Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2024 – 08:09 PM JST

PDB ID	:	8X6Q
Title	:	Crystal structure of OsHSL1 L204F/F298L/I335F complexed with 2-acetyl-cyclohexane-2,4-dione
Authors	:	Lin, H.-Y.; Dong, J.; Yang, G.-F.
Deposited on	:	2023-11-21
Resolution	:	2.39 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 ⓘ 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 ⓘ) were used in the production of this report:

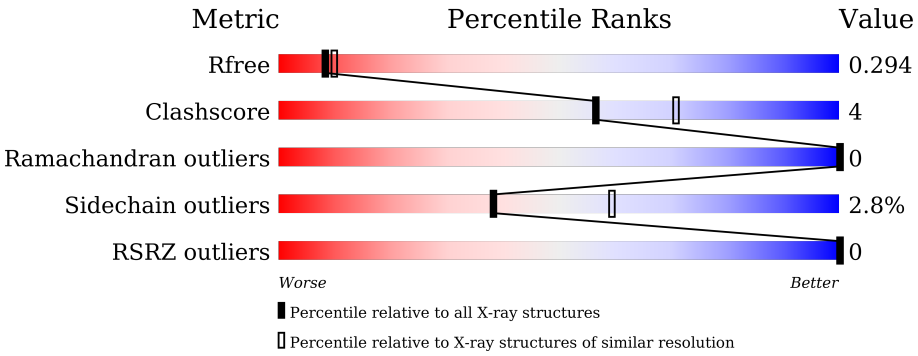
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.39 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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 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	348	86% 12% •
1	B	348	88% 11% •
1	C	348	84% 14% ••
1	D	348	86% 13% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y8R	A	401	-	X	-	-
2	Y8R	C	401	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11590 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.

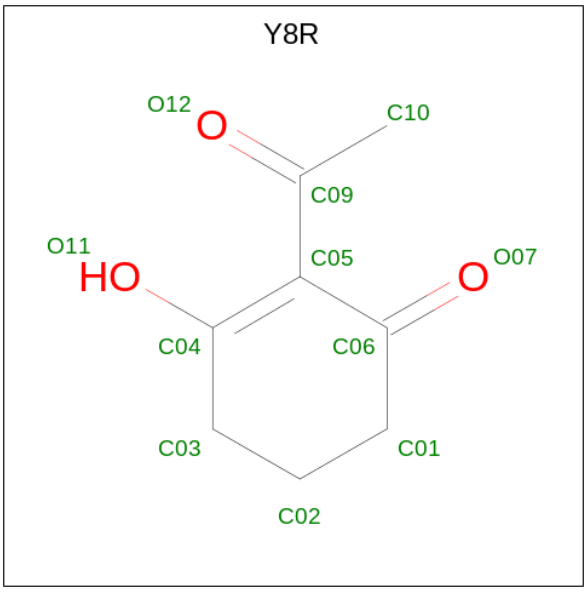
- Molecule 1 is a protein called HPPD Inhibitor Sensitive 1-like 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2794	1770	496	522	6			
1	B	348	Total	C	N	O	S	0	0	0
			2810	1779	498	527	6			
1	C	346	Total	C	N	O	S	0	0	0
			2787	1767	493	521	6			
1	D	348	Total	C	N	O	S	0	0	0
			2798	1772	497	523	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	PHE	LEU	engineered mutation	UNP Q8H620
A	298	LEU	PHE	engineered mutation	UNP Q8H620
A	335	PHE	ILE	engineered mutation	UNP Q8H620
B	204	PHE	LEU	engineered mutation	UNP Q8H620
B	298	LEU	PHE	engineered mutation	UNP Q8H620
B	335	PHE	ILE	engineered mutation	UNP Q8H620
C	204	PHE	LEU	engineered mutation	UNP Q8H620
C	298	LEU	PHE	engineered mutation	UNP Q8H620
C	335	PHE	ILE	engineered mutation	UNP Q8H620
D	204	PHE	LEU	engineered mutation	UNP Q8H620
D	298	LEU	PHE	engineered mutation	UNP Q8H620
D	335	PHE	ILE	engineered mutation	UNP Q8H620

- Molecule 2 is 2-ethanoyl-3-oxidanyl-cyclohex-2-en-1-one (three-letter code: Y8R) (formula: $C_8H_{10}O_3$).

