Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2023 – 07:08 AM EDT

PDB ID	:	3RZL
Title	:	Duplex Interrogation by a Direct DNA Repair Protein in the Search of Damage
Authors	:	Yi, C.; Chen, B.; Qi, B.; Zhang, W.; Jia, G.; Zhang, L.; Li, C.; Dinner, A.; Yang, C.; He, C.
Deposited on	:	2011-05-11
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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 (i)) were used in the production of this report:

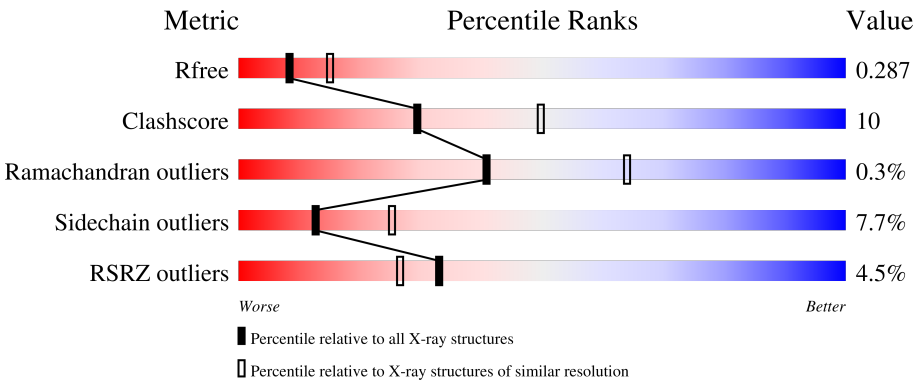
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	208	3%, 76%, 14%, •, 7%
1	D	208	6%, 62%, 31%, •, •
2	B	13	46%, 15%, 38%
2	E	13	8%, 38%, 38%, 23%
3	C	13	54%, 38%, 8%

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Mol	Chain	Length	Quality of chain
3	F	13	8% 69% 23%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4288 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 Alpha-ketoglutarate-dependent dioxygenase alkB homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	194	1585	1016	289	277	3	0	3	0
1	D	199	1625	1040	297	285	3	0	4	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	SER	-	expression tag	UNP Q6NS38
A	55	HIS	-	expression tag	UNP Q6NS38
A	67	SER	CYS	engineered mutation	UNP Q6NS38
A	165	SER	CYS	engineered mutation	UNP Q6NS38
A	169	CYS	GLY	engineered mutation	UNP Q6NS38
A	192	SER	CYS	engineered mutation	UNP Q6NS38
D	54	SER	-	expression tag	UNP Q6NS38
D	55	HIS	-	expression tag	UNP Q6NS38
D	67	SER	CYS	engineered mutation	UNP Q6NS38
D	165	SER	CYS	engineered mutation	UNP Q6NS38
D	169	CYS	GLY	engineered mutation	UNP Q6NS38
D	192	SER	CYS	engineered mutation	UNP Q6NS38

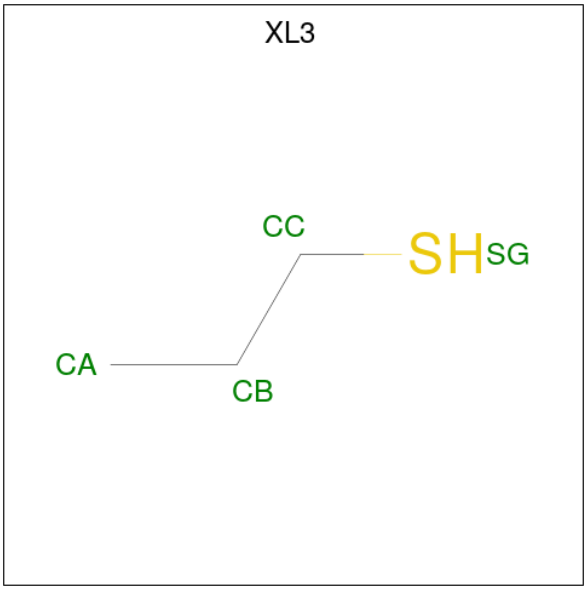
- Molecule 2 is a DNA chain called 5'-D(*AP*TP*GP*TP*AP*TP*CP*AP*CP*TP*GP*CP *G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	13	263	127	47	77	12	0	0	0
2	E	13	263	127	47	77	12	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*TP*CP*GP*CP*AP*GP*TP*IP*AP*TP*AP*CP *A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	263	127	49	75	12	0	0	0
3	F	13	263	127	49	75	12	0	0	0

