	0.97	0.10	-0.50	27,27,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	988	D	904	26/26	0.96	0.10	-0.59	23,27,32,36	0
6	EDO	A	12	4/4	0.98	0.12	-1.36	24,27,29,30	0
3	MG	B	625	1/1	0.98	0.09	-1.75	22,22,22,22	0
3	MG	C	625	1/1	0.98	0.07	-2.56	24,24,24,24	0
3	MG	D	625	1/1	0.98	0.09	-2.77	22,22,22,22	0
3	MG	A	625	1/1	0.99	0.06	-3.46	22,22,22,22	0
2	ZN	A	624	1/1	1.00	0.04	-4.80	33,33,33,33	0
2	ZN	B	624	1/1	0.99	0.03	-5.98	34,34,34,34	0
2	ZN	D	624	1/1	1.00	0.04	-6.15	32,32,32,32	0
2	ZN	C	624	1/1	1.00	0.03	-8.86	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.