



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:11 am BST

PDB ID : 4CG4  
Title : Crystal structure of the CHS-B30.2 domains of TRIM20  
Authors : Weinert, C.; Morger, D.; Djekic, A.; Mittl, P.R.E.; Gruetter, M.G.  
Deposited on : 2013-11-20  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

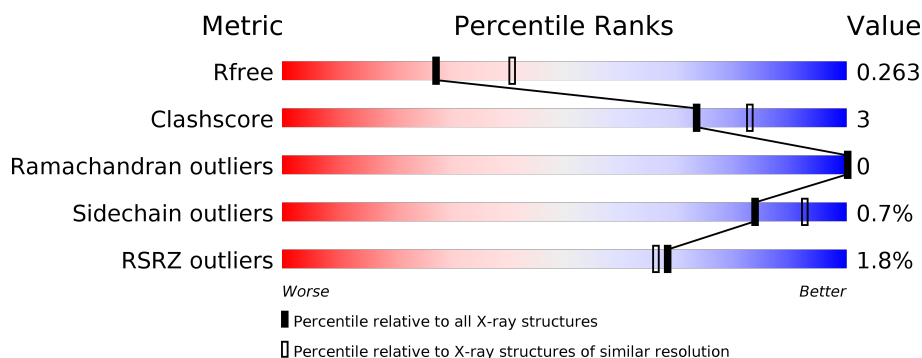
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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  $\leq 5\%$ . 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	377	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	377	<div> <div></div> <div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>
1	C	377	<div> <div></div> <div> <div>91%</div> <div>8%</div> </div> </div>
1	D	377	<div> <div></div> <div> <div>93%</div> <div>7%</div> <div>•</div> </div> </div>
1	E	377	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
1	F	377	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</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
2	SO4	D	1789	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36045 atoms, of which 18001 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 PYRIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	H	N	O	S	0	0	0
			6032	1919	3020	515	567	11			
1	B	364	Total	C	H	N	O	S	0	0	0
			5845	1860	2927	500	547	11			
1	C	376	Total	C	H	N	O	S	0	0	0
			6017	1917	3008	515	566	11			
1	D	377	Total	C	H	N	O	S	0	0	0
			6027	1919	3015	515	567	11			
1	E	374	Total	C	H	N	O	S	0	0	0
			5959	1899	2976	511	562	11			
1	F	376	Total	C	H	N	O	S	0	0	0
			6022	1917	3013	515	566	11			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	ACE	-	expression tag	UNP O15553
A	413	SER	-	expression tag	UNP O15553
A	782	ALA	-	expression tag	UNP O15553
A	783	LEU	-	expression tag	UNP O15553
A	784	GLU	-	expression tag	UNP O15553
A	785	VAL	-	expression tag	UNP O15553
A	786	LEU	-	expression tag	UNP O15553
A	787	PHE	-	expression tag	UNP O15553
A	788	GLN	-	expression tag	UNP O15553
B	412	ACE	-	expression tag	UNP O15553
B	413	SER	-	expression tag	UNP O15553
B	782	ALA	-	expression tag	UNP O15553
B	783	LEU	-	expression tag	UNP O15553
B	784	GLU	-	expression tag	UNP O15553
B	785	VAL	-	expression tag	UNP O15553
B	786	LEU	-	expression tag	UNP O15553
B	787	PHE	-	expression tag	UNP O15553

