wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 09:00 PM EDT

PDB ID	:	1XP4
Title	:	Crystal structure of a peptidoglycan synthesis regulatory factor (PBP3) from Streptococcus pneumoniae
Authors	:	Morlot, C.; Pernot, L.; Le Gouellec, A.; Di Guilmi, A.M.; Vernet, T.; Dideberg, O.; Dessen, A.
Deposited on	:	2004-10-08
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

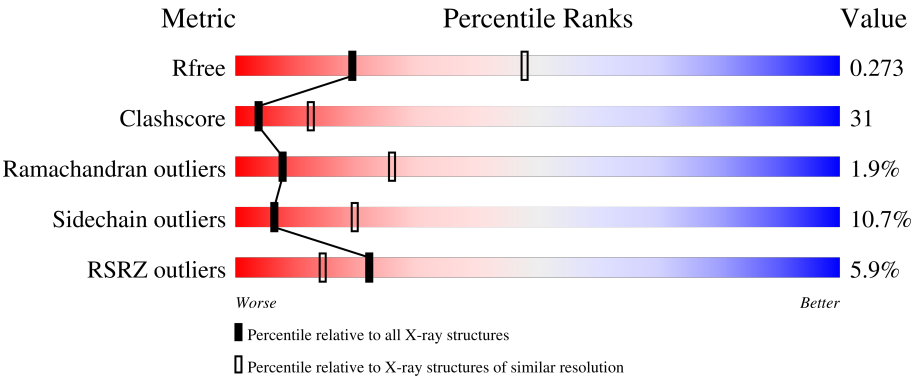
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	5% 57% 32% 5% • •
1	B	379	7% 48% 31% 7% • 11%
1	C	379	4% 56% 32% 5% • 5%
1	D	379	5% 45% 33% 5% • 15%

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	IOD	A	468	-	-	X	-
3	IOD	B	472	-	-	X	-
3	IOD	C	476	-	-	X	-
3	IOD	D	481	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11150 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 D-alanyl-D-alanine carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	Se	0	0	0
			2821	1775	457	580	9			
1	B	339	Total	C	N	O	Se	49	0	0
			2602	1642	420	531	9			
1	C	359	Total	C	N	O	Se	72	0	0
			2750	1731	445	565	9			
1	D	321	Total	C	N	O	Se	27	0	0
			2480	1571	398	502	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MSE	MET	modified residue	UNP Q8DQ99
A	141	MSE	MET	modified residue	UNP Q8DQ99
A	142	MSE	MET	modified residue	UNP Q8DQ99
A	216	MSE	MET	modified residue	UNP Q8DQ99
A	224	MSE	MET	modified residue	UNP Q8DQ99
A	228	MSE	MET	modified residue	UNP Q8DQ99
A	259	MSE	MET	modified residue	UNP Q8DQ99
A	286	MSE	MET	modified residue	UNP Q8DQ99
A	386	MSE	MET	modified residue	UNP Q8DQ99
B	101	MSE	MET	modified residue	UNP Q8DQ99
B	141	MSE	MET	modified residue	UNP Q8DQ99
B	142	MSE	MET	modified residue	UNP Q8DQ99
B	216	MSE	MET	modified residue	UNP Q8DQ99
B	224	MSE	MET	modified residue	UNP Q8DQ99
B	228	MSE	MET	modified residue	UNP Q8DQ99
B	259	MSE	MET	modified residue	UNP Q8DQ99
B	286	MSE	MET	modified residue	UNP Q8DQ99
B	386	MSE	MET	modified residue	UNP Q8DQ99
C	101	MSE	MET	modified residue	UNP Q8DQ99
C	141	MSE	MET	modified residue	UNP Q8DQ99
C	142	MSE	MET	modified residue	UNP Q8DQ99

