



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2017 – 11:33 PM EST

PDB ID : 6ELQ  
Title : Carbon Monoxide Dehydrogenase IV from Carboxydotherrmus hydrogenofor-  
mans  
Authors : Domnik, L.; Goetzl, S.; Jeoung, J.H.; Dobbek, H.  
Deposited on : 2017-09-29  
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](mailto: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.

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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 : rb-20030736  
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) : rb-20030736

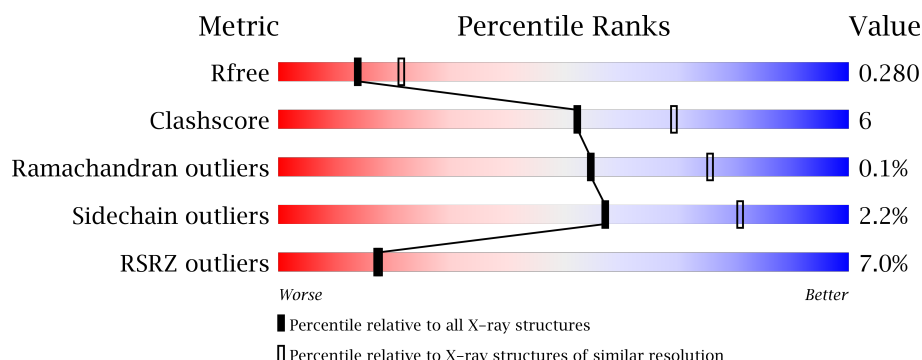
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 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))
$R_{free}$	100719	4636 (2.54-2.50)
Clashscore	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)
RSRZ outliers	101464	4669 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	633	<div> <div>4%</div> <div>85%</div> <div>14%</div> </div>
1	B	633	<div> <div>16%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	X	633	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BF8	B	5002	-	-	X	-

## 2 Entry composition [i](#)

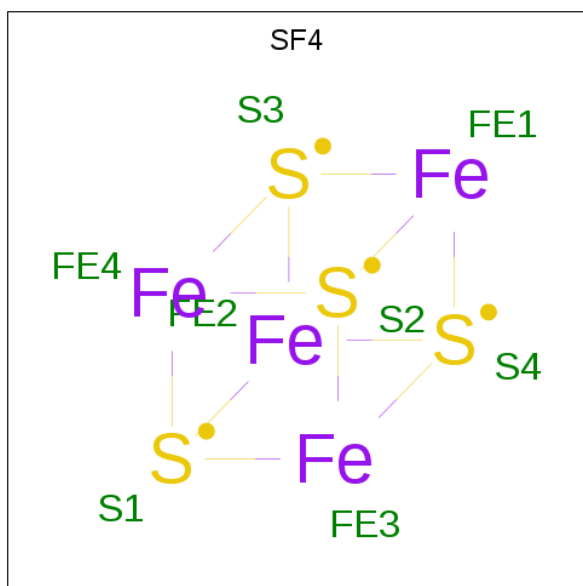
There are 4 unique types of molecules in this entry. The entry contains 14594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carbon Monoxide Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	630	Total	C	N	O	S	0	0	0
			4762	3020	821	894	27			
1	A	630	Total	C	N	O	S	0	0	0
			4762	3020	821	894	27			
1	B	630	Total	C	N	O	S	0	0	0
			4762	3020	821	894	27			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



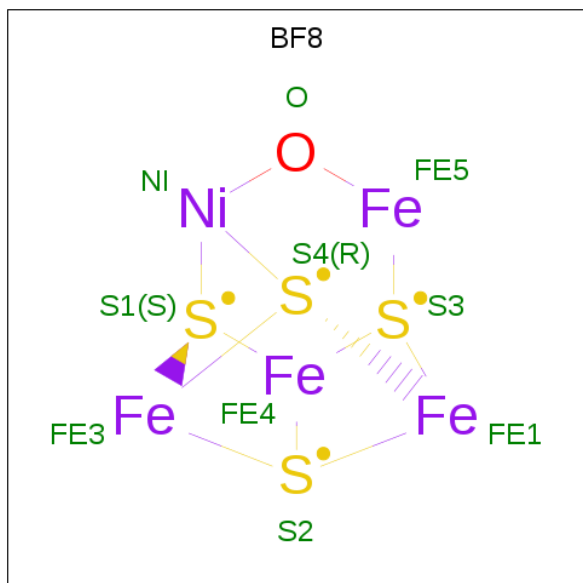
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FE(4)-NI(1)-S(5) CLUSTER with Oxygen (three-letter code: BF8) (formula:  $\text{Fe}_4\text{NiOS}_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	Fe	Ni	O	S	0	0
			10	4	1	1	4		
3	A	1	Total	Fe	Ni	O	S	0	0
			10	4	1	1	4		
3	B	1	Total	Fe	Ni	O	S	0	0
			10	4	1	1	4		