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Chain	Residue	Modelled	Actual	Comment	Reference
B	788	GLN	-	expression tag	UNP O15553
C	412	ACE	-	expression tag	UNP O15553
C	413	SER	-	expression tag	UNP O15553
C	782	ALA	-	expression tag	UNP O15553
C	783	LEU	-	expression tag	UNP O15553
C	784	GLU	-	expression tag	UNP O15553
C	785	VAL	-	expression tag	UNP O15553
C	786	LEU	-	expression tag	UNP O15553
C	787	PHE	-	expression tag	UNP O15553
C	788	GLN	-	expression tag	UNP O15553
D	412	ACE	-	expression tag	UNP O15553
D	413	SER	-	expression tag	UNP O15553
D	782	ALA	-	expression tag	UNP O15553
D	783	LEU	-	expression tag	UNP O15553
D	784	GLU	-	expression tag	UNP O15553
D	785	VAL	-	expression tag	UNP O15553
D	786	LEU	-	expression tag	UNP O15553
D	787	PHE	-	expression tag	UNP O15553
D	788	GLN	-	expression tag	UNP O15553
E	412	ACE	-	expression tag	UNP O15553
E	413	SER	-	expression tag	UNP O15553
E	782	ALA	-	expression tag	UNP O15553
E	783	LEU	-	expression tag	UNP O15553
E	784	GLU	-	expression tag	UNP O15553
E	785	VAL	-	expression tag	UNP O15553
E	786	LEU	-	expression tag	UNP O15553
E	787	PHE	-	expression tag	UNP O15553
E	788	GLN	-	expression tag	UNP O15553
F	412	ACE	-	expression tag	UNP O15553
F	413	SER	-	expression tag	UNP O15553
F	782	ALA	-	expression tag	UNP O15553
F	783	LEU	-	expression tag	UNP O15553
F	784	GLU	-	expression tag	UNP O15553
F	785	VAL	-	expression tag	UNP O15553
F	786	LEU	-	expression tag	UNP O15553
F	787	PHE	-	expression tag	UNP O15553
F	788	GLN	-	expression tag	UNP O15553

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



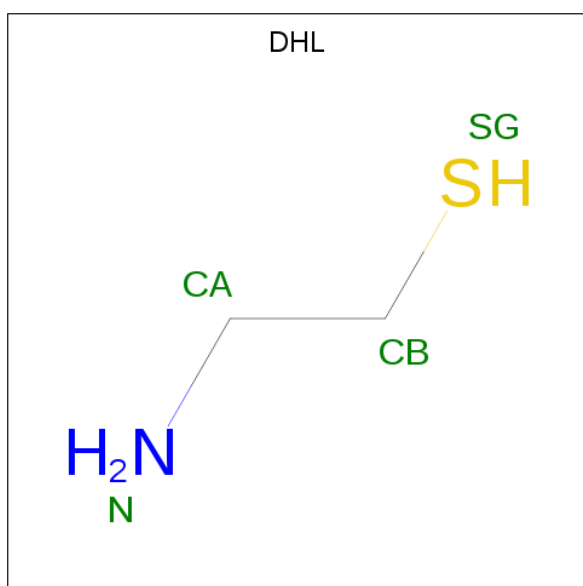
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is 2-AMINO-ETHANETHIOL (three-letter code: DHL) (formula:  $C_2H_7NS$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	H	N	S	0	0
			10	2	6	1	1		
4	C	1	Total	C	H	N	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	H	N	S	0	0
			10	2	6	1	1		
4	E	1	Total	C	H	N	S	0	0
			10	2	6	1	1		
4	F	1	Total	C	H	N	S	0	0
			10	2	6	1	1		

- Molecule 5 is water.

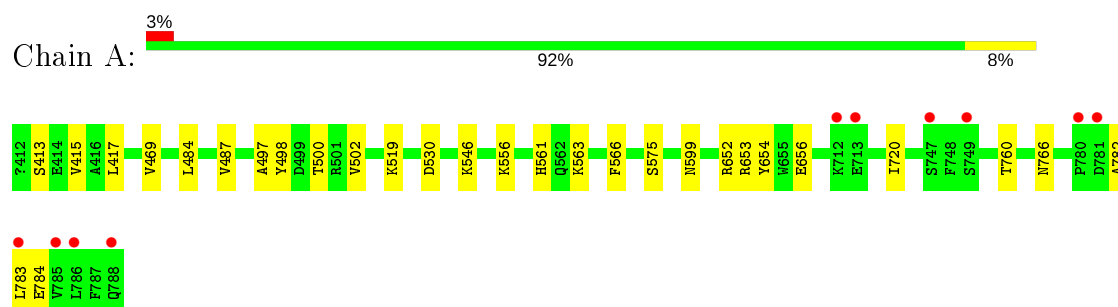
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	6	Total	O	0	0
			6	6		
5	C	9	Total	O	0	0
			9	9		
5	D	3	Total	O	0	0
			3	3		
5	E	7	Total	O	0	0
			7	7		
5	F	1	Total	O	0	0
			1	1		