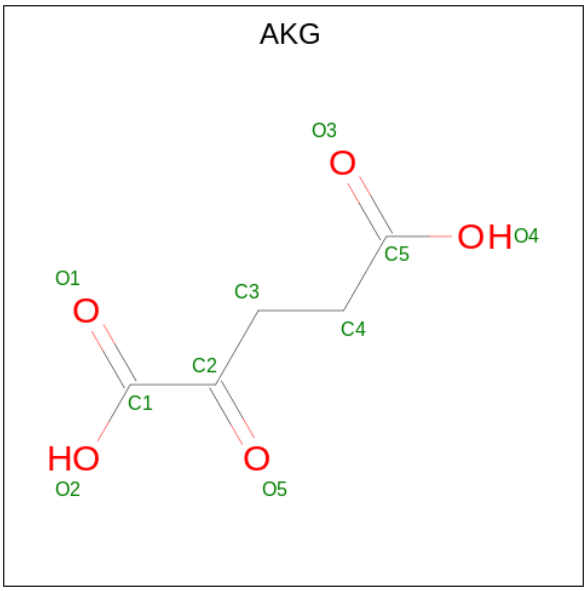


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 8 3	0	0
2	B	1	Total C O 11 8 3	0	0
2	C	1	Total C O 11 8 3	0	0
2	D	1	Total C O 11 8 3	0	0

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0
3	D	1	Total Co 1 1	0	0

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 5 5	0	0
4	B	1	Total C O 10 5 5	0	0
4	C	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	0

- Molecule 5 is water.

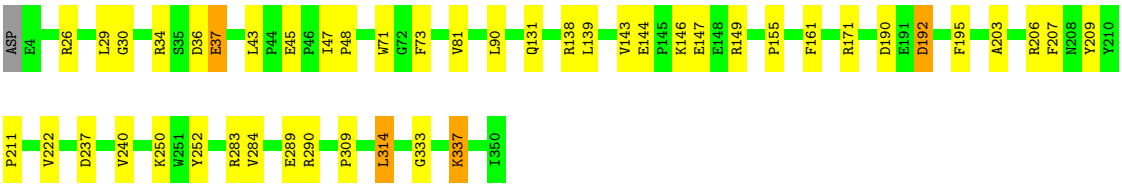
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	68	Total O 68 68	0	0
5	B	81	Total O 81 81	0	0
5	C	78	Total O 78 78	0	0
5	D	86	Total O 86 86	0	0

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.

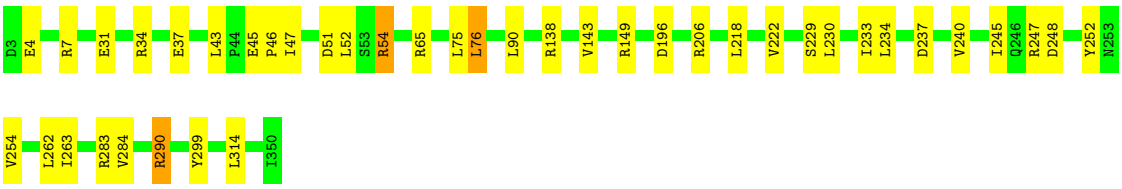
• Molecule 1: HPPD Inhibitor Sensitive 1-like 1 protein

Chain A:



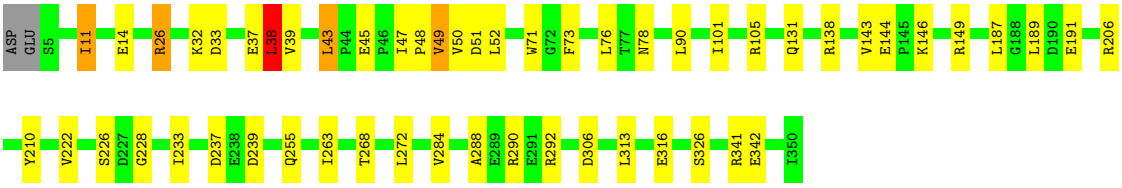
• Molecule 1: HPPD Inhibitor Sensitive 1-like 1 protein

Chain B:



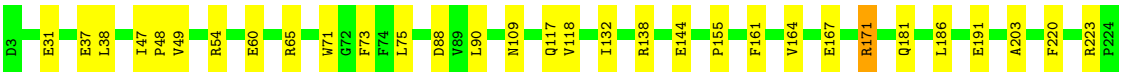
• Molecule 1: HPPD Inhibitor Sensitive 1-like 1 protein