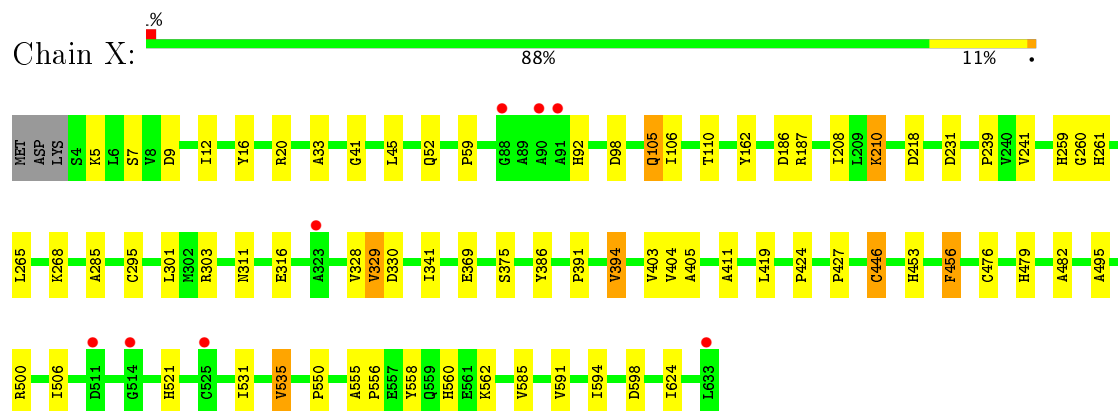
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	123	Total	O	0	0
			123	123		
4	A	77	Total	O	0	0
			77	77		
4	B	38	Total	O	0	0
			38	38		

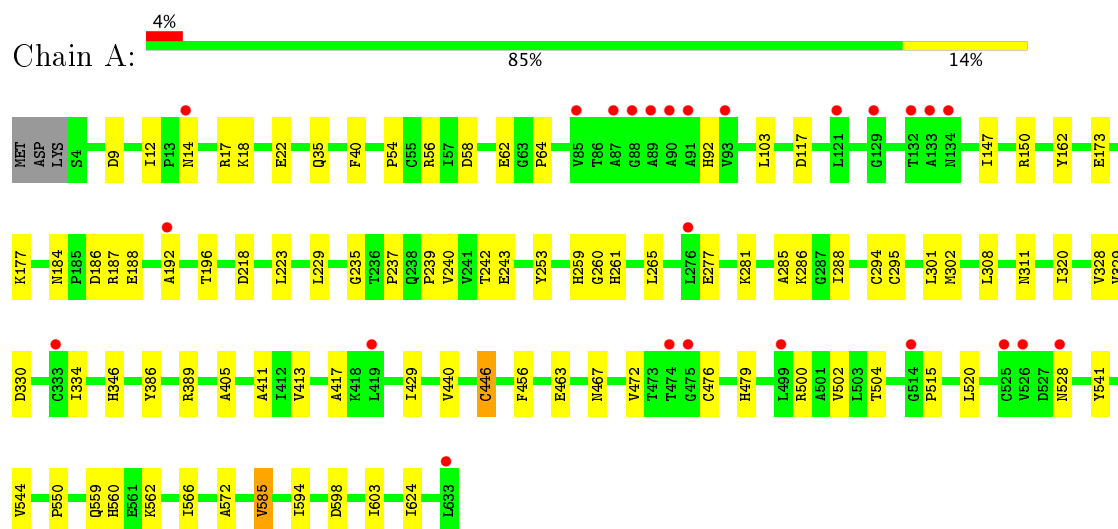
### 3 Residue-property plots [i](#)

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

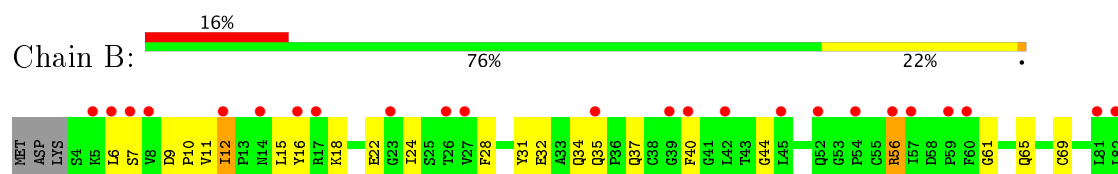
#### • Molecule 1: Carbon Monoxide Dehydrogenase

