



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 AM GMT

PDB ID : 3GZD  
Title : Human selenocysteine lyase, P1 crystal form  
Authors : Karlberg, T.; Hogbom, M.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Schutz, P.; Siponen, M.I.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Schuler, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2009-04-07  
Resolution : 1.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

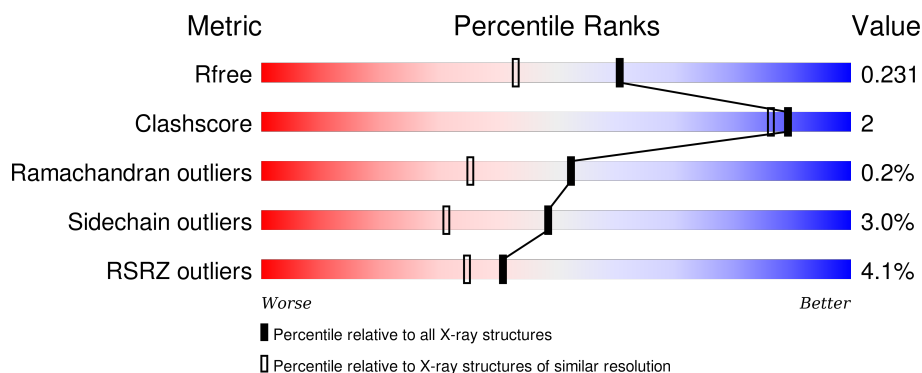
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 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	440	<div> <div>3%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
1	B	440	<div> <div>4%</div> <div>83%</div> <div>6%</div> <div>11%</div> </div>
1	D	440	<div> <div>3%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>
2	C	440	<div> <div>5%</div> <div>83%</div> <div>6%</div> <div>10%</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
4	NO3	A	600	-	X	-	X
4	NO3	B	600	-	X	-	-
4	NO3	C	600	-	X	-	-
4	NO3	D	600	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13184 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 Selenocysteine lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	2	0
			3064	1929	549	571	15			
1	B	392	Total	C	N	O	S	0	1	0
			3027	1906	540	568	13			
1	D	397	Total	C	N	O	S	0	2	0
			3063	1927	547	574	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	SER	-	EXPRESSION TAG	UNP Q96I15
A	7	MET	-	EXPRESSION TAG	UNP Q96I15
A	175	THR	ALA	SEE REMARK 999	UNP Q96I15
B	6	SER	-	EXPRESSION TAG	UNP Q96I15
B	7	MET	-	EXPRESSION TAG	UNP Q96I15
B	175	THR	ALA	SEE REMARK 999	UNP Q96I15
D	6	SER	-	EXPRESSION TAG	UNP Q96I15
D	7	MET	-	EXPRESSION TAG	UNP Q96I15
D	175	THR	ALA	SEE REMARK 999	UNP Q96I15

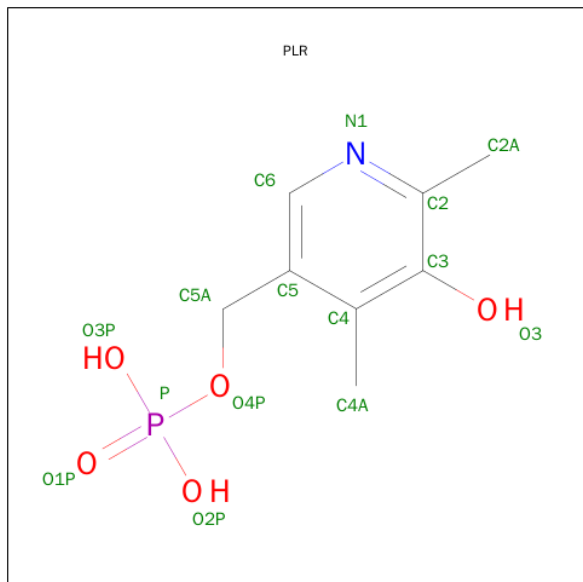
- Molecule 2 is a protein called Selenocysteine lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	396	Total	C	N	O	S	0	2	0
			3056	1923	547	572	14			