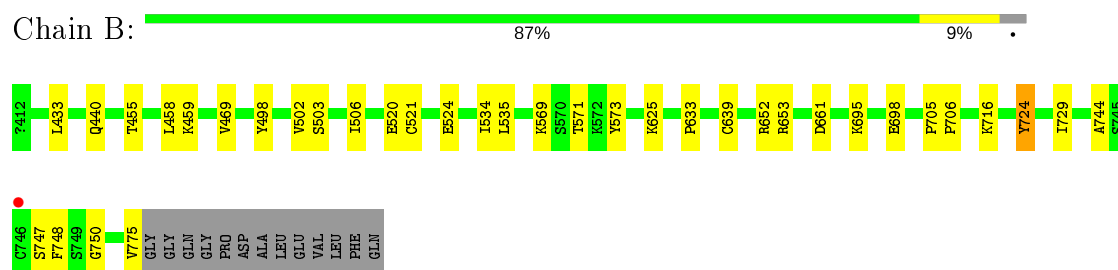
### 3 Residue-property plots [i](#)

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.

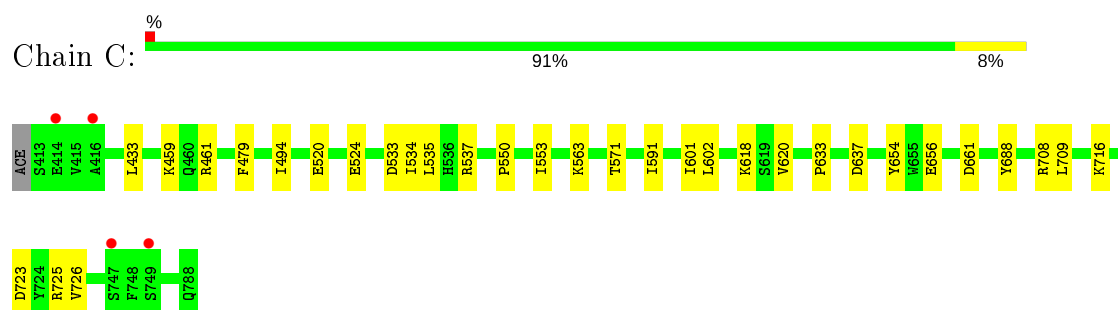
#### • Molecule 1: PYRIN



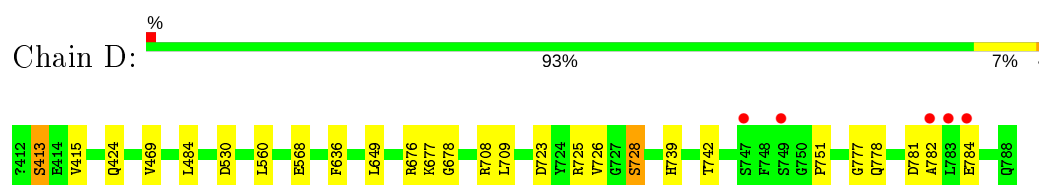
#### • Molecule 1: PYRIN



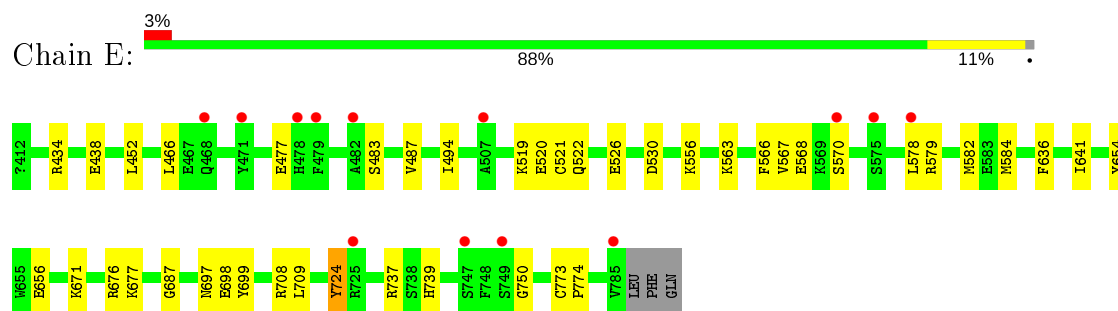
#### • Molecule 1: PYRIN



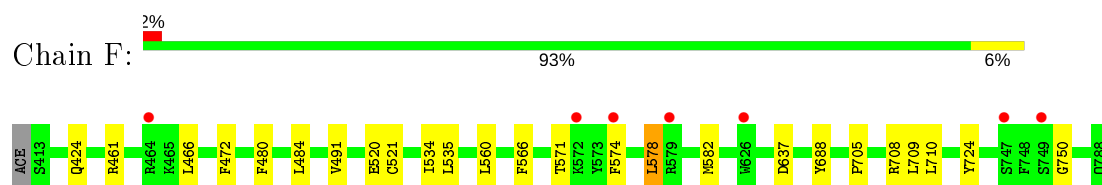
#### • Molecule 1: PYRIN



- Molecule 1: PYRIN



- Molecule 1: PYRIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.82Å 388.21Å 70.88Å 90.00° 116.52° 90.00°	Depositor
Resolution (Å)	48.53 – 2.40 48.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.53-2.40) 99.0 (48.53-2.40)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.211 , 0.261 0.213 , 0.263	Depositor DCC
$R_{free}$ test set	6471 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	36045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DHL, SO4, ACE, 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	0.58	0/3075	0.68	0/4153