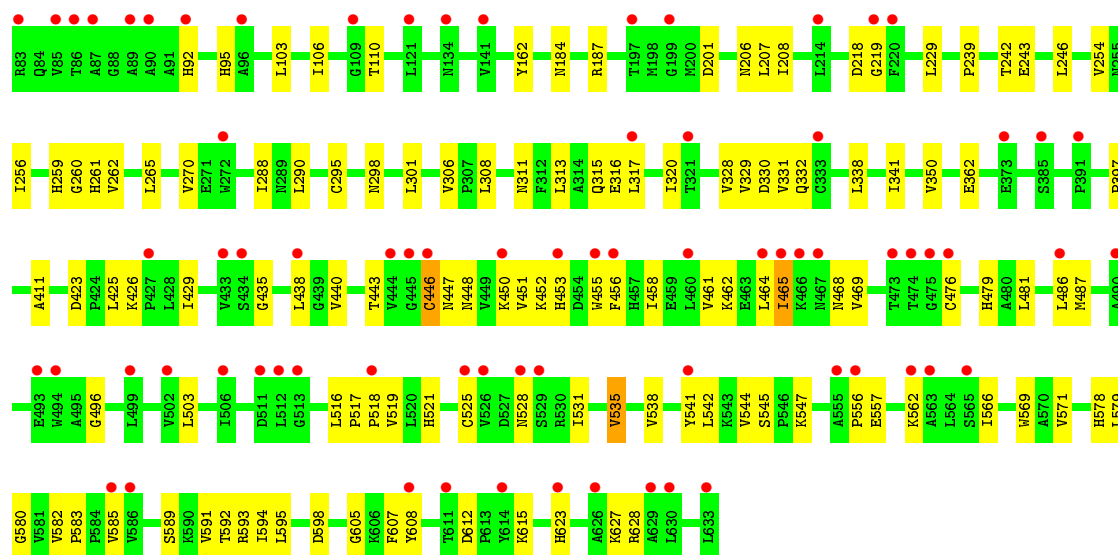


#### • Molecule 1: Carbon Monoxide Dehydrogenase



#### • Molecule 1: Carbon Monoxide Dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.15Å 209.15Å 93.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.63 – 2.52 45.63 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.63-2.52) 99.9 (45.63-2.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1168: ???)	Depositor
R, $R_{free}$	0.235 , 0.275 0.240 , 0.280	Depositor DCC
$R_{free}$ test set	2113 reflections (2.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.092 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SF4, BF8

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	0.24	0/4846	0.42	0/6591
1	B	0.25	0/4846	0.42	0/6591
1	X	0.25	0/4846	0.42	0/6591
All	All	0.25	0/14538	0.42	0/19773

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4762	0	4867	49	0
1	B	4762	0	4866	97	1
1	X	4762	0	4866	40	0
2	A	16	0	0	0	0
2	B	16	0	0	2	0
2	X	8	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	4	0
3	X	10	0	0	1	0
4	A	77	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	38	0	0	0	0
4	X	123	0	0	0	0
All	All	14594	0	14599	182	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 6.

