



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:21 am GMT

PDB ID : 5HCC
Title : Ternary complex of human Complement C5 with Ornithodoros moubata OmCI and Dermacentor andersoni RaCI3.
Authors : Jore, M.M.; Johnson, S.; Lea, S.M.
Deposited on : 2016-01-04
Resolution : 2.59 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

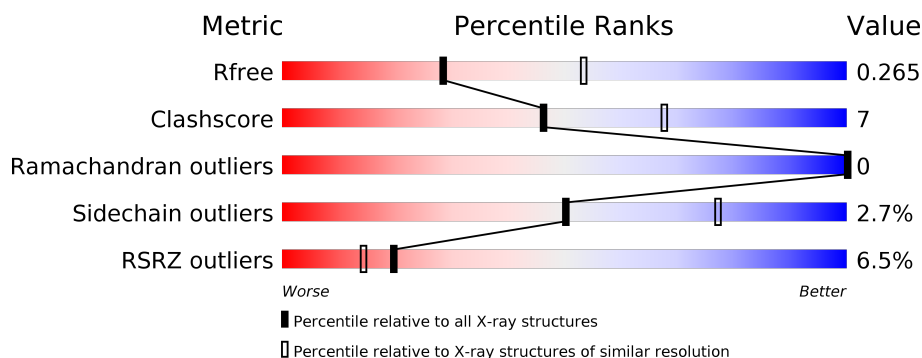
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 $\leq 5\%$. 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	B	656	<div> <div>4%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
2	A	998	<div> <div>8%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
3	C	165	<div> <div>4%</div> <div>80%</div> <div>9%</div> <div>10%</div> </div>
4	D	81	<div> <div>%</div> <div>46%</div> <div>11%</div> <div>42%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	2003	-	-	-	X
5	EDO	A	2005	-	-	-	X
5	EDO	B	701	-	-	-	X
5	EDO	C	201	-	-	-	X
8	DIO	A	2007	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14646 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	647	Total	C	N	O	S	0	0	0
			5116	3281	819	1003	13			

- Molecule 2 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	982	Total	C	N	O	S	0	0	0
			7776	4973	1298	1464	41			

- Molecule 3 is a protein called Complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1160	715	195	239	11			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	initiating methionine	UNP Q5YD59
C	5	ALA	-	expression tag	UNP Q5YD59
C	6	SER	-	expression tag	UNP Q5YD59
C	7	HIS	-	expression tag	UNP Q5YD59
C	8	HIS	-	expression tag	UNP Q5YD59
C	9	HIS	-	expression tag	UNP Q5YD59
C	10	HIS	-	expression tag	UNP Q5YD59
C	11	HIS	-	expression tag	UNP Q5YD59
C	12	HIS	-	expression tag	UNP Q5YD59
C	13	HIS	-	expression tag	UNP Q5YD59
C	14	HIS	-	expression tag	UNP Q5YD59
C	15	HIS	-	expression tag	UNP Q5YD59
C	16	HIS	-	expression tag	UNP Q5YD59
C	17	SER	-	expression tag	UNP Q5YD59

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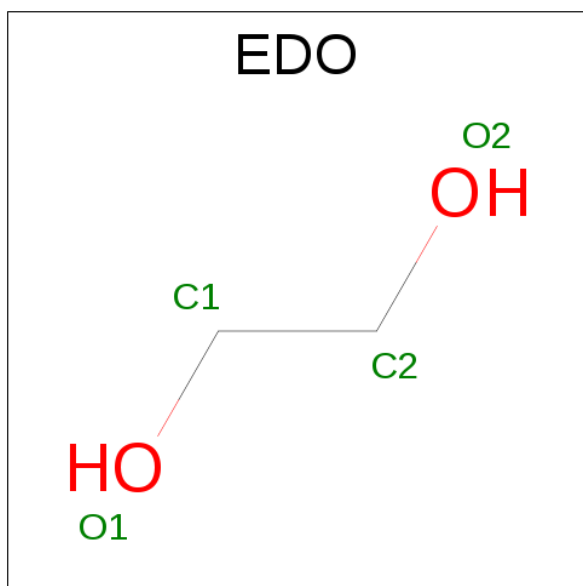
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP Q5YD59
C	78	GLN	ASN	engineered mutation	UNP Q5YD59
C	102	GLN	ASN	engineered mutation	UNP Q5YD59

- Molecule 4 is a protein called Dermacentor andersoni RaCI3.