- Molecule 4 is propane-1-thiol (three-letter code: XL3) (formula: C_3H_8S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	S		
4	B	1	4	3	1	0	0
4	E	1	4	3	1	0	0

- Molecule 5 is water.

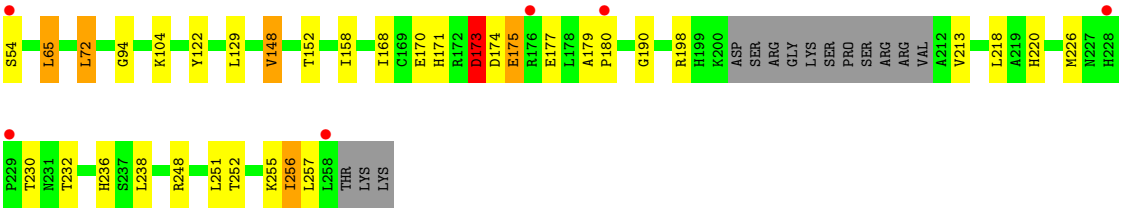
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	13	13	13	0	0
5	C	1	1	1	0	0
5	D	3	3	3	0	0
5	F	1	1	1	0	0

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.

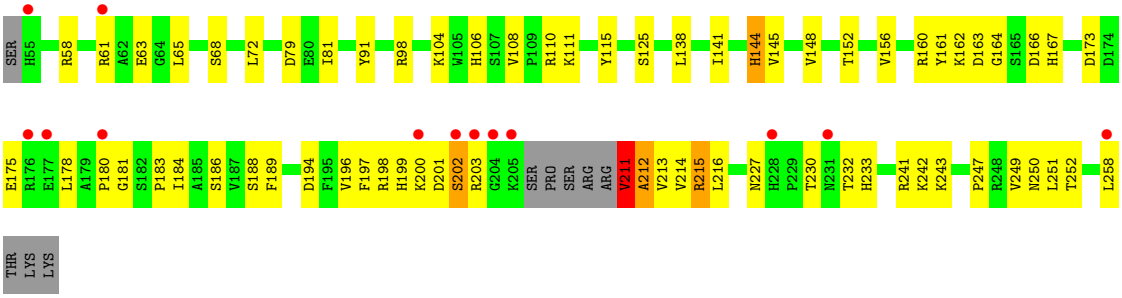
• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase alkB homolog 2

Chain A:



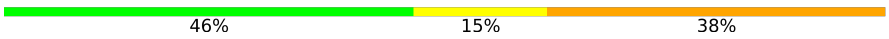
• Molecule 1: Alpha-ketoglutarate-dependent dioxygenase alkB homolog 2

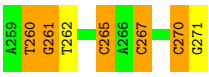
Chain D:



• Molecule 2: 5'-D(*AP*TP*GP*TP*AP*TP*CP*AP*CP*TP*GP*CP*G)-3'

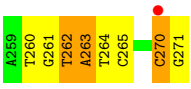
Chain B:





• Molecule 2: 5'-D(*AP*TP*GP*TP*AP*TP*CP*AP*CP*TP*GP*CP*G)-3'

Chain E:



• Molecule 3: 5'-D(*TP*CP*GP*CP*AP*GP*TP*IP*AP*TP*AP*CP*A)-3'

Chain C:

• Molecule 3: 5'-D(*TP*CP*GP*CP*AP*GP*TP*IP*AP*TP*AP*CP*A)-3'

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.93Å 65.01Å 167.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 94.5 (19.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.221 , 0.289 0.217 , 0.287	Depositor DCC
R_{free} test set	944 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4288	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: XL3