1	B	0.64	2/2979 (0.1%)	0.70	1/4024 (0.0%)
1	C	0.57	0/3074	0.67	0/4151
1	D	0.58	0/3075	0.68	0/4153
1	E	0.57	0/3045	0.71	0/4114
1	F	0.58	1/3074 (0.0%)	0.70	0/4151
All	All	0.59	3/18322 (0.0%)	0.69	1/24746 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	705	PRO	N-CD	5.56	1.55	1.47
1	F	705	PRO	N-CD	5.16	1.55	1.47
1	B	706	PRO	N-CD	5.07	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	PRO	C-N-CD	5.41	139.76	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	782	ALA	Peptide

## 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	3012	3020	3021	20	0
1	B	2918	2927	2934	26	0
1	C	3009	3008	3015	23	0
1	D	3012	3015	3020	24	0
1	E	2983	2976	2992	36	0
1	F	3009	3013	3016	21	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	2	0
2	E	15	0	0	0	0
2	F	5	0	0	0	0
3	B	4	6	6	0	0
3	D	4	6	6	0	0
4	C	8	12	12	1	0
4	D	4	6	6	2	0
4	E	4	6	6	1	0
4	F	4	6	6	1	0
5	A	7	0	0	0	0
5	B	6	0	0	0	0
5	C	9	0	0	1	0
5	D	3	0	0	0	0
5	E	7	0	0	0	0
5	F	1	0	0	0	0
All	All	18044	18001	18040	120	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 3.