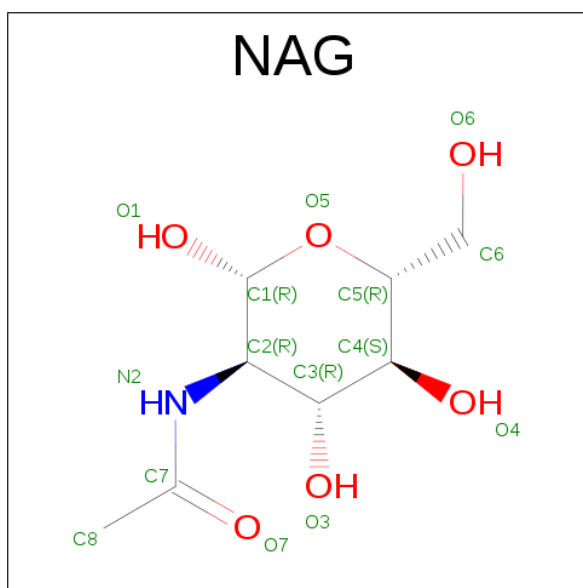
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	47	Total	C	N	O	S	0	0	0
			351	210	65	69	7			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



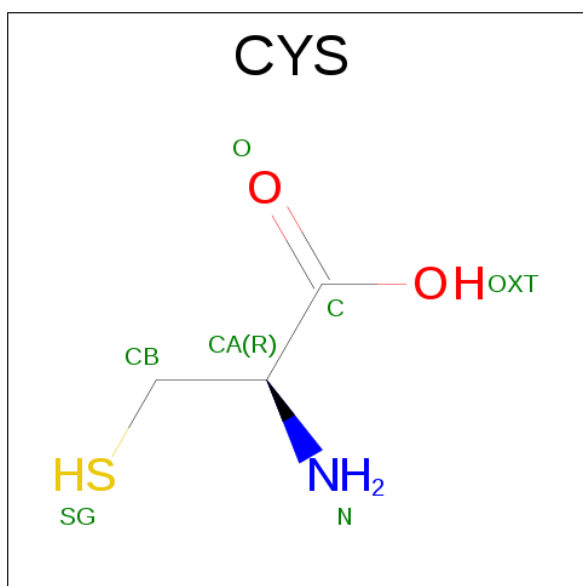
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



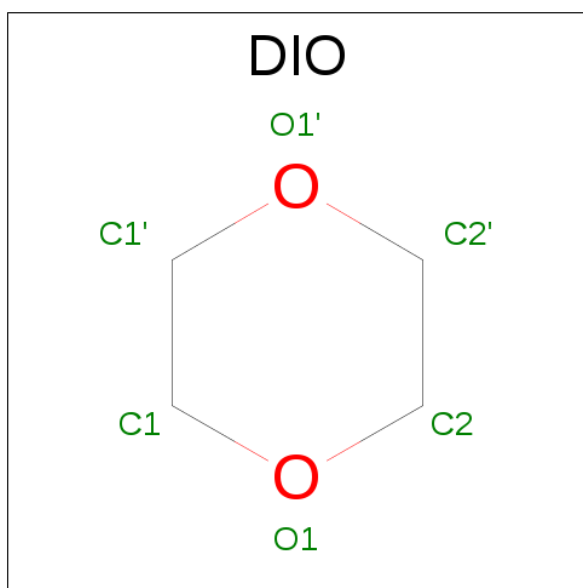
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

- Molecule 8 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	62	Total	O	0	0
			62	62		
9	A	105	Total	O	0	0
			105	105		
9	C	3	Total	O	0	0
			3	3		
9	D	5	Total	O	0	0
			5	5		

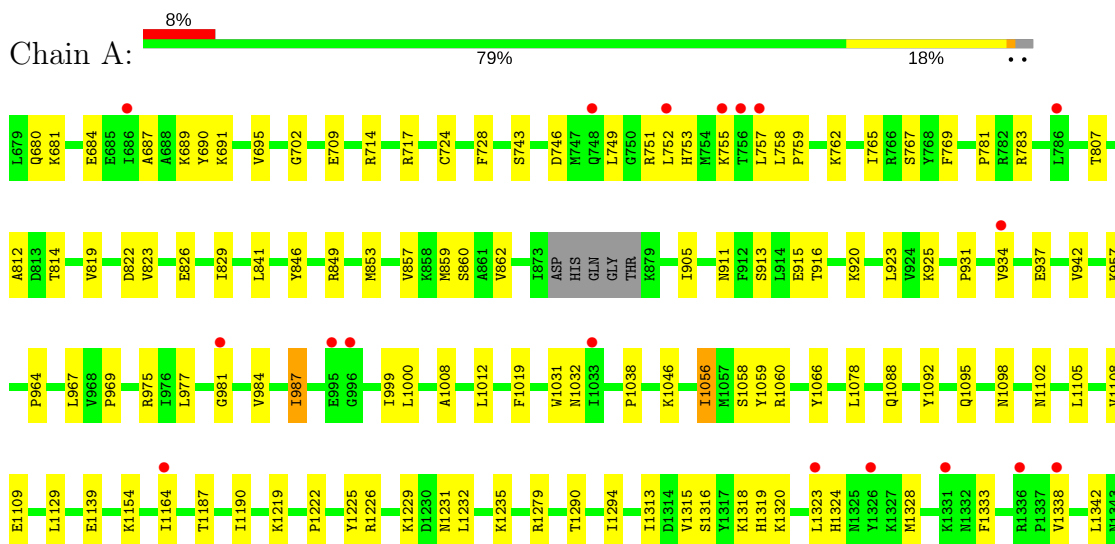
3 Residue-property plots

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.