All (182) 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:261:HIS:CE1	3:B:5002:BF8:S3	2.73	0.80
1:B:435:GLY:HA2	1:B:628:ARG:HH22	1.47	0.79
1:B:446:CYS:HA	1:B:476:CYS:HB2	1.69	0.74
1:B:594:ILE:HA	1:B:598:ASP:HB2	1.70	0.73
1:B:612:ASP:HB3	1:B:615:LYS:HB2	1.72	0.72
1:X:33:ALA:HB1	1:A:64:PRO:HG3	1.71	0.71
1:B:465:ILE:HG21	1:B:518:PRO:HB2	1.76	0.67
1:B:259:HIS:HB3	1:B:329:VAL:HG12	1.76	0.66
1:X:45:LEU:HD12	1:X:59:PRO:HG3	1.76	0.66
1:A:117:ASP:HB2	1:A:235:GLY:HA2	1.78	0.66
1:X:7:SER:HB2	1:X:453:HIS:HB3	1.81	0.62
1:B:40:PHE:HB2	2:B:5001:SF4:S3	2.39	0.62
1:B:208:ILE:HD11	1:B:591:VAL:HG13	1.79	0.62
1:B:487:MET:SD	1:B:521:HIS:HB2	2.38	0.62
1:B:481:LEU:HD13	1:B:519:VAL:HG11	1.82	0.62
1:X:186:ASP:HB3	1:A:186:ASP:HB3	1.82	0.60
1:B:571:VAL:HG13	1:B:605:GLY:HA3	1.83	0.60
1:B:7:SER:HB3	1:B:453:HIS:HB3	1.84	0.59
1:X:105:GLN:NE2	1:X:369:GLU:OE2	2.35	0.59
1:B:481:LEU:HD23	1:B:486:LEU:HD13	1.83	0.59
1:B:254:VAL:HB	1:B:288:ILE:HD13	1.85	0.58
1:B:468:ASN:OD1	1:B:496:GLY:HA3	2.04	0.58
1:B:585:VAL:HG21	1:B:595:LEU:HD12	1.85	0.58
1:X:446:CYS:HA	1:X:476:CYS:HB2	1.85	0.57
1:X:594:ILE:HA	1:X:598:ASP:HB2	1.87	0.57
1:A:239:PRO:HD3	1:A:411:ALA:HB1	1.87	0.56
1:B:11:VAL:HG11	1:B:246:LEU:HD13	1.85	0.56
1:A:18:LYS:NZ	1:A:22:GLU:OE2	2.38	0.56
1:B:103:LEU:HD22	1:B:229:LEU:HD22	1.87	0.56
1:B:330:ASP:OD1	1:B:331:VAL:N	2.37	0.55
1:B:583:PRO:HG2	1:B:585:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:311:ASN:HB3	1:X:479:HIS:HB2	1.88	0.55
1:A:594:ILE:HA	1:A:598:ASP:HB2	1.89	0.54
1:B:316:GLU:HB3	1:B:341:ILE:HD13	1.89	0.54
1:B:265:LEU:HD21	1:B:328:VAL:HG22	1.90	0.54
1:X:495:ALA:O	1:X:500:ARG:NH1	2.40	0.54
1:A:446:CYS:HA	1:A:476:CYS:HB2	1.88	0.53
1:B:270:VAL:HG22	1:B:290:LEU:HD13	1.90	0.53
1:A:260:GLY:HA3	1:A:330:ASP:OD1	2.08	0.53
1:A:9:ASP:HB3	1:A:12:ILE:HG12	1.91	0.53
1:A:504:THR:HG22	1:A:515:PRO:HB3	1.90	0.53
1:A:92:HIS:ND1	1:A:218:ASP:OD1	2.35	0.52
1:B:313:LEU:HB3	1:B:453:HIS:CD2	2.44	0.52
1:B:259:HIS:O	1:B:329:VAL:HA	2.10	0.52
1:B:315:GLN:HG3	1:B:338:LEU:HD21	1.92	0.52
1:B:12:ILE:HG13	1:B:317:LEU:HD12	1.91	0.52
1:A:472:VAL:HG12	1:A:520:LEU:HB2	1.90	0.51
1:X:260:GLY:HA3	1:X:330:ASP:OD1	2.11	0.51
1:X:316:GLU:HB3	1:X:341:ILE:HD13	1.91	0.51
1:B:579:LEU:HD22	1:B:583:PRO:HG3	1.92	0.51
1:B:239:PRO:HD3	1:B:411:ALA:HB1	1.92	0.51
1:A:277:GLU:OE1	1:A:288:ILE:N	2.43	0.51
1:X:239:PRO:HD3	1:X:411:ALA:HB1	1.93	0.51
1:A:463:GLU:OE1	1:A:467:ASN:ND2	2.44	0.50
1:B:525:CYS:O	1:B:528:ASN:ND2	2.44	0.50
1:A:311:ASN:HB3	1:A:479:HIS:CB	2.41	0.50
1:X:231:ASP:OD1	1:X:303:ARG:NH2	2.41	0.50
1:A:311:ASN:HB3	1:A:479:HIS:HB2	1.93	0.50
1:B:443:THR:HG21	1:B:461:VAL:HG22	1.92	0.50
1:B:487:MET:HA	1:B:517:PRO:HB3	1.92	0.50