There are 3 discrepancies between the modelled and reference sequences:

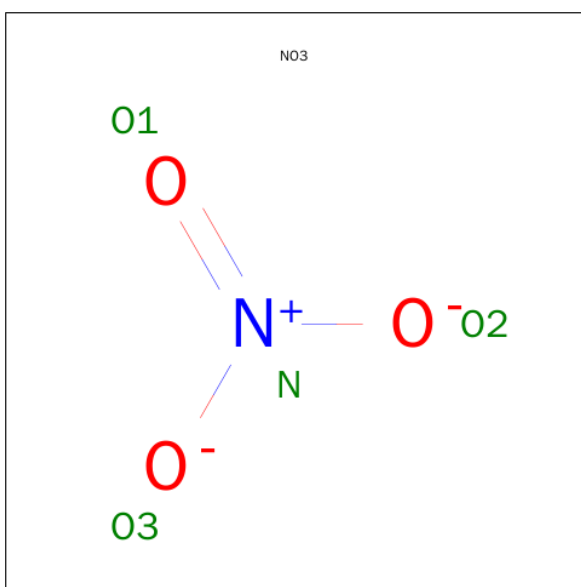
Chain	Residue	Modelled	Actual	Comment	Reference
C	6	SER	-	EXPRESSION TAG	UNP Q96I15
C	7	MET	-	EXPRESSION TAG	UNP Q96I15
C	175	THR	ALA	SEE REMARK 999	UNP Q96I15

- Molecule 3 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula:  $C_8H_{12}NO_5P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula:  $NO_3$ ).

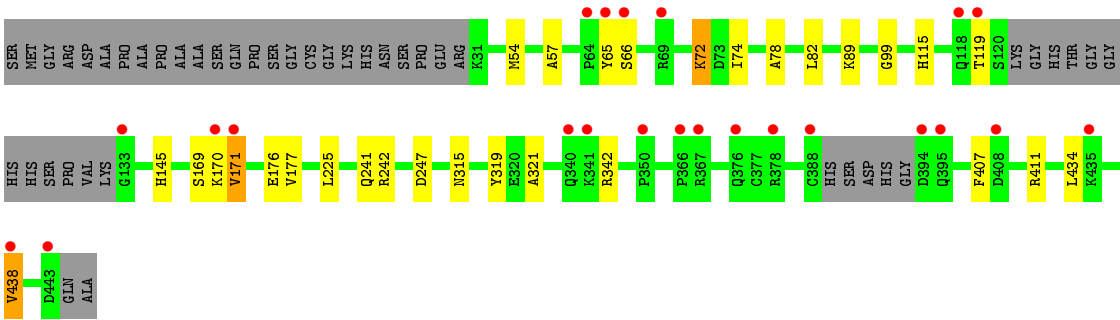


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		
4	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		
5	B	208	Total	O	0	0
			208	208		
5	C	234	Total	O	0	0
			234	234		
5	D	204	Total	O	0	0
			204	204		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.64Å 72.20Å 89.43Å 83.91° 68.39° 86.96°	Depositor
Resolution (Å)	29.59 – 1.80 29.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.59-1.80) 91.3 (29.59-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0035	Depositor
R, $R_{free}$	0.184 , 0.217 0.198 , 0.231	Depositor DCC
$R_{free}$ test set	6724 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 134466 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PLR, CSS, NO3

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	0.67	0/3121	0.70	0/4234
1	B	0.70	0/3085	0.76	2/4187 (0.0%)
1	D	0.65	0/3120	0.71	0/4233
2	C	0.69	0/3120	0.70	0/4234
All	All	0.68	0/12446	0.72	2/16888 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	B	290	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	3064	0	3083	20	0
1	B	3027	0	3036	17	0
1	D	3063	0	3072	14	0
2	C	3056	0	3071	18	0
3	A	15	0	7	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	8	2	0
3	C	15	0	7	2	0
3	D	15	0	9	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	252	0	0	0	0
5	B	208	0	0	0	0
5	C	234	0	0	3	0
5	D	204	0	0	0	0
All	All	13184	0	12293	60	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 2.