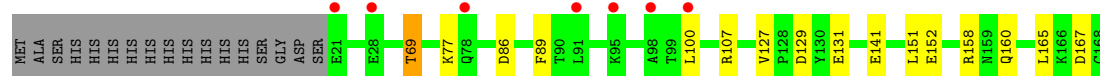
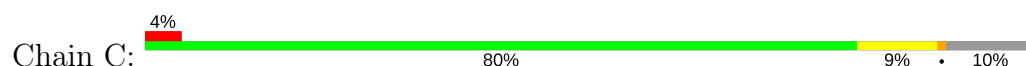
• Molecule 1: Complement C5



• Molecule 2: Complement C5



- Molecule 3: Complement inhibitor



- Molecule 4: Dermacentor andersoni RaCI3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.87Å 140.28Å 211.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.57 – 2.59 93.93 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (66.57-2.59) 99.4 (93.93-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.231 , 0.267 0.228 , 0.265	Depositor DCC
R_{free} test set	4814 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14646	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, NAG, 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	B	0.27	0/5234	0.47	0/7119
2	A	0.29	0/7933	0.47	1/10740 (0.0%)
3	C	0.25	0/1183	0.44	0/1599
4	D	0.28	0/355	0.50	0/480
All	All	0.28	0/14705	0.47	1/19938 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1515	LYS	N-CA-C	-5.24	96.84	111.00