All (120) 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:E:522:GLN:HB3	1:E:526:GLU:HG3	1.51	0.91
1:C:533:ASP:OD1	1:C:537:ARG:NH1	2.05	0.90
1:E:708:ARG:NH1	1:E:709:LEU:O	2.05	0.90
1:D:484:LEU:HD23	1:D:560:LEU:HD13	1.68	0.74
1:E:434:ARG:NH1	1:E:438:GLU:OE2	2.23	0.71
1:E:724:TYR:OH	1:E:750:GLY:O	2.10	0.68
1:E:697:ASN:O	1:E:708:ARG:NH2	2.28	0.67
1:C:637:ASP:OD2	5:C:2003:HOH:O	2.14	0.66
1:A:546:LYS:HA	1:B:440:GLN:HG2	1.82	0.61
1:D:678:GLY:O	4:D:3:DHL:N	2.34	0.60
1:C:459:LYS:HB2	1:D:484:LEU:HD13	1.83	0.60
1:B:661:ASP:OD1	1:B:716:LYS:HE3	2.03	0.58
1:E:698:GLU:HA	1:E:708:ARG:NH2	2.19	0.58
1:A:519:LYS:NZ	1:A:530:ASP:OD1	2.34	0.58
1:F:708:ARG:NH1	1:F:709:LEU:O	2.37	0.58
1:A:530:ASP:N	1:A:530:ASP:OD1	2.36	0.58
1:E:520:GLU:OE2	1:F:424:GLN:OE1	2.23	0.56
1:D:413:SER:HB2	1:D:415:VAL:HG12	1.87	0.55
1:E:530:ASP:OD1	1:E:530:ASP:N	2.37	0.55
1:B:503:SER:O	1:B:506:ILE:HG13	2.07	0.55
1:A:599:ASN:HB3	1:A:784:GLU:OE1	2.07	0.55
1:A:484:LEU:HD21	1:B:459:LYS:HG3	1.89	0.55
1:A:561:HIS:CD2	1:B:458:LEU:HD11	2.42	0.54
1:F:484:LEU:CD1	1:F:560:LEU:HD11	2.38	0.54
1:D:725:ARG:NH2	2:D:1789:SO4:S	2.81	0.53
1:B:775:VAL:HG23	1:B:775:VAL:O	2.07	0.53
1:B:775:VAL:HG21	1:C:591:ILE:CD1	2.38	0.53
1:C:661:ASP:OD1	1:C:716:LYS:HE3	2.08	0.53
1:C:494:ILE:HD13	1:C:550:PRO:HG2	1.91	0.53
1:A:498:TYR:CZ	1:A:502:VAL:HG11	2.44	0.52
1:E:519:LYS:NZ	1:E:530:ASP:OD1	2.34	0.52
1:C:520:GLU:OE2	1:D:424:GLN:NE2	2.43	0.52
1:B:569:LYS:NZ	1:B:573:TYR:OH	2.42	0.52
1:C:524:GLU:OE2	1:D:413:SER:OG	2.27	0.51
1:D:781:ASP:HB3	1:D:784:GLU:OE2	2.11	0.51
1:A:497:ALA:O	1:A:500:THR:HG22	2.10	0.51
1:B:633:PRO:HB3	1:C:433:LEU:HD22	1.92	0.51
1:D:725:ARG:HG3	1:D:726:VAL:HG13	1.92	0.51
1:D:636:PHE:CE1	1:D:676:ARG:HD3	2.46	0.51
1:E:578:LEU:HD12	1:F:566:PHE:CZ	2.47	0.50
1:C:461:ARG:NH2	1:D:568:GLU:OE1	2.45	0.50
1:C:723:ASP:OD1	1:C:725:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:578:LEU:HD11	1:F:566:PHE:CE2	2.47	0.49
1:D:636:PHE:CZ	1:D:676:ARG:HD3	2.48	0.48
1:F:480:PHE:O	1:F:484:LEU:HD13	2.14	0.48
1:F:574:PHE:CE1	1:F:578:LEU:HD11	2.49	0.48
1:A:487:VAL:HG11	1:B:455:THR:HG21	1.95	0.48