Chain C:



• Molecule 1: HPPD Inhibitor Sensitive 1-like 1 protein

Chain D:




H225
I233
L234
D237
R247
D248
V256
L262
I263
R278
S279
R290
D306
R323
S326
R343
L348
K349
I350

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.93Å 58.89Å 140.24Å 89.97° 90.00° 111.98°	Depositor
Resolution (Å)	36.40 – 2.39 36.40 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.5 (36.40-2.39) 97.6 (36.40-2.39)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.249 , 0.295 0.250 , 0.294	Depositor DCC
R_{free} test set	2621 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 23.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l 0.357 for -h,-k,l 0.000 for -h,h+k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11590	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 19.96 % 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 9.6627e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, Y8R, CO

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	0.25	0/2856	0.41	0/3871
1	B	0.25	0/2872	0.42	0/3891
1	C	0.34	2/2849 (0.1%)	0.45	2/3861 (0.1%)
1	D	0.25	0/2860	0.41	0/3877
All	All	0.27	2/11437 (0.0%)	0.42	2/15500 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	VAL	C-O	-5.35	1.13	1.23
1	C	48	PRO	N-CD	5.05	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	45	GLU	C-N-CD	6.13	141.28	128.40
1	C	38	LEU	CA-CB-CG	6.01	129.13	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2794	0	2744	23	0
1	B	2810	0	2763	24	0
1	C	2787	0	2742	33	0
1	D	2798	0	2744	23	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	1	0
2	D	11	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	1	0
4	C	10	0	4	1	0
4	D	10	0	4	0	0
5	A	68	0	0	0	0
5	B	81	0	0	2	0
5	C	78	0	0	2	0
5	D	86	0	0	1	0
All	All	11590	0	11009	100	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 4.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HB2	1:B:76:LEU:HD21	1.66	0.76
1:C:26:ARG:NH1	1:C:131:GLN:O	2.23	0.71
1:D:132:ILE:O	1:D:223:ARG:NH1	2.24	0.69
1:A:26:ARG:NH1	1:A:131:GLN:O	2.27	0.67
1:C:11:ILE:HD11	1:C:14:GLU:HG2	1.77	0.66
1:C:189:LEU:HD11	1:C:313:LEU:HG	1.78	0.66
1:C:51:ASP:OD1	1:C:78:ASN:ND2	2.28	0.66
1:D:54:ARG:HG3	1:D:60:GLU:HG3	1.79	0.64
1:B:45:GLU:HG3	1:C:288:ALA:HB3	1.79	0.64
1:C:38:LEU:HD23	1:C:39:VAL:H	1.65	0.61
1:C:43:LEU:HD12	1:C:47:ILE:HG22	1.83	0.59
1:B:34:ARG:HD2	1:B:218:LEU:HA	1.85	0.59
1:A:29:LEU:O	1:A:34:ARG:NH2	2.35	0.59
1:C:316:GLU:HA	1:D:118:VAL:HG21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD22	1:A:237:ASP:HB2	1.87	0.57
1:A:143:VAL:HA	1:A:149:ARG:HD2	1.85	0.56
1:A:146:LYS:HA	1:A:149:ARG:HD3	1.88	0.56
1:D:233:ILE:HG12	1:D:263:ILE:HD12	1.87	0.56
1:D:306:ASP:OD2	1:D:326:SER:HA	2.04	0.56
1:A:146:LYS:HE2	1:B:196:ASP:OD2	2.05	0.56
1:C:90:LEU:HD22	1:C:237:ASP:HB2	1.90	0.54
1:C:306:ASP:OD2	1:C:326:SER:HA	2.07	0.54
1:A:206:ARG:HD3	4:A:403:AKG:O1	2.08	0.54
1:B:234:LEU:HB3	1:B:262:LEU:HB3	1.89	0.53
1:A:240:VAL:HG21	1:A:290:ARG:HH11	1.72	0.53
1:C:11:ILE:HG13	1:C:11:ILE:O	2.07	0.53
1:B:75:LEU:HD12	1:B:262:LEU:HD23	1.91	0.53
1:B:233:ILE:HG12	1:B:263:ILE:HD12	1.90	0.52
1:D:90:LEU:HD22	1:D:237:ASP:HB2	1.92	0.52
1:A:192:ASP:HA	1:A:195:PHE:HB2	1.92	0.52
1:B:290:ARG:NH2	5:B:514:HOH:O	2.42	0.52
1:B:65:ARG:NH1	5:B:509:HOH:O	2.39	0.51
1:A:47:ILE:HD12	1:A:48:PRO:HD2	1.93	0.50
1:B:90:LEU:HD22	1:B:237:ASP:HB2	1.93	0.50
1:C:290:ARG:NH2	5:C:508:HOH:O	2.38	0.50