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	B	5116	0	5022	82	0
2	A	7776	0	7822	117	0
3	C	1160	0	1085	8	0
4	D	351	0	332	6	0
5	A	12	0	18	3	0
5	B	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	6	0	0
5	D	4	0	6	0	0
6	A	28	0	25	0	0
7	A	6	0	3	0	0
8	A	6	0	8	3	0
9	A	105	0	0	2	0
9	B	62	0	0	1	0
9	C	3	0	0	0	0
9	D	5	0	0	0	0
All	All	14646	0	14339	206	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 (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1515:LYS:HG2	2:A:1516:ILE:HA	1.61	0.82
2:A:1515:LYS:HE3	2:A:1516:ILE:HG23	1.60	0.81
1:B:373:VAL:HG21	1:B:388:VAL:HG11	1.64	0.78
1:B:469:TRP:HA	1:B:484:ILE:HA	1.67	0.77
3:C:77:LYS:NZ	3:C:167:ASP:O	2.22	0.72
1:B:359:THR:HG21	1:B:372:LYS:H	1.55	0.71
2:A:1576:LYS:HE2	2:A:1601:ILE:HD11	1.73	0.71
2:A:942:VAL:HG21	2:A:957:LYS:HG2	1.72	0.71
2:A:1625:LEU:HB2	2:A:1636:ILE:HG23	1.72	0.70
2:A:1556:GLU:HB3	2:A:1622:LYS:HE2	1.73	0.69
1:B:384:GLY:HA3	1:B:413:VAL:HG23	1.75	0.68
1:B:487:THR:HG22	1:B:523:TYR:HB3	1.75	0.68
1:B:268:THR:HG22	1:B:287:MET:HG2	1.75	0.67
1:B:655:THR:HG22	1:B:657:ALA:H	1.58	0.66
2:A:751:ARG:O	2:A:755:LYS:HB2	1.96	0.65
2:A:1517:GLN:NE2	2:A:1604:VAL:O	2.27	0.65
2:A:695:VAL:HG21	2:A:724:CYS:HA	1.77	0.65
1:B:251:LYS:HG2	1:B:296:ILE:HG12	1.78	0.65
3:C:107:ARG:NH1	3:C:131:GLU:OE1	2.30	0.64
2:A:1612:VAL:HB	2:A:1615:ARG:HD2	1.80	0.64
2:A:1532:CYS:HA	2:A:1640:ASP:HA	1.78	0.63
2:A:1226:ARG:NH1	3:C:141:GLU:OE1	2.31	0.63
2:A:1370:THR:HG21	2:A:1506:THR:HB	1.80	0.62
2:A:975:ARG:NH2	2:A:1344:ASP:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASN:O	2:A:1058:SER:OG	2.14	0.62
1:B:25:ILE:O	1:B:653:PHE:HA	1.98	0.62
2:A:1060:ARG:NH1	5:A:2003:EDO:O1	2.31	0.62
1:B:72:HIS:O	1:B:77:ASN:ND2	2.34	0.60
2:A:1432:ILE:HG13	2:A:1511:THR:HG21	1.83	0.60
1:B:386:VAL:H	1:B:411:THR:HB	1.67	0.60
2:A:934:VAL:HG23	2:A:1508:PHE:CZ	2.38	0.59
2:A:905:ILE:HD13	2:A:931:PRO:HG3	1.85	0.58
2:A:749:LEU:HD23	2:A:752:LEU:HD12	1.86	0.57
2:A:1154:LYS:NZ	8:A:2007:DIO:H12	2.19	0.57
2:A:857:VAL:HA	2:A:913:SER:O	2.03	0.57
3:C:129:ASP:OD1	3:C:158:ARG:NH2	2.37	0.57
2:A:1544:SER:O	2:A:1546:GLU:N	2.33	0.57
1:B:569:ASN:ND2	1:B:598:SER:HB2	2.20	0.56
2:A:1622:LYS:HE3	2:A:1642:LEU:HD23	1.86	0.56
1:B:414:ASP:OD1	1:B:414:ASP:N	2.39	0.56
1:B:444:GLU:O	1:B:449:ARG:NH2	2.39	0.56
2:A:977:LEU:HD21	2:A:1315:VAL:HG11	1.89	0.55
1:B:104:LEU:O	1:B:114:SER:HA	2.07	0.55
1:B:503:ILE:HB	1:B:511:HIS:HB2	1.89	0.55
1:B:38:ASN:ND2	1:B:82:SER:OG	2.31	0.55
1:B:165:ASP:OD2	1:B:195:ARG:NH1	2.36	0.54
2:A:934:VAL:HG22	2:A:1492:THR:HG21	1.89	0.54
1:B:132:LYS:HD2	1:B:609:VAL:HG11	1.88	0.54
2:A:1012:LEU:HD21	2:A:1056:ILE:HD12	1.90	0.54
2:A:743:SER:OG	2:A:746:ASP:OD1	2.20	0.54
2:A:1129:LEU:HD13	2:A:1139:GLU:HB3	1.89	0.54
2:A:1320:LYS:HG2	2:A:1342:LEU:HD13	1.88	0.53
1:B:204:LYS:NZ	4:D:28:GLU:OE1	2.33	0.53
1:B:38:ASN:HD21	1:B:82:SER:HG	1.53	0.53
2:A:1548:ARG:HH11	2:A:1644:TRP:HH2	1.57	0.53
2:A:822:ASP:HB2	2:A:849:ARG:HG3	1.90	0.53
2:A:823:VAL:HA	2:A:846:TYR:O	2.09	0.53
1:B:22:THR:HA	1:B:656:ASN:HD21	1.73	0.53
4:D:21:ARG:HD3	4:D:29:ARG:HE	1.74	0.53
2:A:1219:LYS:HB2	2:A:1225:TYR:HB2	1.90	0.52
1:B:412:ARG:N	1:B:417:VAL:O	2.35	0.52
2:A:1516:ILE:HG22	2:A:1517:GLN:H	1.75	0.52
2:A:1315:VAL:HG12	2:A:1348:VAL:HG22	1.92	0.52
2:A:1066:TYR:HB3	2:A:1078:LEU:HD23	1.91	0.51
1:B:273:GLU:OE2	1:B:321:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1548:ARG:NH1	2:A:1646:GLU:OE1	2.43	0.51
1:B:463:SER:HA	1:B:490:SER:HB2	1.93	0.51
1:B:469:TRP:HZ3	1:B:559:VAL:HB	1.75	0.51