1:X:531:ILE:O	1:X:535:VAL:HG13	2.11	0.49
1:B:61:GLY:HA2	1:B:65:GLN:CD	2.32	0.49
1:B:531:ILE:O	1:B:535:VAL:HG13	2.12	0.49
1:B:261:HIS:CD2	1:B:295:CYS:HB2	2.48	0.49
1:A:413:VAL:O	1:A:417:ALA:N	2.45	0.49
1:B:562:LYS:O	1:B:566:ILE:HG12	2.13	0.49
1:A:237:PRO:HB3	1:A:302:MET:HB3	1.94	0.49
1:B:201:ASP:OD2	1:B:206:ASN:ND2	2.42	0.49
1:X:261:HIS:CD2	1:X:295:CYS:HB2	2.48	0.49
1:X:419:LEU:HD11	1:X:506:ILE:HA	1.95	0.49
1:B:425:LEU:HB3	1:B:429:ILE:HD12	1.94	0.48
1:B:11:VAL:HG12	1:B:15:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:HG13	1:A:541:TYR:CD1	2.49	0.48
1:B:464:LEU:O	1:B:469:VAL:HB	2.14	0.47
1:B:106:ILE:HA	1:B:110:THR:HG22	1.97	0.47
1:X:241:VAL:HG22	1:X:404:VAL:HG22	1.96	0.47
1:B:313:LEU:HB3	1:B:453:HIS:HD2	1.80	0.47
1:A:18:LYS:HE3	1:A:320:ILE:O	2.15	0.47
1:B:301:LEU:HD22	1:B:308:LEU:HD21	1.97	0.47
1:B:313:LEU:HB2	1:B:447:ASN:HB2	1.96	0.47
1:X:311:ASN:HB3	1:X:479:HIS:CB	2.45	0.47
1:B:585:VAL:O	1:B:592:THR:OG1	2.33	0.46
1:A:14:ASN:O	1:A:17:ARG:HG3	2.15	0.46
1:A:550:PRO:HB2	1:A:624:ILE:HG23	1.98	0.46
1:X:456:PHE:CD1	1:X:556:PRO:HB3	2.50	0.46
1:B:184:ASN:HB3	1:B:187:ARG:HB3	1.97	0.46
1:X:265:LEU:HD21	1:X:328:VAL:HG22	1.98	0.46
1:X:9:ASP:HB3	1:X:12:ILE:HG12	1.97	0.46
1:A:173:GLU:O	1:A:177:LYS:HG2	2.15	0.46
1:A:184:ASN:HB3	1:A:187:ARG:HB3	1.98	0.46
1:B:18:LYS:NZ	1:B:22:GLU:OE2	2.40	0.46
1:B:31:TYR:CZ	1:B:450:LYS:HA	2.51	0.46
1:B:34:GLN:O	1:B:37:GLN:HG3	2.16	0.45
1:B:525:CYS:SG	3:B:5002:BF8:O	2.75	0.45
1:B:6:LEU:HD11	1:B:16:TYR:CD2	2.52	0.45
1:B:92:HIS:ND1	1:B:218:ASP:OD2	2.33	0.45
1:B:32:GLU:HA	1:B:35:GLN:HG3	1.99	0.45
1:B:623:HIS:CE1	1:B:627:LYS:HE2	2.52	0.45
1:B:95:HIS:CD2	1:B:262:VAL:HG22	2.51	0.45
1:B:350:VAL:HA	1:B:362:GLU:O	2.16	0.45
1:A:265:LEU:HD21	1:A:328:VAL:HG22	1.99	0.45
1:B:11:VAL:HG13	1:B:397:PRO:HG3	1.99	0.45
1:B:256:ILE:HB	1:B:290:LEU:HD23	1.99	0.45
1:B:311:ASN:HB3	1:B:479:HIS:CB	2.47	0.45
1:B:311:ASN:HB3	1:B:479:HIS:HB3	1.97	0.45
1:X:259:HIS:HB3	1:X:329:VAL:HG23	1.99	0.45
1:B:545:SER:OG	1:B:547:LYS:HG2	2.17	0.45
1:X:403:VAL:HG11	1:X:482:ALA:HB1	1.98	0.45
1:B:328:VAL:HA	1:B:350:VAL:HG23	1.99	0.44
1:B:69:CYS:HB3	2:B:5000:SF4:S4	2.56	0.44
1:B:458:ILE:O	1:B:462:LYS:HG3	2.17	0.44
1:B:219:GLY:HA3	1:B:569:TRP:CD1	2.52	0.44
1:B:578:HIS:HA	1:B:608:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD22	1:A:308:LEU:HD11	1.99	0.44
1:B:316:GLU:O	1:B:320:ILE:HG12	2.18	0.44
1:A:192:ALA:O	1:A:196:THR:HG23	2.18	0.43
1:A:223:LEU:HD11	1:A:566:ILE:HG12	1.99	0.43
1:B:438:LEU:HD12	1:B:628:ARG:HH11	1.82	0.43
1:X:550:PRO:HB2	1:X:624:ILE:HG23	2.00	0.43
1:A:35:GLN:NE2	4:A:5112:HOH:O	2.51	0.43
1:B:40:PHE:O	1:B:44:GLY:N	2.50	0.43
1:X:424:PRO:O	1:X:427:PRO:HD2	2.18	0.43