1:B:43:LEU:HD23	1:B:47:ILE:HG22	1.93	0.49
1:D:144:GLU:HB2	1:D:203:ALA:HB3	1.94	0.49
1:C:33:ASP:OD1	1:C:341:ARG:NH1	2.44	0.49
1:A:250:LYS:HG2	1:A:252:TYR:CZ	2.47	0.49
1:D:71:TRP:CZ3	1:D:247:ARG:HG2	2.47	0.49
1:C:52:LEU:HB2	1:C:76:LEU:HD11	1.95	0.48
1:B:37:GLU:HA	1:B:283:ARG:NH2	2.29	0.48
1:A:309:PRO:HB2	1:A:314:LEU:HD21	1.96	0.47
1:C:222:VAL:HG12	1:C:284:VAL:HB	1.96	0.47
1:A:139:LEU:HB3	1:A:207:PHE:HB2	1.95	0.47
1:A:333:GLY:O	1:A:337:LYS:HE2	2.14	0.47
1:C:233:ILE:HG12	1:C:263:ILE:HD12	1.96	0.47
1:D:234:LEU:HB3	1:D:262:LEU:HB3	1.96	0.46
1:B:31:GLU:OE1	1:B:34:ARG:NH1	2.49	0.46
1:D:65:ARG:NH2	1:D:186:LEU:O	2.47	0.46
1:C:228:GLY:N	2:C:401:Y8R:O12	2.43	0.46
1:D:279:SER:O	1:D:343:ARG:NH2	2.48	0.46
1:C:49:VAL:HG12	1:C:50:VAL:N	2.31	0.46
1:C:187:LEU:HB3	1:C:189:LEU:HD13	1.98	0.46
1:D:88:ASP:OD2	1:D:164:VAL:HG21	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:CD1	1:C:47:ILE:HG22	2.46	0.45
1:C:268:THR:O	1:C:272:LEU:HG	2.17	0.45
1:A:71:TRP:HB3	1:A:73:PHE:CE2	2.52	0.45
1:B:247:ARG:HB3	1:B:252:TYR:HE2	1.82	0.45
1:B:4:GLU:OE2	1:B:7:ARG:HG3	2.16	0.45
1:C:206:ARG:HD3	4:C:403:AKG:O1	2.17	0.45
1:D:49:VAL:HG22	1:D:75:LEU:HB2	1.99	0.45
1:D:167:GLU:O	1:D:171:ARG:HG2	2.16	0.44
1:C:342:GLU:H	1:C:342:GLU:CD	2.21	0.44
1:D:155:PRO:HD2	1:D:161:PHE:CE2	2.53	0.44
1:C:71:TRP:HB3	1:C:73:PHE:CE2	2.52	0.44
1:D:47:ILE:HG13	1:D:48:PRO:HD2	2.00	0.44
1:A:155:PRO:HD2	1:A:161:PHE:CE2	2.53	0.44
1:A:37:GLU:HA	1:A:283:ARG:NH2	2.33	0.44
1:C:143:VAL:HG23	1:C:144:GLU:HG2	2.00	0.44
1:B:51:ASP:CG	1:B:54:ARG:HD3	2.38	0.43
1:B:229:SER:HB2	1:B:299:TYR:O	2.18	0.43
1:B:240:VAL:HG21	1:B:290:ARG:NE	2.33	0.43
1:B:45:GLU:HA	1:B:46:PRO:HA	1.82	0.43
1:A:144:GLU:HB2	1:A:203:ALA:HB3	2.00	0.43
1:C:38:LEU:HD23	1:C:39:VAL:N	2.32	0.43
1:A:36:ASP:O	1:A:283:ARG:NH2	2.31	0.42
1:D:225:HIS:CD2	2:D:401:Y8R:C01	3.02	0.42
1:D:37:GLU:HG3	1:D:220:PHE:CE1	2.54	0.42
1:D:181:GLN:HG2	1:D:191:GLU:OE2	2.20	0.42
1:D:323:ARG:NH1	1:D:348:LEU:HA	2.34	0.42
1:B:240:VAL:HG11	1:B:290:ARG:NH2	2.35	0.42
1:C:101:ILE:O	1:C:105:ARG:HG3	2.20	0.42
1:A:222:VAL:HG12	1:A:284:VAL:HB	2.01	0.42
1:C:146:LYS:HE3	1:C:149:ARG:NH1	2.35	0.42
1:D:278:ARG:NH2	5:D:517:HOH:O	2.51	0.42
1:A:30:GLY:O	1:A:34:ARG:HG3	2.20	0.42
1:D:71:TRP:HB3	1:D:73:PHE:CE2	2.55	0.42
1:A:81:VAL:HG22	1:A:171:ARG:HB3	2.01	0.41
1:A:209:TYR:O	1:A:211:PRO:HD3	2.19	0.41
1:B:245:ILE:HG13	1:B:254:VAL:HG21	2.01	0.41
1:B:206:ARG:HD3	4:B:403:AKG:O2	2.20	0.41
1:D:109:ASN:HB2	1:D:117:GLN:O	2.21	0.41
1:C:226:SER:O	5:C:501:HOH:O	2.22	0.41
1:B:143:VAL:O	1:B:149:ARG:HD3	2.20	0.41
1:C:210:TYR:HB2	1:C:292:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:HD3	1:C:32:LYS:HA	1.94	0.41
1:C:146:LYS:HE2	1:C:146:LYS:HB3	1.92	0.40
1:C:239:ASP:O	1:C:255:GLN:NE2	2.46	0.40
1:B:222:VAL:HG12	1:B:284:VAL:HB	2.03	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	345/348 (99%)	335 (97%)	10 (3%)	0	100	100
1	B	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
1	C	344/348 (99%)	332 (96%)	12 (4%)	0	100	100
1	D	346/348 (99%)	337 (97%)	9 (3%)	0	100	100
All	All	1381/1392 (99%)	1344 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	299/302 (99%)	289 (97%)	10 (3%)	33	53
1	B	302/302 (100%)	295 (98%)	7 (2%)	45	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	299/302 (99%)	292 (98%)	7 (2%)	45 66
1	D	299/302 (99%)	290 (97%)	9 (3%)	36 57
All	All	1199/1208 (99%)	1166 (97%)	33 (3%)	38 59