2:A:1095:GLN:OE1	5:A:2005:EDO:O1	2.28	0.51
1:B:352:TYR:HE1	1:B:383:VAL:HG11	1.76	0.50
1:B:364:LYS:HB3	1:B:367:ILE:HD13	1.93	0.50
2:A:1187:THR:HA	2:A:1190:ILE:HG22	1.91	0.50
2:A:1290:THR:O	2:A:1294:ILE:HG12	2.10	0.50
2:A:975:ARG:HA	2:A:1362:THR:O	2.12	0.50
2:A:969:PRO:HG3	2:A:1601:ILE:HG21	1.94	0.50
1:B:476:LEU:HB2	1:B:563:ILE:HG12	1.94	0.50
1:B:417:VAL:HG21	1:B:473:HIS:CD2	2.47	0.50
1:B:547:THR:OG1	1:B:548:GLY:N	2.45	0.50
2:A:1324:HIS:HE1	2:A:1338:VAL:HG11	1.76	0.50
1:B:573:VAL:HG12	1:B:592:MET:HG2	1.94	0.50
1:B:80:GLN:NE2	1:B:514:THR:OG1	2.45	0.50
1:B:451:GLY:O	1:B:674:ARG:NH2	2.45	0.49
2:A:1019:PHE:CZ	2:A:1088:GLN:HB3	2.46	0.49
1:B:395:ILE:HG12	1:B:401:THR:HG22	1.94	0.49
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.94	0.49
2:A:987:ILE:HD13	2:A:1294:ILE:HG23	1.94	0.49
1:B:503:ILE:HG12	1:B:540:LEU:HD13	1.93	0.49
2:A:1618:LEU:O	2:A:1645:ILE:HA	2.13	0.49
2:A:942:VAL:CG2	2:A:957:LYS:HG2	2.40	0.49
1:B:539:ARG:NH2	1:B:635:GLY:O	2.46	0.49
2:A:841:LEU:HD12	2:A:859:MET:HE1	1.95	0.49
1:B:469:TRP:CD1	1:B:482:LEU:HD11	2.48	0.49
1:B:498:HIS:CE1	1:B:516:GLU:HG2	2.48	0.49
2:A:714:ARG:HA	2:A:717:ARG:HH21	1.78	0.48
1:B:29:LYS:HD2	1:B:652:THR:HG23	1.95	0.48
3:C:152:GLU:HG2	3:C:160:GLN:HE22	1.78	0.48
2:A:1598:ILE:HD12	2:A:1637:TYR:HE1	1.77	0.48
1:B:221:GLU:OE1	2:A:762:LYS:NZ	2.44	0.48
2:A:1567:SER:HB2	2:A:1578:LYS:HD2	1.94	0.48
2:A:1450:PHE:CZ	2:A:1475:VAL:HB	2.48	0.48
2:A:1316:SER:HA	2:A:1323:LEU:H	1.78	0.48
2:A:1154:LYS:HZ2	8:A:2007:DIO:H12	1.78	0.48
2:A:1031:TRP:HB3	2:A:1038:PRO:HB3	1.95	0.48
2:A:1576:LYS:HG2	2:A:1601:ILE:HG12	1.96	0.47
2:A:1535:MET:HG3	2:A:1645:ILE:HD11	1.96	0.47
1:B:359:THR:HG21	1:B:372:LYS:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:SER:OG	1:B:491:PRO:O	2.17	0.47
2:A:681:LYS:HA	2:A:684:GLU:HB2	1.96	0.47
2:A:829:ILE:HG13	2:A:925:LYS:HG2	1.96	0.47
2:A:981:GLY:HA3	2:A:1333:PHE:HB2	1.96	0.47
1:B:318:LEU:HA	1:B:321:LYS:HG3	1.96	0.47
2:A:1108:VAL:HG21	2:A:1164:ILE:HG22	1.97	0.47
2:A:1235:LYS:NZ	2:A:1413:GLU:OE1	2.45	0.47
2:A:915:GLU:HG2	2:A:920:LYS:HG3	1.95	0.47
2:A:1652:THR:HG22	2:A:1658:GLN:HB2	1.97	0.47
2:A:1222:PRO:HG2	3:C:165:LEU:HD11	1.97	0.47
2:A:823:VAL:HG21	2:A:853:MET:SD	2.55	0.47
2:A:1032:ASN:N	2:A:1032:ASN:OD1	2.48	0.46
1:B:180:ILE:HG13	1:B:182:ILE:H	1.79	0.46
2:A:751:ARG:O	2:A:755:LYS:CB	2.63	0.46
1:B:160:VAL:HG22	1:B:175:GLU:HB3	1.96	0.46
1:B:25:ILE:HB	1:B:654:LEU:HB2	1.97	0.46
1:B:331:GLU:OE2	1:B:333:THR:OG1	2.27	0.46
1:B:383:VAL:O	1:B:411:THR:HG21	2.15	0.46
2:A:984:VAL:HG23	2:A:987:ILE:HD12	1.98	0.46
1:B:571:LEU:HG	2:A:812:ALA:HB2	1.98	0.46
4:D:42:ILE:HG22	4:D:44:GLU:H	1.80	0.46
1:B:540:LEU:O	1:B:558:SER:HA	2.16	0.45
1:B:354:LEU:HD23	1:B:435:VAL:HG23	1.97	0.45
1:B:59:TYR:HA	1:B:60:PRO:HA	1.79	0.45
1:B:115:LYS:HB2	1:B:654:LEU:HD21	1.97	0.45
2:A:937:GLU:HG3	2:A:1364:VAL:HG22	1.96	0.45
2:A:1565:ILE:HD11	2:A:1611:LEU:HD13	1.98	0.45
2:A:1318:LYS:HE3	2:A:1319:HIS:CE1	2.52	0.45
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.98	0.45
1:B:469:TRP:O	1:B:469:TRP:CD1	2.70	0.45
1:B:29:LYS:HA	1:B:652:THR:HG23	1.99	0.45
1:B:144:ARG:NH2	1:B:602:LEU:O	2.46	0.45
2:A:1313:ILE:HD12	2:A:1328:MET:HE3	1.98	0.45
2:A:1088:GLN:HG2	8:A:2007:DIO:H1'2	1.98	0.44
1:B:417:VAL:HG21	1:B:473:HIS:NE2	2.32	0.44
1:B:465:LEU:HD11	1:B:486:VAL:HG13	1.98	0.44
2:A:1554:LYS:HG3	2:A:1556:GLU:H	1.82	0.44
1:B:311:SER:O	1:B:313:TYR:N	2.51	0.44
2:A:1402:ILE:HG13	2:A:1479:ILE:HD13	1.99	0.44
4:D:58:LEU:HD12	4:D:58:LEU:HA	1.82	0.44