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	0.66	0/1635	0.78	1/2213 (0.0%)
1	D	0.61	0/1677	0.84	7/2268 (0.3%)
2	B	1.15	0/294	1.73	8/452 (1.8%)
2	E	1.07	0/294	1.79	9/452 (2.0%)
3	C	1.20	1/270 (0.4%)	2.05	12/412 (2.9%)
3	F	3.70	16/270 (5.9%)	2.53	24/412 (5.8%)
All	All	1.18	17/4440 (0.4%)	1.28	61/6209 (1.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	272	DT	N1-C2	36.64	1.67	1.38
3	F	272	DT	C4-C5	32.30	1.74	1.45
3	F	272	DT	C5-C7	12.95	1.57	1.50
3	F	272	DT	N1-C6	11.98	1.46	1.38
3	F	272	DT	C5-C6	10.70	1.41	1.34
3	F	272	DT	C3'-C2'	8.57	1.62	1.52
3	F	280	DA	P-O5'	-8.47	1.51	1.59
3	F	272	DT	C4'-O4'	7.67	1.52	1.45
3	F	274	DG	N3-C4	7.37	1.40	1.35
3	F	273	DC	C4-C5	7.33	1.48	1.43
3	F	273	DC	N1-C2	6.77	1.47	1.40
3	F	272	DT	C4-O4	6.42	1.29	1.23
3	F	272	DT	C2-O2	6.05	1.27	1.22
3	F	272	DT	C2'-C1'	6.02	1.58	1.52
3	F	274	DG	C6-N1	5.60	1.43	1.39
3	F	272	DT	C1'-N1	5.19	1.55	1.49
3	C	280	DA	P-OP1	-5.05	1.40	1.49

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	272	DT	C5-C6-N1	-16.19	113.98	123.70
3	F	272	DT	C6-C5-C7	-16.02	113.29	122.90
3	C	282	DA	C1'-O4'-C4'	-11.71	98.39	110.10
3	C	282	DA	O4'-C4'-C3'	-11.20	99.28	106.00
1	D	181	GLY	N-CA-C	10.93	140.41	113.10
3	F	272	DT	O4'-C1'-N1	10.13	115.09	108.00
3	F	272	DT	N3-C2-O2	-9.85	116.39	122.30
3	F	280	DA	O5'-P-OP2	-9.48	97.16	105.70
3	C	280	DA	P-O5'-C5'	9.28	135.75	120.90
2	B	261	DG	O4'-C1'-N9	-9.09	101.64	108.00
3	F	278	DT	O4'-C1'-N1	8.69	114.08	108.00
2	B	260	DT	O4'-C1'-N1	8.66	114.06	108.00
2	B	270	DC	P-O3'-C3'	8.61	130.04	119.70
3	F	272	DT	N3-C4-O4	-7.92	115.15	119.90
2	B	260	DT	P-O3'-C3'	7.66	128.89	119.70
3	C	283	DC	O4'-C1'-N1	7.46	113.22	108.00
3	F	280	DA	P-O5'-C5'	7.44	132.81	120.90
2	E	260	DT	O4'-C1'-N1	-7.42	102.81	108.00
3	F	272	DT	C6-N1-C2	7.41	125.00	121.30
3	C	282	DA	N9-C1'-C2'	7.40	126.67	112.60
1	D	211	VAL	CB-CA-C	7.38	125.42	111.40
3	F	272	DT	C4-C5-C7	7.34	123.40	119.00
3	F	284	DA	O4'-C4'-C3'	-7.16	101.64	104.50
3	C	272	DT	C4-C5-C7	7.14	123.28	119.00
3	F	284	DA	O5'-P-OP1	-6.99	99.41	105.70
3	F	272	DT	C4-C5-C6	6.97	122.18	118.00
2	E	262	DT	O4'-C1'-N1	6.94	112.86	108.00
2	E	270	DC	O4'-C1'-N1	6.90	112.83	108.00
3	C	283	DC	P-O3'-C3'	6.85	127.92	119.70
2	B	265	DC	O4'-C1'-N1	-6.71	103.30	108.00
3	F	272	DT	C2-N3-C4	-6.62	123.22	127.20
1	D	201	ASP	CB-CA-C	6.58	123.57	110.40
3	C	272	DT	C6-C5-C7	-6.45	119.03	122.90
3	F	274	DG	P-O3'-C3'	6.31	127.28	119.70
3	F	281	DT	O4'-C1'-N1	6.22	112.35	108.00
3	F	272	DT	O4'-C1'-C2'	6.21	110.87	105.90
2	E	260	DT	C4-C5-C7	5.99	122.59	119.00
3	C	274	DG	P-O3'-C3'	5.83	126.70	119.70
1	D	202	SER	N-CA-CB	-5.78	101.84	110.50
2	B	267	DC	O4'-C4'-C3'	-5.76	102.19	104.50
3	F	283	DC	N1-C2-O2	5.76	122.36	118.90
2	B	260	DT	C5-C4-O4	-5.76	120.87	124.90
3	F	276	DA	C3'-C2'-C1'	-5.71	95.65	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	265	DC	O4'-C1'-N1	-5.65	104.04	108.00
3	F	277	DG	C1'-O4'-C4'	-5.65	104.45	110.10
2	E	263	DA	P-O3'-C3'	5.61	126.43	119.70
2	E	262	DT	C1'-O4'-C4'	-5.61	104.49	110.10
1	A	173	ASP	CB-CG-OD1	5.54	123.29	118.30
3	F	278	DT	C1'-O4'-C4'	-5.48	104.62	110.10
1	D	61	ARG	CB-CA-C	-5.47	99.47	110.40
1	D	212	ALA	CB-CA-C	5.41	118.22	110.10
2	E	264	DT	C5-C4-O4	-5.40	121.12	124.90
1	D	202	SER	N-CA-C	5.31	125.35	111.00
2	E	260	DT	C6-C5-C7	-5.27	119.74	122.90
3	C	272	DT	O4'-C1'-C2'	-5.23	101.71	105.90
3	F	272	DT	C6-N1-C1'	-5.20	112.60	120.40
2	B	260	DT	N3-C4-O4	5.20	123.02	119.90
3	C	283	DC	C3'-C2'-C1'	-5.16	96.30	102.50
3	F	274	DG	C5-C6-O6	-5.16	125.51	128.60
3	C	283	DC	N1-C2-O2	5.07	121.94	118.90
3	F	283	DC	N3-C2-O2	-5.05	118.37	121.90