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	43	LEU
1	A	45	GLU
1	A	138	ARG
1	A	147	GLU
1	A	190	ASP
1	A	192	ASP
1	A	289	GLU
1	A	314	LEU
1	A	337	LYS
1	B	54	ARG
1	B	76	LEU
1	B	138	ARG
1	B	230	LEU
1	B	248	ASP
1	B	290	ARG
1	B	314	LEU
1	C	11	ILE
1	C	26	ARG
1	C	37	GLU
1	C	38	LEU
1	C	43	LEU
1	C	138	ARG
1	C	191	GLU
1	D	31	GLU
1	D	38	LEU
1	D	138	ARG
1	D	171	ARG
1	D	247	ARG
1	D	248	ASP
1	D	256	VAL
1	D	290	ARG
1	D	323	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	AKG	B	403	3	9,9,9	1.30	1 (11%)	11,11,11	1.65	3 (27%)
2	Y8R	D	401	-	11,11,11	3.63	4 (36%)	14,15,15	5.74	8 (57%)
4	AKG	A	403	3	9,9,9	1.35	1 (11%)	11,11,11	1.63	3 (27%)
4	AKG	C	403	3	9,9,9	1.28	1 (11%)	11,11,11	1.67	3 (27%)
2	Y8R	B	401	-	11,11,11	3.64	4 (36%)	14,15,15	5.74	8 (57%)
4	AKG	D	403	3	9,9,9	1.35	1 (11%)	11,11,11	1.58	4 (36%)
2	Y8R	A	401	-	11,11,11	4.09	6 (54%)	14,15,15	4.59	9 (64%)
2	Y8R	C	401	-	11,11,11	3.55	4 (36%)	14,15,15	6.67	10 (71%)