2:A:687:ALA:O	2:A:691:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1008:ALA:HB2	2:A:1059:TYR:CG	2.54	0.43
2:A:1464:LEU:HD23	2:A:1467:ILE:HG12	1.99	0.43
2:A:765:ILE:HG13	2:A:767:SER:H	1.84	0.43
2:A:860:SER:HB3	2:A:911:ASN:H	1.83	0.43
2:A:1386:ILE:HA	2:A:1386:ILE:HD12	1.86	0.43
1:B:363:LEU:HB2	1:B:456:ALA:HA	2.00	0.43
1:B:243:PHE:O	1:B:303:SER:HB2	2.19	0.43
2:A:1279:ARG:HD2	9:A:2137:HOH:O	2.19	0.43
2:A:905:ILE:HG21	2:A:931:PRO:HG3	2.00	0.43
2:A:1046:LYS:NZ	2:A:1092:TYR:O	2.52	0.43
2:A:826:GLU:HG2	2:A:846:TYR:HE1	1.84	0.43
1:B:392:ALA:HB1	1:B:431:LEU:HD11	2.01	0.43
3:C:69:THR:HA	3:C:89:PHE:O	2.19	0.43
2:A:1645:ILE:HG13	2:A:1645:ILE:O	2.17	0.43
1:B:106:VAL:O	1:B:112:SER:HA	2.18	0.43
2:A:1516:ILE:CG2	2:A:1518:LYS:HG2	2.49	0.42
2:A:758:LEU:HB2	2:A:759:PRO:HD3	2.01	0.42
2:A:1516:ILE:HG22	2:A:1517:GLN:N	2.34	0.42
9:B:849:HOH:O	5:A:2005:EDO:H11	2.18	0.42
1:B:228:SER:O	1:B:252:ALA:HA	2.19	0.42
2:A:1232:LEU:HB2	2:A:1235:LYS:HD3	2.02	0.42
2:A:680:GLN:HG3	2:A:753:HIS:NE2	2.35	0.42
2:A:709:GLU:OE1	2:A:717:ARG:NH2	2.52	0.42
1:B:609:VAL:HG12	2:A:769:PHE:CG	2.55	0.42
2:A:691:LYS:HE2	2:A:757:LEU:HD13	2.02	0.42
2:A:964:PRO:HG2	2:A:967:LEU:HB2	2.01	0.42
2:A:999:ILE:HG13	2:A:1000:LEU:HG	2.01	0.42
3:C:86:ASP:O	3:C:100:LEU:HD13	2.20	0.41
1:B:159:THR:O	1:B:175:GLU:HA	2.20	0.41
1:B:224:LEU:HD12	1:B:225:PRO:HD2	2.01	0.41
1:B:539:ARG:NH1	1:B:631:ASP:OD2	2.53	0.41
2:A:1229:LYS:HD2	2:A:1231:ASN:O	2.20	0.41
2:A:702:GLY:HA2	2:A:728:PHE:CE2	2.56	0.41
4:D:35:PRO:HG2	4:D:38:CYS:SG	2.61	0.41
2:A:1105:LEU:O	2:A:1109:GLU:HB2	2.20	0.41
1:B:267:ILE:HD13	1:B:299:VAL:HG21	2.02	0.41
2:A:1616:GLN:OE1	2:A:1650:ARG:NH2	2.54	0.41
2:A:689:LYS:HD3	2:A:690:TYR:CE1	2.55	0.41
2:A:781:PRO:C	2:A:783:ARG:H	2.24	0.41
2:A:1384:GLN:O	2:A:1400:LYS:HA	2.20	0.41
2:A:1563:VAL:HG12	2:A:1581:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASP:C	1:B:319:ASN:H	2.24	0.41
1:B:375:VAL:HG11	1:B:386:VAL:HG11	2.02	0.41
2:A:1378:TYR:CE2	2:A:1409:LYS:HG2	2.56	0.41
1:B:481:HIS:CE1	1:B:529:PRO:HB3	2.56	0.41
1:B:484:ILE:HG22	1:B:526:ILE:O	2.21	0.41
4:D:43:ARG:NH2	4:D:56:TYR:OH	2.49	0.41
2:A:819:VAL:HG21	9:A:2104:HOH:O	2.20	0.41
2:A:1379:LEU:HD22	2:A:1493:PHE:CE2	2.55	0.40
2:A:923:LEU:HD11	2:A:925:LYS:HZ3	1.86	0.40
1:B:592:MET:SD	1:B:602:LEU:HD11	2.61	0.40
2:A:1577:TYR:CE1	2:A:1611:LEU:HB2	2.56	0.40
1:B:460:LEU:HD12	1:B:460:LEU:HA	1.87	0.40
2:A:1540:ASP:HB3	2:A:1543:ILE:HD13	2.02	0.40
1:B:256:TYR:HA	2:A:846:TYR:HE2	1.86	0.40
1:B:128:ILE:HB	1:B:215:ALA:HB2	2.03	0.40
2:A:1098:ASN:O	2:A:1102:ASN:ND2	2.52	0.40
2:A:1515:LYS:CE	2:A:1516:ILE:HG23	2.41	0.40
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B	643/656 (98%)	616 (96%)	27 (4%)	0	100	100
2	A	976/998 (98%)	925 (95%)	51 (5%)	0	100	100
3	C	146/165 (88%)	138 (94%)	8 (6%)	0	100	100
4	D	45/81 (56%)	44 (98%)	1 (2%)	0	100	100
All	All	1810/1900 (95%)	1723 (95%)	87 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	B	574/581 (99%)	558 (97%)	16 (3%)	49	76
2	A	872/885 (98%)	848 (97%)	24 (3%)	49	76
3	C	128/143 (90%)	125 (98%)	3 (2%)	56	81
4	D	41/71 (58%)	40 (98%)	1 (2%)	54	80
All	All	1615/1680 (96%)	1571 (97%)	44 (3%)	50	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	ASP
1	B	103	TYR
1	B	264	ASP
1	B	289	ASN
1	B	354	LEU
1	B	414	ASP
1	B	460	LEU
1	B	470	THR
1	B	471	ASP
1	B	472	ASN
1	B	473	HIS
1	B	474	LYS
1	B	494	ASP
1	B	495	LYS
1	B	550	GLN
1	B	672	ILE
2	A	807	THR
2	A	814	THR
2	A	862	VAL
2	A	916	THR
2	A	987	ILE
2	A	1056	ILE
2	A	1370	THR
2	A	1515	LYS