1:E:578:LEU:CD1	1:F:566:PHE:CZ	2.97	0.48
1:E:522:GLN:HB3	1:E:526:GLU:CG	2.35	0.47
1:E:579:ARG:O	1:E:582:MET:HG2	2.14	0.47
1:F:724:TYR:OH	1:F:750:GLY:O	2.27	0.47
1:D:725:ARG:NH2	2:D:1789:SO4:O2	2.48	0.47
1:D:530:ASP:N	1:D:530:ASP:OD1	2.47	0.47
1:E:578:LEU:HD23	1:F:472:PHE:CE2	2.51	0.46
1:A:469:VAL:HG21	1:B:571:THR:HG22	1.97	0.46
1:B:433:LEU:HD22	1:C:633:PRO:HB3	1.96	0.46
1:F:688:TYR:OH	4:F:5:DHL:HB3	2.16	0.46
1:C:725:ARG:HG3	1:C:726:VAL:HG13	1.98	0.46
1:B:520:GLU:O	1:B:521:CYS:HB2	2.16	0.46
1:E:578:LEU:CD2	1:F:472:PHE:CE2	2.98	0.46
1:D:778:GLN:O	1:E:737:ARG:NH1	2.44	0.46
1:A:487:VAL:HG22	1:A:556:LYS:HB3	1.97	0.45
1:A:575:SER:HB2	1:B:469:VAL:HG22	1.97	0.45
1:E:654:TYR:CE2	1:E:656:GLU:HG3	2.52	0.45
1:C:571:THR:HA	1:D:469:VAL:HG21	1.99	0.45
1:E:477:GLU:HG3	1:F:466:LEU:CD2	2.47	0.45
1:E:487:VAL:HG22	1:E:556:LYS:HB3	1.99	0.45
1:C:654:TYR:CE2	1:C:656:GLU:HG3	2.51	0.44
1:D:649:LEU:HD23	1:D:751:PRO:HB3	2.00	0.44
1:D:777:GLY:H	1:E:737:ARG:NH1	2.16	0.44
1:D:484:LEU:CD2	1:D:560:LEU:HD13	2.41	0.44
1:E:570:SER:HB3	1:F:578:LEU:HD21	2.00	0.44
1:A:413:SER:OG	1:B:524:GLU:OE2	2.27	0.44
1:C:534:ILE:HG23	1:C:535:LEU:N	2.33	0.44
1:B:744:ALA:O	1:B:747:SER:OG	2.32	0.44
1:C:708:ARG:NH1	1:C:709:LEU:O	2.50	0.44
1:B:652:ARG:O	1:B:653:ARG:HD3	2.18	0.44
1:E:579:ARG:HA	1:E:582:MET:HG2	1.99	0.44
1:C:602:LEU:HD13	1:C:620:VAL:HB	2.00	0.43
1:E:636:PHE:CD2	1:E:641:ILE:HD11	2.53	0.43
1:D:677:LYS:O	4:D:3:DHL:N	2.52	0.43
1:A:654:TYR:CE2	1:A:656:GLU:HG3	2.54	0.43
1:E:773:CYS:HA	1:E:774:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:520:GLU:HG3	1:F:521:CYS:N	2.33	0.43
1:B:534:ILE:HG23	1:B:535:LEU:N	2.34	0.43
1:E:671:LYS:HE2	1:E:687:GLY:CA	2.49	0.43
1:C:479:PHE:CZ	1:C:563:LYS:HE2	2.53	0.43
1:E:677:LYS:O	4:E:4:DHL:HA3	2.19	0.43
1:A:760:THR:O	1:A:766:ASN:HB3	2.18	0.42
1:B:498:TYR:O	1:B:502:VAL:HG12	2.19	0.42
1:D:708:ARG:NH1	1:D:709:LEU:O	2.52	0.42
1:E:699:TYR:H	1:E:708:ARG:NH1	2.17	0.42
1:B:569:LYS:HZ2	1:B:573:TYR:HE2	1.67	0.42
1:B:748:PHE:C	1:B:748:PHE:CD1	2.93	0.42
1:E:699:TYR:O	1:E:708:ARG:NH1	2.52	0.42
1:A:413:SER:O	1:A:417:LEU:HG	2.20	0.42