All (60) 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:50:MET:CE	1:B:54:MET:HE3	1.99	0.91
1:A:50:MET:HE3	1:B:54:MET:HE3	1.58	0.86
2:C:145:HIS:HB2	3:C:500:PLR:H2A3	1.65	0.79
1:A:50:MET:HE3	1:B:54:MET:CE	2.17	0.73
1:A:50:MET:CE	1:B:54:MET:CE	2.70	0.69
1:A:145:HIS:HB2	3:A:500:PLR:H2A3	1.76	0.68
1:A:369:GLN:HG3	1:A:411:ARG:HG2	1.77	0.65
2:C:115:HIS:O	2:C:119:THR:HG23	1.98	0.63
2:C:321:ALA:HB2	5:C:497:HOH:O	1.97	0.62
1:D:145:HIS:HB2	3:D:500:PLR:H2A3	1.82	0.61
1:B:65:TYR:O	1:B:66:SER:C	2.37	0.59
1:A:326:VAL:CG2	1:A:418:VAL:HG21	2.33	0.58
2:C:99:GLY:HA3	3:C:500:PLR:H5A1	1.86	0.57
1:A:218:GLN:NE2	1:D:218:GLN:OE1	2.38	0.57
2:C:241:GLN:NE2	5:C:530:HOH:O	2.36	0.56
1:A:369:GLN:O	1:A:372:VAL:HG13	2.05	0.56
1:D:366:PRO:HD2	1:D:367:ARG:NH1	2.21	0.55
2:C:242:ARG:NH1	2:C:247:ASP:OD2	2.42	0.53
1:A:119:THR:HG22	1:A:119:THR:O	2.10	0.52
2:C:54:MET:HE3	1:D:54:MET:HE1	1.92	0.52
1:B:145:HIS:HB2	3:B:500:PLR:H2A3	1.92	0.51
2:C:170:LYS:HG3	2:C:170:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:HA3	3:A:500:PLR:H5A1	1.93	0.51
1:A:50:MET:HE2	1:B:54:MET:HE3	1.85	0.51
1:D:177:VAL:HG22	1:D:212:ARG:NH1	2.26	0.50
1:D:367:ARG:H	1:D:367:ARG:CD	2.26	0.49
1:D:216:LEU:HD22	1:D:220:ARG:HG3	1.94	0.48
1:A:50:MET:HE2	1:B:54:MET:CE	2.43	0.48
1:B:78:ALA:O	1:B:82:LEU:HD23	2.14	0.47
2:C:78:ALA:O	2:C:82:LEU:HD23	2.14	0.47
1:A:326:VAL:HG23	1:A:418:VAL:HG21	1.96	0.46
1:A:64:PRO:HA	1:A:69:ARG:CD	2.46	0.46
2:C:65:TYR:O	2:C:66:SER:C	2.53	0.46
2:C:434:LEU:O	2:C:438:VAL:HG13	2.16	0.45
2:C:315:ASN:HB2	2:C:319:TYR:CZ	2.51	0.45
1:D:433:ASP:O	1:D:436:GLN:HG3	2.16	0.45
1:A:256:VAL:HG11	3:A:500:PLR:H5A2	1.99	0.44
1:B:405:VAL:HG12	1:B:410:ALA:HB2	1.99	0.44
1:B:436:GLN:OE1	1:B:440:GLN:NE2	2.49	0.44
1:D:258:HIS:CE1	1:D:259:LYS:HE3	2.52	0.44
1:A:108:HIS:CG	1:A:282:MET:HG2	2.52	0.44
1:B:118:GLN:C	1:B:120:SER:H	2.22	0.43
1:B:342:ARG:NH1	1:B:442:GLU:OE2	2.50	0.43
2:C:57:ALA:CB	2:C:74:ILE:HD12	2.49	0.43
1:A:64:PRO:HA	1:A:69:ARG:HD3	2.01	0.43
1:B:70:LYS:O	1:B:74:ILE:HG12	2.19	0.43
2:C:407:PHE:O	2:C:411:ARG:HG3	2.19	0.42
1:B:108:HIS:CG	1:B:282:MET:HG2	2.54	0.42
2:C:72:LYS:HE3	2:C:72:LYS:HA	2.00	0.42
1:B:108:HIS:CD2	1:B:282:MET:HG2	2.54	0.42
2:C:54:MET:HE1	1:D:54:MET:HE3	2.02	0.42
1:A:322:HIS:NE2	1:A:422:THR:O	2.51	0.42
2:C:169:SER:OG	2:C:171:VAL:HG13	2.20	0.42
2:C:177:VAL:HG23	5:C:607:HOH:O	2.19	0.42
1:D:315:ASN:HB2	1:D:319:TYR:CZ	2.55	0.42
1:B:259:LYS:NZ	3:B:500:PLR:O3	2.51	0.41
1:D:177:VAL:HG11	1:D:208:GLU:CD	2.40	0.41
1:D:150:LEU:HD23	1:D:150:LEU:HA	1.94	0.41
1:D:367:ARG:H	1:D:367:ARG:HD2	1.85	0.40
1:A:146:ASP:OD2	1:A:389:HIS:NE2	2.55	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	392/440 (89%)	383 (98%)	9 (2%)	0	100	100
1	B	387/440 (88%)	374 (97%)	12 (3%)	1 (0%)	46	29
1	D	392/440 (89%)	382 (97%)	8 (2%)	2 (0%)	34	17
2	C	392/440 (89%)	381 (97%)	11 (3%)	0	100	100
All	All	1563/1760 (89%)	1520 (97%)	40 (3%)	3 (0%)	52	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	119	THR
1	B	64	PRO
1	D	64	PRO