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Mol	Chain	Res	Type
2	A	1516	ILE
2	A	1519	VAL
2	A	1526	LYS
2	A	1546	GLU
2	A	1562	LYS
2	A	1581	LEU
2	A	1589	GLU
2	A	1601	ILE
2	A	1636	ILE
2	A	1645	ILE
2	A	1650	ARG
2	A	1651	ASP
2	A	1654	CYS
2	A	1657	CYS
2	A	1658	GLN
2	A	1664	LEU
3	C	69	THR
3	C	127	VAL
3	C	151	LEU
4	D	58	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
6	NAG	A	2001	2,6	14,14,15	0.32	0	15,19,21	0.51	0
6	NAG	A	2002	6	14,14,15	0.24	0	15,19,21	0.52	0
5	EDO	A	2003	-	3,3,3	0.37	0	2,2,2	0.60	0
5	EDO	A	2004	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	A	2005	-	3,3,3	0.44	0	2,2,2	0.40	0
7	CYS	A	2006	2	5,5,6	1.00	0	2,5,7	1.09	0
8	DIO	A	2007	-	6,6,6	0.66	0	6,6,6	0.50	0
5	EDO	B	701	-	3,3,3	0.47	0	2,2,2	0.21	0
5	EDO	B	702	-	3,3,3	0.48	0	2,2,2	0.17	0
5	EDO	C	201	-	3,3,3	0.47	0	2,2,2	0.26	0
5	EDO	D	101	-	3,3,3	0.46	0	2,2,2	0.30	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
6	NAG	A	2001	2,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2002	6	-	0/6/23/26	0/1/1/1
5	EDO	A	2003	-	-	0/1/1/1	0/0/0/0
5	EDO	A	2004	-	-	0/1/1/1	0/0/0/0
5	EDO	A	2005	-	-	0/1/1/1	0/0/0/0
7	CYS	A	2006	2	-	0/1/4/6	0/0/0/0
8	DIO	A	2007	-	-	0/0/6/6	0/1/1/1
5	EDO	B	701	-	-	0/1/1/1	0/0/0/0
5	EDO	B	702	-	-	0/1/1/1	0/0/0/0
5	EDO	C	201	-	-	0/1/1/1	0/0/0/0
5	EDO	D	101	-	-	0/1/1/1	0/0/0/0