1:A:652:ARG:O	1:A:653:ARG:HD3	2.20	0.42
1:E:563:LYS:O	1:E:567:VAL:HG23	2.20	0.42
1:A:563:LYS:O	1:A:566:PHE:HB3	2.20	0.42
1:D:723:ASP:OD1	1:D:725:ARG:HG2	2.19	0.42
1:E:434:ARG:HH11	1:E:434:ARG:HG3	1.85	0.41
1:E:466:LEU:HD12	1:F:571:THR:HG21	2.02	0.41
1:B:625:LYS:HD3	1:B:625:LYS:N	2.35	0.41
1:B:775:VAL:HG21	1:C:591:ILE:HD12	2.01	0.41
1:D:739:HIS:NE2	1:D:742:THR:OG1	2.43	0.41
1:A:782:ALA:HA	1:A:783:LEU:HA	1.91	0.41
1:B:695:LYS:HE2	1:B:698:GLU:OE1	2.19	0.41
1:F:484:LEU:HD11	1:F:560:LEU:HD11	2.02	0.41
1:C:688:TYR:OH	4:C:1:DHL:HB3	2.20	0.41
1:E:568:GLU:OE1	1:F:461:ARG:NE	2.50	0.41
1:E:452:LEU:HD21	1:F:491:VAL:CG2	2.50	0.41
1:E:566:PHE:CE1	1:F:582:MET:HG2	2.56	0.41
1:B:729:ILE:HG13	1:B:748:PHE:HE2	1.86	0.41
1:F:534:ILE:HG23	1:F:535:LEU:N	2.35	0.41
1:B:724:TYR:OH	1:B:750:GLY:O	2.23	0.40
1:C:601:ILE:HG22	1:C:618:LYS:HE2	2.03	0.40
1:E:584:MET:HG3	1:E:739:HIS:HB3	2.03	0.40
1:A:720:ILE:HD12	1:A:720:ILE:N	2.37	0.40
1:C:550:PRO:HD2	1:C:553:ILE:HD12	2.04	0.40
1:D:726:VAL:HG23	1:D:728:SER:OG	2.21	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	A	375/377 (100%)	366 (98%)	9 (2%)	0	100	100
1	B	362/377 (96%)	358 (99%)	4 (1%)	0	100	100
1	C	374/377 (99%)	369 (99%)	5 (1%)	0	100	100
1	D	375/377 (100%)	369 (98%)	6 (2%)	0	100	100
1	E	372/377 (99%)	366 (98%)	6 (2%)	0	100	100
1	F	374/377 (99%)	370 (99%)	4 (1%)	0	100	100
All	All	2232/2262 (99%)	2198 (98%)	34 (2%)	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	A	331/331 (100%)	330 (100%)	1 (0%)	92	97
1	B	322/331 (97%)	320 (99%)	2 (1%)	86	94
1	C	331/331 (100%)	331 (100%)	0	100	100
1	D	331/331 (100%)	329 (99%)	2 (1%)	86	94
1	E	328/331 (99%)	323 (98%)	5 (2%)	65	80
1	F	331/331 (100%)	328 (99%)	3 (1%)	78	90
All	All	1974/1986 (99%)	1961 (99%)	13 (1%)	84	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	VAL
1	B	639	CYS
1	B	724	TYR
1	D	413	SER
1	D	728	SER
1	E	483	SER
1	E	494	ILE
1	E	521	CYS
1	E	676	ARG
1	E	724	TYR
1	F	578	LEU
1	F	637	ASP
1	F	710	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	HIS
1	B	558	GLN
1	B	561	HIS
1	E	558	GLN
1	F	555	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 ⓘ