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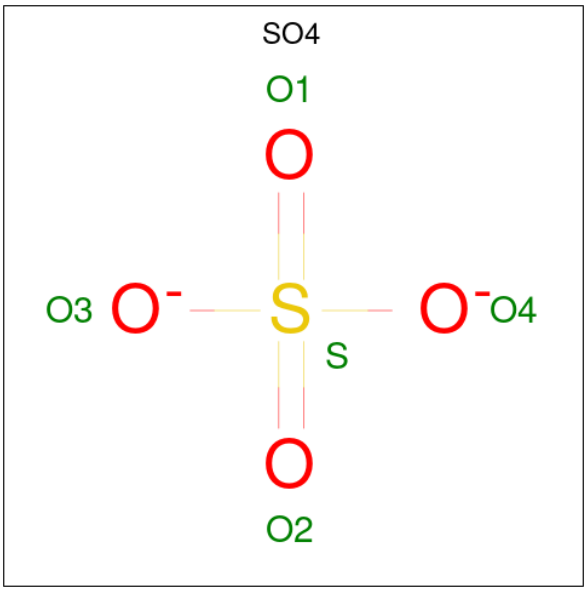
Chain	Residue	Modelled	Actual	Comment	Reference
C	216	MSE	MET	modified residue	UNP Q8DQ99
C	224	MSE	MET	modified residue	UNP Q8DQ99
C	228	MSE	MET	modified residue	UNP Q8DQ99
C	259	MSE	MET	modified residue	UNP Q8DQ99
C	286	MSE	MET	modified residue	UNP Q8DQ99
C	386	MSE	MET	modified residue	UNP Q8DQ99
D	101	MSE	MET	modified residue	UNP Q8DQ99
D	141	MSE	MET	modified residue	UNP Q8DQ99
D	142	MSE	MET	modified residue	UNP Q8DQ99
D	216	MSE	MET	modified residue	UNP Q8DQ99
D	224	MSE	MET	modified residue	UNP Q8DQ99
D	228	MSE	MET	modified residue	UNP Q8DQ99
D	259	MSE	MET	modified residue	UNP Q8DQ99
D	286	MSE	MET	modified residue	UNP Q8DQ99
D	386	MSE	MET	modified residue	UNP Q8DQ99

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total I 4 4	0	0
3	B	4	Total I 4 4	0	0
3	C	4	Total I 4 4	0	0
3	D	4	Total I 4 4	0	0

- Molecule 4 is water.

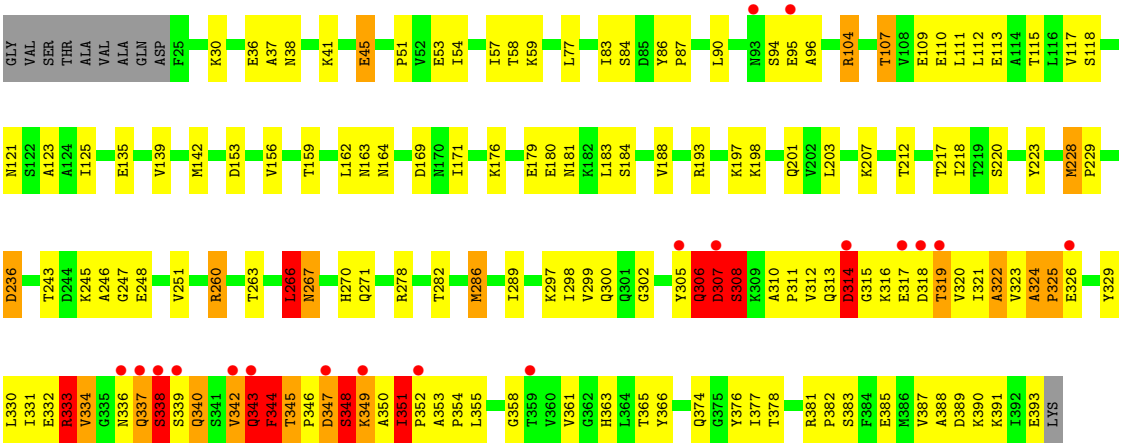
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	139	Total O 139 139	1	0
4	B	98	Total O 98 98	0	0
4	C	121	Total O 121 121	0	0
4	D	103	Total O 103 103	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