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2003	EDO	1	0
5	A	2005	EDO	2	0
8	A	2007	DIO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	647/656 (98%)	0.64	29 (4%) 34 26	36, 73, 125, 178	0
2	A	982/998 (98%)	0.79	81 (8%) 12 8	32, 61, 138, 213	0
3	C	148/165 (89%)	0.57	7 (4%) 32 25	45, 77, 113, 133	0
4	D	47/81 (58%)	0.32	1 (2%) 64 58	44, 66, 98, 136	0
All	All	1824/1900 (96%)	0.70	118 (6%) 20 14	32, 66, 133, 213	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1517	GLN	11.5
2	A	1518	LYS	10.8
2	A	1671	ILE	7.6
2	A	1672	PHE	5.9
2	A	1667	PHE	5.7
2	A	1669	GLU	5.4
2	A	1673	LEU	5.3
2	A	1642	LEU	5.3
2	A	996	GLY	5.3
1	B	469	TRP	5.0
2	A	1625	LEU	5.0
2	A	1601	ILE	4.8
2	A	1676	CYS	4.6
1	B	623	VAL	4.6
1	B	624	PHE	4.5
1	B	476	LEU	4.2
2	A	1588	GLY	4.2
2	A	1664	LEU	4.2
2	A	1657	CYS	4.1
3	C	21	GLU	4.0
2	A	1521	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	A	1635	TYR	3.9
2	A	1585	TYR	3.8
1	B	620	LEU	3.8
2	A	1520	CYS	3.6
2	A	1651	ASP	3.6
2	A	1668	ALA	3.6
2	A	1519	VAL	3.5
2	A	1516	ILE	3.5
2	A	1524	ALA	3.5
2	A	1620	MET	3.5
2	A	1666	GLU	3.4
2	A	1650	ARG	3.4
2	A	1557	ILE	3.3
2	A	756	THR	3.3
2	A	1623	GLU	3.3
2	A	1622	LYS	3.3
2	A	1514	ILE	3.2
2	A	757	LEU	3.2
1	B	625	GLN	3.2
2	A	1605	THR	3.1
1	B	95	GLY	3.1
2	A	1584	ILE	3.1
2	A	1652	THR	3.1
3	C	28	GLU	3.0
2	A	1647	TYR	3.0
2	A	1589	GLU	3.0
2	A	1560	ALA	3.0
2	A	995	GLU	3.0
2	A	1627	ILE	3.0
2	A	1331	LYS	2.9
2	A	934	VAL	2.9
2	A	755	LYS	2.9
2	A	686	ILE	2.9
2	A	1648	TRP	2.9
1	B	256	TYR	2.9
4	D	14	CYS	2.8
1	B	523	TYR	2.8
2	A	1656	SER	2.8
2	A	748	GLN	2.7
2	A	752	LEU	2.7
1	B	444	GLU	2.7
2	A	1637	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	1346	LEU	2.7
2	A	1559	TYR	2.7
2	A	1033	ILE	2.7
2	A	1674	ASN	2.7
2	A	1591	VAL	2.7
2	A	1164	ILE	2.7
1	B	255	PHE	2.6
2	A	1522	GLY	2.6
1	B	224	LEU	2.6
2	A	1663	ASN	2.6
2	A	1590	ALA	2.6
3	C	100	LEU	2.5
2	A	1644	TRP	2.5
2	A	1547	THR	2.5
3	C	78	GLN	2.5
2	A	1558	ALA	2.5
1	B	30	ILE	2.5
2	A	1675	GLY	2.5
2	A	1412	ARG	2.4
3	C	95	LYS	2.4
1	B	284	GLN	2.4
1	B	348	VAL	2.4
2	A	1552	ALA	2.4
2	A	1662	ALA	2.4
1	B	397	VAL	2.3
1	B	470	THR	2.3
2	A	1326	TYR	2.3
2	A	1561	TYR	2.3
2	A	1579	ALA	2.3
1	B	673	LEU	2.3
1	B	373	VAL	2.3
1	B	431	LEU	2.3
3	C	91	LEU	2.3
1	B	276	LYS	2.3
1	B	73	LEU	2.2
1	B	549	GLU	2.2
2	A	1336	ARG	2.2
1	B	312	TYR	2.2
1	B	107	VAL	2.1
2	A	786	LEU	2.1
2	A	1661	LEU	2.1
2	A	1338	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	2.1
2	A	1633	PHE	2.1
2	A	1653	THR	2.1
1	B	477	LEU	2.1
2	A	1634	ARG	2.1
2	A	1670	ASP	2.1
3	C	98	ALA	2.0
2	A	981	GLY	2.0
2	A	1515	LYS	2.0
2	A	1583	ASP	2.0
1	B	525	SER	2.0
2	A	1323	LEU	2.0
1	B	399	GLN	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	2005	4/4	0.86	0.49	9.17	81,81,83,84	0
8	DIO	A	2007	6/6	0.95	0.34	8.32	73,75,78,79	0
5	EDO	B	701	4/4	0.77	0.28	5.89	88,89,89,90	0
5	EDO	C	201	4/4	0.95	0.28	3.79	59,60,60,61	0
5	EDO	A	2003	4/4	0.89	0.24	3.10	40,44,45,51	0
5	EDO	A	2004	4/4	0.81	0.23	1.31	65,67,68,69	0
5	EDO	B	702	4/4	0.89	0.28	0.99	80,81,82,82	0
7	CYS	A	2006	6/7	0.83	0.23	-0.28	115,119,124,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	2001	14/15	0.93	0.12	-3.22	51,67,73,82	0
6	NAG	A	2002	14/15	0.88	0.14	-	87,90,96,97	0
5	EDO	D	101	4/4	0.94	0.37	-	70,73,75,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.