15 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	SO4	B	1777	-	4,4,4	0.23	0	6,6,6	0.42	0
4	DHL	C	1	1	2,3,3	0.98	0	1,2,2	0.72	0
4	DHL	F	5	1	2,3,3	0.81	0	1,2,2	0.86	0
2	SO4	C	1789	-	4,4,4	0.09	0	6,6,6	0.28	0
3	EDO	D	1790	-	3,3,3	0.36	0	2,2,2	0.75	0
4	DHL	C	2	1	2,3,3	0.79	0	1,2,2	0.79	0
3	EDO	B	1778	-	3,3,3	0.46	0	2,2,2	0.30	0
2	SO4	E	1787	-	4,4,4	0.14	0	6,6,6	0.26	0
2	SO4	E	1788	-	4,4,4	0.11	0	6,6,6	0.14	0
4	DHL	D	3	1	2,3,3	0.89	0	1,2,2	1.15	0
2	SO4	B	1776	-	4,4,4	0.16	0	6,6,6	0.45	0
2	SO4	D	1789	-	4,4,4	0.25	0	6,6,6	0.38	0
2	SO4	E	1786	-	4,4,4	0.17	0	6,6,6	0.40	0
4	DHL	E	4	1	2,3,3	0.49	0	1,2,2	0.42	0
2	SO4	F	1789	-	4,4,4	0.09	0	6,6,6	0.48	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	DHL	C	1	1	-	0/1/1/1	-
4	DHL	F	5	1	-	0/1/1/1	-
4	DHL	C	2	1	-	1/1/1/1	-
3	EDO	B	1778	-	-	1/1/1/1	-
4	DHL	D	3	1	-	1/1/1/1	-
4	DHL	E	4	1	-	1/1/1/1	-
3	EDO	D	1790	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	DHL	N-CA-CB-SG
4	E	4	DHL	N-CA-CB-SG
4	D	3	DHL	N-CA-CB-SG
3	B	1778	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	DHL	1	0
4	F	5	DHL	1	0
4	D	3	DHL	2	0
2	D	1789	SO4	2	0
4	E	4	DHL	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	376/377 (99%)	0.12	10 (2%) 54 52	29, 50, 79, 121	0
1	B	363/377 (96%)	-0.01	1 (0%) 94 93	29, 49, 72, 102	0
1	C	376/377 (99%)	-0.02	4 (1%) 80 79	29, 49, 75, 104	0
1	D	376/377 (99%)	0.02	5 (1%) 77 75	32, 50, 79, 113	0
1	E	373/377 (98%)	0.17	13 (3%) 44 43	31, 52, 93, 110	0
1	F	376/377 (99%)	0.20	7 (1%) 66 64	36, 57, 90, 107	0
All	All	2240/2262 (99%)	0.08	40 (1%) 68 66	29, 51, 85, 121	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	782	ALA	6.5
1	A	786	LEU	6.0
1	C	749	SER	5.9
1	A	785	VAL	5.8
1	F	574	PHE	4.9
1	A	783	LEU	4.6
1	E	747	SER	4.2
1	E	482	ALA	4.1
1	E	479	PHE	4.0
1	F	747	SER	3.8
1	F	572	LYS	3.8
1	E	570	SER	3.8
1	E	575	SER	3.6
1	A	747	SER	3.3
1	E	578	LEU	3.2
1	F	749	SER	3.2
1	A	780	PRO	3.2
1	F	626	TRP	3.1
1	A	788	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	749	SER	2.9
1	E	785	VAL	2.9
1	E	468	GLN	2.9
1	A	712	LYS	2.9
1	C	414	GLU	2.8
1	C	747	SER	2.8
1	D	783	LEU	2.8
1	A	781	ASP	2.7
1	E	725	ARG	2.6
1	D	784	GLU	2.6
1	C	416	ALA	2.4
1	E	478	HIS	2.4
1	A	749	SER	2.4
1	D	747	SER	2.3
1	E	507	ALA	2.3
1	D	749	SER	2.2
1	F	579	ARG	2.2
1	A	713	GLU	2.2
1	E	471	TYR	2.1
1	B	746	CYS	2.0
1	F	464	ARG	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	1789	5/5	0.81	0.19	74,79,91,91	0
2	SO4	C	1789	5/5	0.87	0.20	87,94,95,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	1778	4/4	0.90	0.20	39,61,73,84	0
2	SO4	B	1777	5/5	0.92	0.17	58,76,83,85	0
2	SO4	E	1788	5/5	0.92	0.18	91,93,97,101	0
4	DHL	D	3	4/4	0.92	0.22	64,77,88,88	0
4	DHL	C	2	4/4	0.92	0.17	51,61,64,64	0
2	SO4	F	1789	5/5	0.92	0.18	60,64,65,79	0
4	DHL	E	4	4/4	0.94	0.16	30,41,51,51	0
3	EDO	D	1790	4/4	0.95	0.15	39,47,53,64	0
2	SO4	E	1786	5/5	0.96	0.11	56,61,75,77	0
2	SO4	E	1787	5/5	0.96	0.10	76,83,86,96	0
4	DHL	F	5	4/4	0.96	0.15	44,54,75,75	0
4	DHL	C	1	4/4	0.97	0.11	38,45,47,48	0
2	SO4	B	1776	5/5	0.98	0.15	56,61,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.