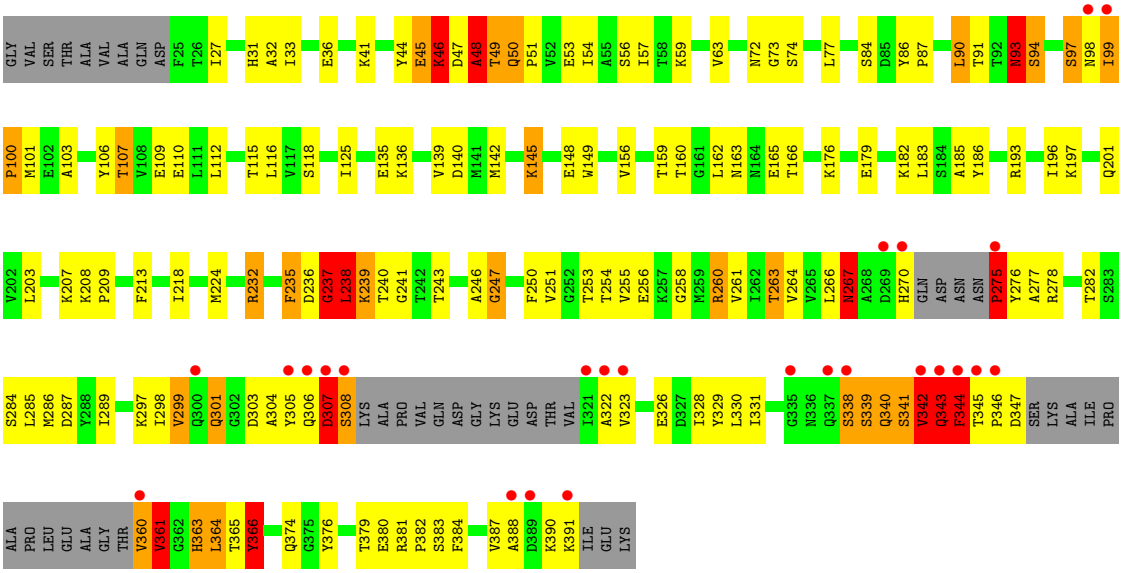
• Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain A:



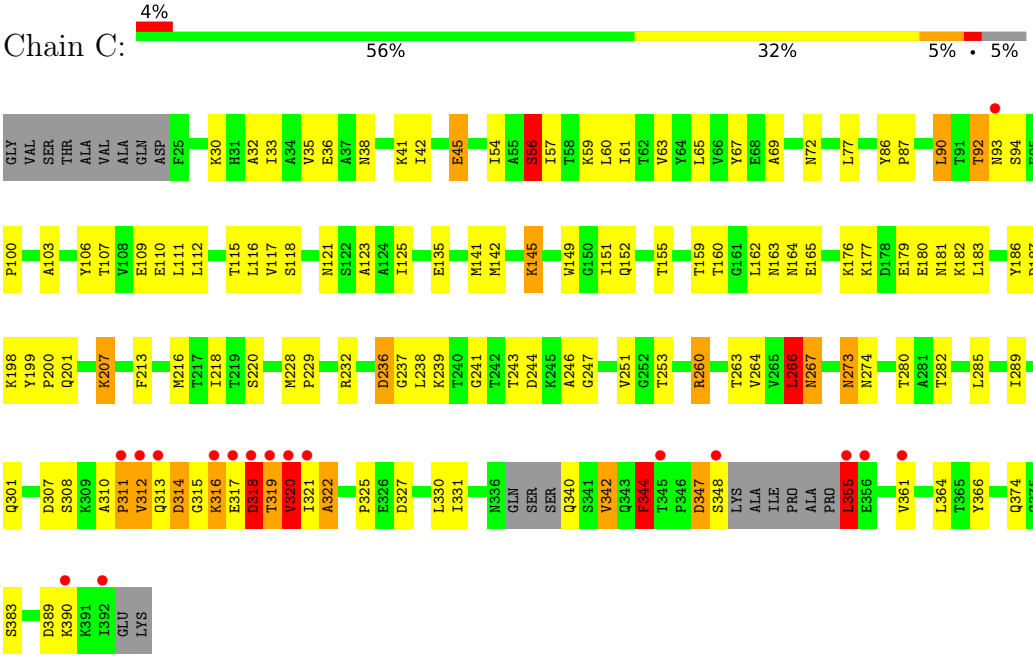
• Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain B:



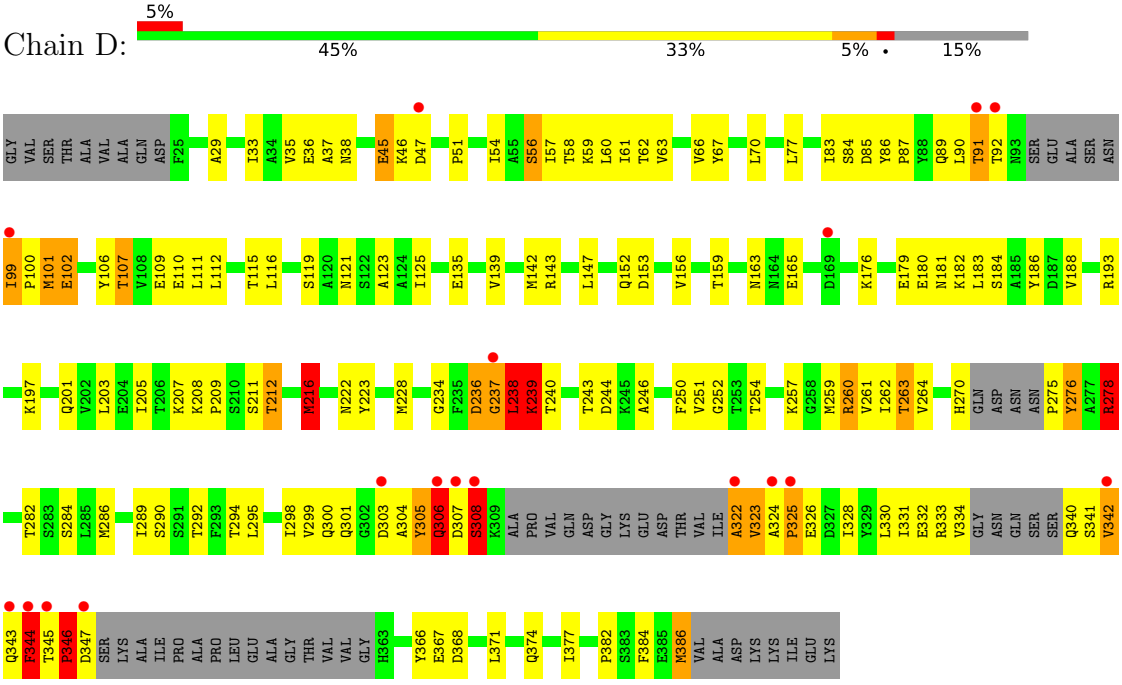
• Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain C:



• Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.61Å 120.84Å 177.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.84 – 2.80 65.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.84-2.80) 99.9 (65.84-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.278 0.234 , 0.273	Depositor DCC
R_{free} test set	3309 reflections (7.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11150	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, IOD

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	0.62	1/2857 (0.0%)	1.02	16/3868 (0.4%)
1	B	0.50	0/2632	0.96	12/3555 (0.3%)
1	C	0.55	1/2782 (0.0%)	0.91	11/3762 (0.3%)
1	D	0.48	0/2508	0.91	11/3384 (0.3%)
All	All	0.54	2/10779 (0.0%)	0.95	50/14569 (0.3%)

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	A	0	14
1	B	0	15
1	C	2	8
1	D	0	6
All	All	2	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	PHE	C-N	18.73	1.77	1.34
1	C	266	LEU	C-O	16.93	1.55	1.23

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SER	O-C-N	-17.82	94.19	122.70
1	C	266	LEU	O-C-N	-17.40	94.86	122.70
1	B	275	PRO	CA-N-CD	-16.95	87.76	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	275	PRO	CA-N-CD	-16.85	87.91	111.50
1	C	311	PRO	CA-N-CD	-14.77	90.82	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	318	ASP	CA
1	C	343	GLN	CA

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LEU	Peptide
1	A	308	SER	Mainchain
1	A	314	ASP	Sidechain
1	A	315	GLY	Peptide
1	A	317	GLU	Mainchain

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	2821	0	2801	178	0
1	B	2602	0	2586	168	1
1	C	2750	0	2728	139	1
1	D	2480	0	2467	173	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	4	0	0	2	0
3	B	4	0	0	2	0
3	C	4	0	0	2	0
3	D	4	0	0	3	0
4	A	139	0	0	6	0
4	B	98	0	0	2	0
4	C	121	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	103	0	0	5	0
All	All	11150	0	10582	646	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 31.