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	1585	0	1576	24	0
1	D	1625	0	1621	38	0
2	B	263	0	148	9	0
2	E	263	0	148	4	0
3	C	263	0	147	3	0
3	F	263	0	147	5	0
4	B	4	0	6	3	0
4	E	4	0	6	0	0
5	A	13	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
All	All	4288	0	3799	77	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 10.

All (77) 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:174:ASP:C	1:A:175:GLU:HG2	1.74	1.03
1:A:174:ASP:O	1:A:175:GLU:HG2	1.62	0.99
1:A:54:SER:HB2	1:A:148:VAL:HG11	1.45	0.97
1:D:200:LYS:HB3	1:D:233:HIS:O	1.66	0.95
1:A:54:SER:HB3	1:A:72:LEU:HD23	1.49	0.94
1:A:65:LEU:HD23	1:A:230:THR:HG23	1.59	0.84
1:D:211:VAL:CG1	1:D:212:ALA:H	1.94	0.81
1:A:174:ASP:O	1:A:175:GLU:CG	2.29	0.79
1:D:173:ASP:OD2	5:D:7:HOH:O	2.01	0.76
2:B:260:DT:H4'	2:B:261:DG:OP1	1.86	0.75
2:B:267:DC:H5	4:B:1:XL3:HBA	1.51	0.74
2:E:261:DG:H4'	2:E:262:DT:OP1	1.89	0.72
2:E:270:DC:H2'	2:E:271:DG:C8	2.25	0.72
3:C:281:DT:H2"	3:C:282:DA:C8	2.30	0.67
2:B:267:DC:C5	4:B:1:XL3:HBA	2.31	0.65
1:D:198:ARG:HG2	1:D:213:VAL:HG22	1.80	0.64
1:A:198[A]:ARG:HG2	1:A:213:VAL:HG22	1.81	0.63
1:D:199:HIS:O	1:D:202:SER:OG	2.17	0.62
1:D:211:VAL:HG13	1:D:212:ALA:H	1.63	0.61
2:B:262:DT:H3	3:C:282:DA:H61	1.49	0.60
2:E:262:DT:H2"	2:E:263:DA:C8	2.35	0.60
2:B:270:DC:H2"	2:B:271:DG:C8	2.36	0.60
1:D:160:ARG:HG3	1:D:249:VAL:HG22	1.83	0.60
1:A:158:ILE:HG12	1:A:251:LEU:HG	1.84	0.60
1:D:211:VAL:HG12	1:D:212:ALA:H	1.67	0.59
1:D:211:VAL:CG1	1:D:212:ALA:N	2.66	0.58
1:A:255[A]:LYS:O	1:A:255[A]:LYS:HG2	2.03	0.58
1:A:122:TYR:HA	1:A:177:GLU:OE2	2.04	0.57
1:A:198[B]:ARG:HG2	1:A:213:VAL:HG22	1.89	0.55
1:D:98:ARG:HA	1:D:106:HIS:O	2.06	0.55
3:F:278:DT:H3'	3:F:279:DI:C4	2.42	0.54
1:D:178:LEU:O	1:D:180:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:PRO:HB3	1:D:227:ASN:HA	1.90	0.53
2:B:267:DC:C5	4:B:1:XL3:CB	2.91	0.53