1:A:40:PHE:CD1	1:A:56:ARG:HB2	2.54	0.43
1:B:525:CYS:HB2	3:B:5002:BF8:O	2.17	0.43
1:B:556:PRO:O	1:B:580:GLY:HA3	2.19	0.43
1:X:210:LYS:HD3	1:X:210:LYS:HA	1.81	0.43
1:A:253:TYR:CE1	1:A:286:LYS:HD3	2.53	0.43
1:A:147:ILE:HG12	1:A:150:ARG:HH21	1.84	0.43
1:A:572:ALA:HA	1:A:603:ILE:HD13	1.99	0.43
1:B:298:ASN:HD21	1:B:479:HIS:HD2	1.65	0.43
1:B:579:LEU:HD11	1:B:607:PHE:HD2	1.84	0.43
1:X:106:ILE:HA	1:X:110:THR:HG22	2.01	0.43
1:A:294:CYS:HB3	1:A:295:CYS:H	1.69	0.43
1:X:208:ILE:HD11	1:X:591:VAL:HG13	2.00	0.43
1:A:103:LEU:HD22	1:A:229:LEU:HD22	1.99	0.43
1:B:201:ASP:HB3	1:B:207:LEU:HD21	2.01	0.43
1:B:18:LYS:HE3	1:B:320:ILE:O	2.19	0.43
1:X:41:GLY:HA3	1:A:54:PRO:HG3	2.00	0.42
1:B:579:LEU:HD11	1:B:607:PHE:CD2	2.53	0.42
1:B:503:LEU:HB3	1:B:516:LEU:HB2	2.01	0.42
1:B:451:VAL:HG11	1:B:456:PHE:HB2	2.01	0.42
1:A:528:ASN:HD22	1:A:566:ILE:HD13	1.85	0.42
1:B:542:LEU:HB2	1:B:544:VAL:HG22	2.01	0.42
1:B:242:THR:OG1	1:B:243:GLU:N	2.52	0.42
1:A:259:HIS:HB3	1:A:329:VAL:HG23	2.02	0.42
1:X:391:PRO:HA	1:X:394:VAL:HG13	2.01	0.42
1:X:239:PRO:HA	1:X:405:ALA:O	2.19	0.42
1:X:555:ALA:HB1	1:X:558:TYR:HB3	2.02	0.42
1:A:285:ALA:HB2	1:A:386:TYR:CE2	2.54	0.42
1:B:313:LEU:HD23	1:B:453:HIS:HB2	2.01	0.42
1:A:261:HIS:CD2	1:A:295:CYS:HB2	2.55	0.42
1:B:9:ASP:HA	1:B:10:PRO:HD3	1.92	0.42
1:X:285:ALA:HB2	1:X:386:TYR:CE2	2.55	0.42
1:B:429:ILE:HD13	1:B:541:TYR:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLY:HA3	1:B:330:ASP:OD1	2.20	0.41
1:B:456:PHE:CD1	1:B:556:PRO:HB3	2.55	0.41
1:X:560:HIS:CE1	1:X:562:LYS:HE2	2.55	0.41
1:A:58:ASP:OD2	1:A:62:GLU:HB2	2.19	0.41
1:B:301:LEU:HD22	1:B:308:LEU:HD11	2.02	0.41
1:B:448:ASN:H	1:B:557:GLU:HB3	1.85	0.41
1:A:346:HIS:CE1	1:A:389:ARG:HG3	2.55	0.41
1:X:92:HIS:ND1	1:X:218:ASP:OD1	2.37	0.41
1:B:24:ILE:HG12	1:B:341:ILE:HG12	2.02	0.41
1:B:525:CYS:CB	3:B:5002:BF8:O	2.69	0.41
1:B:298:ASN:HD21	1:B:479:HIS:CD2	2.39	0.41
1:B:423:ASP:OD1	1:B:426:LYS:N	2.54	0.41
1:X:562:LYS:HE3	3:X:702:BF8:S4	2.60	0.41
1:B:452:LYS:HB3	1:B:455:TRP:HB3	2.03	0.41
1:B:585:VAL:HG23	1:B:591:VAL:HG12	2.03	0.41
1:A:242:THR:OG1	1:A:243:GLU:N	2.53	0.41
1:B:503:LEU:HG	1:B:503:LEU:H	1.65	0.41
1:X:5:LYS:HG2	1:X:5:LYS:H	1.70	0.41
1:A:281:LYS:HA	1:A:285:ALA:O	2.20	0.41
1:A:560:HIS:CE1	1:A:562:LYS:HE2	2.56	0.40
1:X:16:TYR:CZ	1:X:20:ARG:HD2	2.57	0.40
1:A:329:VAL:HG13	1:A:334:ILE:HD13	2.02	0.40
1:X:52:GLN:HG3	1:A:559:GLN:HB2	2.03	0.40
1:A:239:PRO:HA	1:A:405:ALA:O	2.21	0.40
1:B:317:LEU:HD23	1:B:317:LEU:HA	1.89	0.40
1:A:184:ASN:O	1:A:188:GLU:HG2	2.21	0.40
1:B:28:PHE:HE2	1:B:453:HIS:HB2	1.86	0.40
1:X:268:LYS:HB3	1:X:375:SER:OG	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:B:34:GLN:NE2	1:B:56:ARG:O[5_675]	2.19	0.01