The worst 5 of 646 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:A:344:PHE:C	1:A:345:THR:N	1.77	1.38
1:C:243:THR:HG22	1:C:246:ALA:CB	1.63	1.27
1:B:305:TYR:OH	1:B:343:GLN:HB3	1.28	1.25
1:B:237:GLY:HA3	1:B:253:THR:CG2	1.67	1.24
1:B:342:VAL:CG2	1:B:342:VAL:O	1.81	1.24

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:51:PRO:CD	1:C:344:PHE:CZ[3_545]	1.79	0.41

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	367/379 (97%)	329 (90%)	31 (8%)	7 (2%)	8 26
1	B	331/379 (87%)	290 (88%)	33 (10%)	8 (2%)	6 20
1	C	353/379 (93%)	320 (91%)	29 (8%)	4 (1%)	14 41
1	D	309/379 (82%)	280 (91%)	22 (7%)	7 (2%)	6 21
All	All	1360/1516 (90%)	1219 (90%)	115 (8%)	26 (2%)	8 26

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASP
1	A	337	GLN
1	B	93	ASN
1	B	247	GLY
1	B	306	GLN

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	310/308 (101%)	279 (90%)	31 (10%)	7	22
1	B	286/308 (93%)	247 (86%)	39 (14%)	3	11
1	C	302/308 (98%)	275 (91%)	27 (9%)	9	28
1	D	272/308 (88%)	244 (90%)	28 (10%)	7	21
All	All	1170/1232 (95%)	1045 (89%)	125 (11%)	6	20

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	307	ASP
1	D	244	ASP
1	C	56	SER
1	D	239	LYS
1	D	306	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	274	ASN
1	D	306	GLN
1	D	300	GLN
1	B	340	GLN
1	C	273	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	SO4	D	467	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	C	466	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	B	465	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	A	464	-	4,4,4	0.27	0	6,6,6	0.14	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	344:PHE	C	345:THR	N	1.77

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	360/379 (94%)	0.09	19 (5%)	26	17	7, 20, 65, 82	0
1	B	323/379 (85%)	0.23	25 (7%)	13	7	9, 22, 72, 85	0
1	C	341/379 (89%)	0.17	17 (4%)	28	19	9, 23, 67, 88	0
1	D	309/379 (81%)	0.05	18 (5%)	23	15	7, 20, 61, 88	0
All	All	1333/1516 (87%)	0.14	79 (5%)	22	14	7, 22, 68, 88	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	GLN	8.0
1	A	318	ASP	7.6
1	C	316	LYS	6.5
1	C	318	ASP	5.9
1	A	338	SER	5.8

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 monosaccharides 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IOD	C	478	1/1	0.85	0.12	76,76,76,76	1
3	IOD	A	470	1/1	0.92	0.11	66,66,66,66	1
2	SO4	B	465	5/5	0.92	0.18	48,49,51,52	0
3	IOD	B	475	1/1	0.94	0.11	56,56,56,56	1
2	SO4	C	466	5/5	0.94	0.20	60,61,63,63	0
3	IOD	C	479	1/1	0.94	0.12	44,44,44,44	1
2	SO4	A	464	5/5	0.95	0.20	48,52,54,54	0
3	IOD	D	482	1/1	0.95	0.09	56,56,56,56	1
2	SO4	D	467	5/5	0.96	0.19	38,39,41,41	0
3	IOD	B	474	1/1	0.97	0.24	9,9,9,9	1
3	IOD	D	483	1/1	0.97	0.15	44,44,44,44	1
3	IOD	A	471	1/1	0.98	0.14	38,38,38,38	1
3	IOD	B	473	1/1	0.99	0.08	43,43,43,43	0
3	IOD	D	480	1/1	0.99	0.11	43,43,43,43	0
3	IOD	C	477	1/1	0.99	0.10	38,38,38,38	0
3	IOD	A	469	1/1	0.99	0.12	39,39,39,39	0
3	IOD	B	472	1/1	1.00	0.12	19,19,19,19	0
3	IOD	D	481	1/1	1.00	0.13	17,17,17,17	0
3	IOD	A	468	1/1	1.00	0.15	19,19,19,19	0
3	IOD	C	476	1/1	1.00	0.12	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.