1:A:256:ILE:HG22	1:A:257:LEU:N	2.24	0.52
2:B:262:DT:H3	3:C:282:DA:N6	2.06	0.52
1:D:196:VAL:HG22	1:D:215[B]:ARG:HG2	1.92	0.52
1:D:108:VAL:HG23	1:D:110:ARG:O	2.11	0.51
1:A:218:LEU:HD12	1:A:248:ARG:NH2	2.27	0.50
1:A:170:GLU:HA	1:A:236:HIS:O	2.11	0.50
1:A:54:SER:HB3	1:A:72:LEU:CD2	2.34	0.50
1:D:258:LEU:O	1:D:258:LEU:HG	2.12	0.49
1:A:174:ASP:O	1:A:174:ASP:OD1	2.29	0.49
1:D:141:ILE:O	1:D:145:VAL:HG23	2.13	0.49
1:D:58:ARG:O	1:D:68:SER:HA	2.12	0.49
1:A:72:LEU:HD21	1:A:148:VAL:HG21	1.95	0.49
1:D:161:TYR:CD2	1:D:161:TYR:N	2.82	0.48
1:D:164:GLY:HA3	1:D:241:ARG:O	2.14	0.48
1:D:162:LYS:HG2	1:D:166:ASP:OD2	2.13	0.48
1:A:190:GLY:H	1:A:220:HIS:CE1	2.32	0.48
1:D:144:HIS:O	1:D:148:VAL:HG23	2.15	0.46
1:D:211:VAL:HG13	1:D:212:ALA:N	2.28	0.46
3:F:282:DA:H1'	3:F:283:DC:H5'	1.98	0.46
1:D:250:ASN:HD21	1:D:252:THR:HG23	1.80	0.46
1:D:197:PHE:HB2	1:D:214:VAL:HB	1.99	0.45
1:A:255[A]:LYS:O	1:A:255[A]:LYS:CG	2.65	0.44
1:A:173:ASP:HB2	1:A:236:HIS:HE1	1.82	0.44
1:D:81:ILE:HG21	1:D:189:PHE:CZ	2.52	0.44
1:D:178:LEU:HD11	1:D:184:ILE:HD11	2.00	0.43
1:A:94:GLY:HA3	3:F:283:DC:OP2	2.18	0.43
1:A:168:ILE:HG22	1:A:238:LEU:HB3	2.01	0.43
1:D:242:LYS:HB2	3:F:272:DT:H5'	2.01	0.43
1:D:194:ASP:OD2	1:D:215[B]:ARG:NH2	2.46	0.43
1:D:115:TYR:HB2	1:D:156:VAL:CG1	2.49	0.43
1:D:175:GLU:HA	1:D:175:GLU:OE1	2.19	0.42
2:E:262:DT:H2"	2:E:263:DA:N7	2.34	0.42
1:A:179:ALA:HB1	1:A:180:PRO:HD2	2.01	0.42
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.89	0.42
1:D:91:TYR:CD1	1:D:111:LYS:HB3	2.55	0.41
1:D:243:LYS:HE2	3:F:272:DT:H4'	2.02	0.41
1:D:186:SER:HA	1:D:251:LEU:O	2.20	0.41
2:B:270:DC:H2"	2:B:271:DG:O5'	2.20	0.41
1:D:162:LYS:HG3	1:D:163:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ALA:O	1:D:213:VAL:HG23	2.21	0.41
1:A:171:HIS:HB3	2:B:265:DC:O4'	2.21	0.40
1:D:161:TYR:O	1:D:247:PRO:HA	2.21	0.40
1:D:110:ARG:HD3	1:D:167:HIS:O	2.22	0.40