### 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	330/359 (92%)	320 (97%)	10 (3%)	48	31
1	B	327/359 (91%)	320 (98%)	7 (2%)	61	47
1	D	330/359 (92%)	314 (95%)	16 (5%)	31	14
2	C	330/360 (92%)	323 (98%)	7 (2%)	61	47
All	All	1317/1437 (92%)	1277 (97%)	40 (3%)	48	31

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	69	ARG
1	A	72	LYS
1	A	120	SER
1	A	170	LYS
1	A	216	LEU
1	A	225	LEU
1	A	283	LEU
1	A	293	ARG
1	A	372	VAL
1	B	169	SER
1	B	199	GLU
1	B	216	LEU
1	B	225	LEU
1	B	293	ARG
1	B	314	GLN
1	B	436	GLN
2	C	72	LYS
2	C	89	LYS
2	C	171	VAL
2	C	176	GLU
2	C	225	LEU
2	C	342	ARG
2	C	438	VAL
1	D	48[A]	GLN
1	D	48[B]	GLN
1	D	65	TYR
1	D	72	LYS
1	D	74	ILE
1	D	171	VAL
1	D	176	GLU
1	D	177	VAL
1	D	211	GLN
1	D	216	LEU
1	D	225	LEU
1	D	283	LEU
1	D	314	GLN
1	D	341	LYS
1	D	367	ARG
1	D	390	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
2	C	91	GLN
2	C	241	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSS	A	388	1	4,6,7	0.78	0	3,6,8	2.07	2 (66%)
1	CSS	D	388	1	4,6,7	0.75	0	3,6,8	1.52	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
1	CSS	A	388	1	-	0/1/5/7	0/0/0/0
1	CSS	D	388	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	CSS	O-C-CA	-2.25	119.63	125.49
1	A	388	CSS	CB-SG-SD	2.42	108.70	103.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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$
3	PLR	A	500	1	15,15,15	1.27	2 (13%)	21,22,22	2.50	6 (28%)
4	NO3	A	600	-	3,3,3	3.20	3 (100%)	3,3,3	0.41	0
3	PLR	B	500	1	15,15,15	0.78	0	21,22,22	2.16	7 (33%)
4	NO3	B	600	-	3,3,3	3.32	3 (100%)	3,3,3	0.43	0
3	PLR	C	500	2	15,15,15	0.73	0	21,22,22	1.48	5 (23%)
4	NO3	C	600	-	3,3,3	3.30	3 (100%)	3,3,3	0.39	0
3	PLR	D	500	1	15,15,15	0.98	1 (6%)	21,22,22	1.76	8 (38%)
4	NO3	D	600	-	3,3,3	3.36	3 (100%)	3,3,3	0.44	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
3	PLR	A	500	1	-	0/6/6/6	0/1/1/1
4	NO3	A	600	-	-	0/0/0/0	0/0/0/0
3	PLR	B	500	1	-	0/6/6/6	0/1/1/1
4	NO3	B	600	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLR	C	500	2	-	0/6/6/6	0/1/1/1
4	NO3	C	600	-	-	0/0/0/0	0/0/0/0