## 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	A	628/633 (99%)	605 (96%)	22 (4%)	1 (0%)	51	72
1	B	628/633 (99%)	597 (95%)	30 (5%)	1 (0%)	51	72
1	X	628/633 (99%)	604 (96%)	24 (4%)	0	100	100
All	All	1884/1899 (99%)	1806 (96%)	76 (4%)	2 (0%)	55	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	VAL
1	B	332	GLN

### 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	A	512/515 (99%)	503 (98%)	9 (2%)	64	85
1	B	512/515 (99%)	500 (98%)	12 (2%)	56	80
1	X	512/515 (99%)	499 (98%)	13 (2%)	53	78
All	All	1536/1545 (99%)	1502 (98%)	34 (2%)	57	81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	98	ASP

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Mol	Chain	Res	Type
1	X	105	GLN
1	X	162	TYR
1	X	187	ARG
1	X	210	LYS
1	X	301	LEU
1	X	329	VAL
1	X	394	VAL
1	X	446	CYS
1	X	456	PHE
1	X	521	HIS
1	X	535	VAL
1	X	585	VAL
1	A	162	TYR
1	A	240	VAL
1	A	440	VAL
1	A	446	CYS
1	A	456	PHE
1	A	500	ARG
1	A	502	VAL
1	A	544	VAL
1	A	585	VAL
1	B	12	ILE
1	B	56	ARG
1	B	162	TYR
1	B	306	VAL
1	B	440	VAL
1	B	446	CYS
1	B	465	ILE
1	B	535	VAL
1	B	538	VAL
1	B	582	VAL
1	B	589	SER
1	B	593	ARG

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

### 5.3.3 RNA ⓘ

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](#)

8 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	$\# Z  > 2$
2	SF4	A	5001	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	5002	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BF8	A	5003	1	0,14,14	0.00	-	0,26,26	0.00	-
2	SF4	B	5000	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	5001	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BF8	B	5002	1	0,14,14	0.00	-	0,26,26	0.00	-
2	SF4	X	701	1	0,12,12	0.00	-	0,24,24	0.00	-
3	BF8	X	702	1	0,14,14	0.00	-	0,26,26	0.00	-

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
2	SF4	A	5001	1	-	0/0/48/48	0/6/5/5
2	SF4	A	5002	1	-	0/0/48/48	0/6/5/5
3	BF8	A	5003	1	-	0/0/49/49	0/3/5/5
2	SF4	B	5000	1	-	0/0/48/48	0/6/5/5
2	SF4	B	5001	1	-	0/0/48/48	0/6/5/5
3	BF8	B	5002	1	-	0/0/49/49	0/3/5/5
2	SF4	X	701	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BF8	X	702	1	-	0/0/49/49	0/3/5/5