There are no symmetry-related clashes.

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	193/208 (93%)	176 (91%)	17 (9%)	0	100	100
1	D	199/208 (96%)	185 (93%)	13 (6%)	1 (0%)	29	52
All	All	392/416 (94%)	361 (92%)	30 (8%)	1 (0%)	41	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	230	THR

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	171/181 (94%)	159 (93%)	12 (7%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	175/181 (97%)	160 (91%)	15 (9%)	10	20
All	All	346/362 (96%)	319 (92%)	27 (8%)	13	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	72	LEU
1	A	104	LYS
1	A	129	LEU
1	A	148	VAL
1	A	152	THR
1	A	173	ASP
1	A	175	GLU
1	A	226	MET
1	A	232	THR
1	A	252	THR
1	A	256	ILE
1	D	63	GLU
1	D	65	LEU
1	D	72	LEU
1	D	79	ASP
1	D	104	LYS
1	D	125	SER
1	D	144	HIS
1	D	152	THR
1	D	188	SER
1	D	203	ARG
1	D	211	VAL
1	D	215[A]	ARG
1	D	215[B]	ARG
1	D	216	LEU
1	D	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	250	ASN
1	D	100	GLN
1	D	250	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
4	XL3	B	1	1,2	3,3,3	0.29	0	2,2,2	3.06	1 (50%)
4	XL3	E	1	1,2	3,3,3	0.51	0	2,2,2	4.02	1 (50%)

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	XL3	B	1	1,2	-	1/1/1/1	-
4	XL3	E	1	1,2	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	XL3	CB-CC-SG	-5.68	107.82	113.74
4	B	1	XL3	CB-CC-SG	-4.33	109.23	113.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	XL3	CA-CB-CC-SG
4	B	1	XL3	CA-CB-CC-SG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	XL3	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	194/208 (93%)	-0.17	6 (3%) 49 42	38, 48, 74, 91	0
1	D	199/208 (95%)	0.17	13 (6%) 18 14	41, 62, 94, 137	0
2	B	13/13 (100%)	-0.47	0 100 100	41, 66, 120, 126	0
2	E	13/13 (100%)	-0.01	1 (7%) 13 10	42, 66, 154, 161	0
3	C	12/13 (92%)	-0.58	0 100 100	53, 65, 78, 90	0
3	F	12/13 (92%)	-0.54	0 100 100	62, 78, 99, 111	0
All	All	443/468 (94%)	-0.04	20 (4%) 33 26	38, 56, 92, 161	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	GLY	11.4
1	D	203	ARG	6.9
1	D	205	LYS	4.0
1	D	202	SER	3.8
1	D	200	LYS	3.6
1	D	228	HIS	3.4
1	D	55	HIS	3.3
1	A	176	ARG	3.0
1	D	176	ARG	2.9
2	E	270	DC	2.9
1	A	228	HIS	2.7
1	D	258	LEU	2.6
1	D	231	ASN	2.4
1	D	61	ARG	2.4
1	A	229	PRO	2.3
1	D	177	GLU	2.2
1	A	54	SER	2.2
1	D	180	PRO	2.2
1	A	180	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	XL3	B	1	4/4	0.95	0.16	39,41,42,46	0
4	XL3	E	1	4/4	0.96	0.19	47,47,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.