3	PLR	D	500	1	-	0/6/6/6	0/1/1/1
4	NO3	D	600	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	PLR	C3-C2	-2.84	1.38	1.40
3	A	500	PLR	C5-C4	2.01	1.42	1.40
4	C	600	NO3	O3-N	2.50	1.38	1.25
4	B	600	NO3	O3-N	2.71	1.39	1.25
4	D	600	NO3	O2-N	2.74	1.39	1.25
3	A	500	PLR	C4A-C4	2.88	1.57	1.51
4	C	600	NO3	O2-N	2.96	1.40	1.25
4	A	600	NO3	O2-N	2.97	1.40	1.25
4	A	600	NO3	O3-N	3.12	1.41	1.25
4	D	600	NO3	O3-N	3.21	1.41	1.25
4	B	600	NO3	O2-N	3.24	1.42	1.25
4	A	600	NO3	O1-N	3.49	1.38	1.24
4	B	600	NO3	O1-N	3.91	1.40	1.24
4	D	600	NO3	O1-N	4.02	1.40	1.24
4	C	600	NO3	O1-N	4.21	1.41	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLR	C3-C4-C5	-4.39	113.99	118.78
3	D	500	PLR	O3P-P-O4P	-3.72	95.86	106.56
3	A	500	PLR	C5A-C5-C6	-3.70	112.29	119.28
3	B	500	PLR	C5A-C5-C6	-3.19	113.24	119.28
3	C	500	PLR	O3P-P-O4P	-2.83	98.42	106.56
3	C	500	PLR	C5-C6-N1	-2.76	119.08	123.86
3	B	500	PLR	C4A-C4-C3	-2.39	116.03	120.36
3	D	500	PLR	C5-C6-N1	-2.26	119.94	123.86
3	D	500	PLR	C5A-C5-C6	-2.17	115.17	119.28
3	B	500	PLR	O3P-P-O4P	-2.07	100.61	106.56
3	A	500	PLR	C5-C6-N1	-2.01	120.36	123.86
3	C	500	PLR	O2P-P-O1P	2.02	117.09	110.58
3	D	500	PLR	O4P-C5A-C5	2.05	112.39	108.99
3	B	500	PLR	O2P-P-O1P	2.12	117.40	110.58
3	C	500	PLR	O4P-C5A-C5	2.29	112.78	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	500	PLR	C6-C5-C4	2.35	120.14	118.15
3	D	500	PLR	O3P-P-O2P	2.38	116.46	107.38
3	D	500	PLR	C5A-C5-C4	2.64	125.15	121.65
3	D	500	PLR	C4A-C4-C5	2.65	123.64	120.88
3	D	500	PLR	O2P-P-O1P	2.67	119.18	110.58
3	A	500	PLR	C5A-C5-C4	2.96	125.57	121.65
3	B	500	PLR	O4P-C5A-C5	3.07	114.06	108.99
3	B	500	PLR	C5A-C5-C4	4.06	127.03	121.65
3	A	500	PLR	C6-C5-C4	4.61	122.05	118.15
3	B	500	PLR	C4A-C4-C5	5.77	126.89	120.88
3	A	500	PLR	C4A-C4-C5	7.00	128.18	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PLR	3	0
3	B	500	PLR	2	0
3	C	500	PLR	2	0
3	D	500	PLR	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	396/440 (90%)	-0.03	12 (3%) 54 48	5, 13, 30, 39	0
1	B	392/440 (89%)	0.02	19 (4%) 34 28	4, 13, 29, 38	0