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5000	SF4	1	0
2	B	5001	SF4	1	0
3	B	5002	BF8	4	0
3	X	702	BF8	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	630/633 (99%)	0.19	25 (3%) 39 41	38, 54, 73, 88	0
1	B	630/633 (99%)	0.96	99 (15%) 2 2	43, 69, 95, 106	0
1	X	630/633 (99%)	-0.06	8 (1%) 77 79	36, 46, 60, 75	0
All	All	1890/1899 (99%)	0.37	132 (6%) 17 18	36, 54, 86, 106	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LYS	6.7
1	B	633	LEU	6.4
1	B	40	PHE	6.0
1	B	317	LEU	5.9
1	A	525	CYS	5.2
1	B	6	LEU	5.2
1	B	438	LEU	5.2
1	A	499	LEU	5.0
1	B	525	CYS	5.0
1	B	85	VAL	4.6
1	B	445	GLY	4.6
1	A	514	GLY	4.5
1	B	506	ILE	4.3
1	A	633	LEU	4.1
1	B	476	CYS	4.1
1	B	141	VAL	4.0
1	B	518	PRO	3.9
1	B	450	LYS	3.9
1	B	513	GLY	3.8
1	B	490	ALA	3.8
1	B	630	LEU	3.8
1	B	333	CYS	3.7
1	A	85	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	526	VAL	3.5
1	B	512	LEU	3.5
1	B	16	TYR	3.5
1	B	17	ARG	3.5
1	B	502	VAL	3.5
1	X	514	GLY	3.5
1	B	565	SER	3.4
1	B	57	ILE	3.3
1	B	89	ALA	3.3
1	B	39	GLY	3.2
1	B	499	LEU	3.2
1	B	86	THR	3.1
1	B	475	GLY	3.1
1	B	563	ALA	3.1
1	B	197	THR	3.1
1	B	12	ILE	3.1
1	X	633	LEU	3.1
1	B	87	ALA	3.1
1	B	465	ILE	3.0
1	B	541	TYR	3.0
1	A	134	ASN	3.0
1	B	27	VAL	2.9
1	B	453	HIS	2.9
1	A	89	ALA	2.9
1	B	446	CYS	2.9
1	B	433	VAL	2.9
1	B	444	VAL	2.8
1	B	466	LYS	2.8
1	A	88	GLY	2.8
1	B	528	ASN	2.8
1	B	629	ALA	2.8
1	B	45	LEU	2.8
1	A	333	CYS	2.8
1	B	60	PHE	2.8
1	B	555	ALA	2.8
1	B	460	LEU	2.8
1	B	26	THR	2.8
1	B	81	LEU	2.7
1	A	91	ALA	2.7
1	A	276	LEU	2.7
1	B	608	TYR	2.7
1	X	525	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	7	SER	2.6
1	B	626	ALA	2.6
1	A	87	ALA	2.6
1	A	419	LEU	2.5
1	B	391	PRO	2.5
1	B	464	LEU	2.5
1	B	562	LYS	2.5
1	B	272	TRP	2.5
1	B	474	THR	2.5
1	B	59	PRO	2.5
1	B	82	LEU	2.5
1	B	585	VAL	2.5
1	B	321	THR	2.4
1	B	623	HIS	2.4
1	A	14	ASN	2.4
1	B	42	LEU	2.4
1	B	8	VAL	2.4
1	B	35	GLN	2.4
1	B	214	LEU	2.4
1	A	93	VAL	2.4
1	B	467	ASN	2.4
1	B	556	PRO	2.3
1	A	132	THR	2.3
1	B	486	LEU	2.3
1	B	83	ARG	2.3
1	B	529	SER	2.3
1	A	474	THR	2.3
1	B	56	ARG	2.3
1	B	455	TRP	2.3
1	B	456	PHE	2.3
1	B	473	THR	2.3
1	B	121	LEU	2.3
1	B	52	GLN	2.2
1	B	92	HIS	2.2
1	B	586	VAL	2.2
1	A	528	ASN	2.2
1	B	54	PRO	2.2
1	B	219	GLY	2.2
1	B	373	GLU	2.2
1	B	199	GLY	2.2
1	B	385	SER	2.2
1	A	90	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	ALA	2.1
1	B	434	SER	2.1
1	B	134	ASN	2.1
1	A	475	GLY	2.1
1	B	90	ALA	2.1
1	B	109	GLY	2.1
1	B	493	GLU	2.1
1	B	427	PRO	2.1
1	X	511	ASP	2.1
1	A	129	GLY	2.1
1	X	90	ALA	2.1
1	A	526	VAL	2.1
1	X	88	GLY	2.1
1	B	23	GLY	2.1
1	A	121	LEU	2.1
1	B	220	PHE	2.1
1	B	494	TRP	2.1
1	B	611	THR	2.1
1	X	323	ALA	2.1
1	B	511	ASP	2.1
1	X	91	ALA	2.0
1	A	192	ALA	2.0
1	B	614	TYR	2.0
1	B	96	ALA	2.0
1	B	14	ASN	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	BF8	X	702	10/10	0.97	0.18	-0.41	45,47,55,59	8
2	SF4	X	701	8/8	0.98	0.14	-0.46	34,45,50,50	0
3	BF8	A	5003	10/10	0.97	0.20	-0.57	46,50,59,63	7
3	BF8	B	5002	10/10	0.95	0.23	-0.78	60,66,72,73	6
2	SF4	A	5002	8/8	0.98	0.12	-1.08	34,41,45,48	0
2	SF4	B	5001	8/8	0.93	0.14	-1.38	77,83,104,104	8
2	SF4	A	5001	8/8	0.97	0.10	-1.64	42,44,51,55	0
2	SF4	B	5000	8/8	0.97	0.12	-2.23	64,67,71,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.