1	D	396/440 (90%)	0.05	11 (2%) 56 51	4, 13, 32, 39	0
2	C	396/440 (90%)	0.10	23 (5%) 26 21	3, 14, 31, 41	0
All	All	1580/1760 (89%)	0.04	65 (4%) 41 35	3, 13, 31, 41	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	GLY	5.0
2	C	133	GLY	4.9
1	B	133	GLY	4.8
1	A	133	GLY	4.6
1	A	443	ASP	4.0
2	C	443	ASP	3.8
2	C	170	LYS	3.6
1	D	64	PRO	3.4
1	B	395	GLN	3.4
1	B	66	SER	3.3
1	D	119	THR	3.3
2	C	119	THR	3.2
1	B	443	ASP	3.1
1	B	367	ARG	3.1
1	B	170	LYS	3.0
1	A	439	ALA	3.0
1	A	378	ARG	3.0
1	B	171	VAL	2.9
1	A	63	SER	2.8
1	B	366	PRO	2.8
1	B	119	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	66	SER	2.8
1	B	341	LYS	2.8
1	D	69	ARG	2.8
2	C	394	ASP	2.8
2	C	69	ARG	2.8
1	A	341	LYS	2.7
1	A	119	THR	2.7
1	A	69	ARG	2.7
1	D	65	TYR	2.6
2	C	65	TYR	2.6
1	D	443	ASP	2.6
2	C	171	VAL	2.6
2	C	350	PRO	2.6
1	A	65	TYR	2.5
2	C	408	ASP	2.4
2	C	341	LYS	2.4
2	C	376	GLN	2.4
1	A	366	PRO	2.4
1	B	408	ASP	2.4
1	B	350	PRO	2.4
1	B	118	GLN	2.3
1	D	134	ALA	2.3
1	B	378	ARG	2.3
1	D	63	SER	2.3
1	B	65	TYR	2.3
1	B	274	GLY	2.3
2	C	388	CYS	2.3
1	B	69	ARG	2.3
2	C	66	SER	2.3
1	D	171	VAL	2.2
2	C	438	VAL	2.2
2	C	340	GLN	2.2
1	D	367	ARG	2.2
2	C	395	GLN	2.1
1	A	66	SER	2.1
2	C	366	PRO	2.1
2	C	435	LYS	2.1
1	A	435	LYS	2.1
2	C	378	ARG	2.1
2	C	64	PRO	2.1
1	B	67	ALA	2.1
2	C	367	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	118	GLN	2.1
1	B	340	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
1	CSS	D	388	7/8	0.88	0.15	-	26,26,29,33	0
1	CSS	A	388	7/8	0.85	0.13	-	31,32,35,38	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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(Å <sup>2</sup> )	Q<0.9
4	NO3	A	600	4/4	0.87	0.28	5.46	45,45,46,47	0
3	PLR	B	500	15/15	0.93	0.14	0.89	20,21,22,23	0
3	PLR	D	500	15/15	0.92	0.14	0.66	17,21,22,23	0
3	PLR	A	500	15/15	0.96	0.14	0.62	13,18,24,25	0
3	PLR	C	500	15/15	0.94	0.12	0.28	19,20,21,22	0
4	NO3	C	600	4/4	0.91	0.13	0.26	31,31,31,31	0
4	NO3	B	600	4/4	0.90	0.10	-0.22	33,33,33,33	0
4	NO3	D	600	4/4	0.92	0.10	-1.95	25,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.