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	AKG	B	403	3	-	0/9/9/9	-
2	Y8R	D	401	-	-	4/4/18/18	0/1/1/1
4	AKG	A	403	3	-	4/9/9/9	-
4	AKG	C	403	3	-	2/9/9/9	-
2	Y8R	B	401	-	-	4/4/18/18	0/1/1/1
4	AKG	D	403	3	-	0/9/9/9	-
2	Y8R	A	401	-	-	4/4/18/18	0/1/1/1
2	Y8R	C	401	-	-	4/4/18/18	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	Y8R	O07-C06	9.58	1.42	1.23
2	C	401	Y8R	O07-C06	8.24	1.39	1.23
2	B	401	Y8R	O07-C06	8.23	1.39	1.23
2	D	401	Y8R	O07-C06	8.23	1.39	1.23
2	A	401	Y8R	O12-C09	6.58	1.37	1.23
2	B	401	Y8R	O12-C09	6.03	1.36	1.23
2	D	401	Y8R	O12-C09	6.00	1.36	1.23
2	C	401	Y8R	O12-C09	5.17	1.34	1.23
2	B	401	Y8R	C05-C04	4.80	1.54	1.39
2	D	401	Y8R	C05-C04	4.80	1.54	1.39
2	C	401	Y8R	C05-C04	4.73	1.53	1.39
2	A	401	Y8R	C05-C04	4.58	1.53	1.39
2	C	401	Y8R	C05-C06	3.38	1.53	1.46
2	A	401	Y8R	C05-C06	3.27	1.53	1.46
2	B	401	Y8R	C05-C06	2.97	1.52	1.46
2	D	401	Y8R	C05-C06	2.95	1.52	1.46
2	A	401	Y8R	C05-C09	2.54	1.54	1.46
2	A	401	Y8R	O11-C04	2.24	1.38	1.32
4	D	403	AKG	O5-C2	-2.09	1.18	1.23
4	A	403	AKG	O5-C2	-2.08	1.18	1.23
4	C	403	AKG	O5-C2	-2.05	1.18	1.23
4	B	403	AKG	O5-C2	-2.02	1.19	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	Y8R	C02-C03-C04	-13.74	98.23	112.48
2	C	401	Y8R	O07-C06-C05	-11.91	102.41	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	Y8R	O07-C06-C01	-10.32	103.95	120.86
2	D	401	Y8R	O07-C06-C05	-9.85	105.93	122.75
2	B	401	Y8R	O07-C06-C05	-9.85	105.93	122.75
2	D	401	Y8R	O12-C09-C05	-9.80	102.27	120.41
2	B	401	Y8R	O12-C09-C05	-9.78	102.30	120.41
2	B	401	Y8R	C02-C03-C04	-9.63	102.49	112.48
2	D	401	Y8R	C02-C03-C04	-9.62	102.50	112.48
2	A	401	Y8R	O07-C06-C01	-8.81	106.42	120.86
2	B	401	Y8R	O07-C06-C01	-8.34	107.19	120.86
2	D	401	Y8R	O07-C06-C01	-8.34	107.19	120.86
2	C	401	Y8R	O12-C09-C05	-8.03	105.54	120.41
2	A	401	Y8R	O12-C09-C05	-7.24	107.00	120.41
2	C	401	Y8R	C06-C05-C09	-7.06	103.46	121.46
2	A	401	Y8R	O12-C09-C10	-6.58	105.14	119.73
2	B	401	Y8R	O11-C04-C05	-6.21	109.07	121.91
2	D	401	Y8R	O11-C04-C05	-6.21	109.09	121.91
2	A	401	Y8R	C06-C05-C04	-6.06	112.59	119.27
2	D	401	Y8R	C06-C05-C09	-5.61	107.16	121.46
2	B	401	Y8R	C06-C05-C09	-5.60	107.19	121.46
2	A	401	Y8R	O07-C06-C05	-4.98	114.24	122.75
2	C	401	Y8R	O11-C04-C03	-4.83	103.40	114.49
2	A	401	Y8R	O11-C04-C05	-4.49	112.64	121.91
2	C	401	Y8R	O12-C09-C10	-4.02	110.82	119.73
2	B	401	Y8R	O12-C09-C10	-3.89	111.10	119.73
2	D	401	Y8R	O12-C09-C10	-3.88	111.12	119.73
2	A	401	Y8R	O11-C04-C03	-3.80	105.77	114.49
2	C	401	Y8R	C06-C05-C04	-3.76	115.12	119.27
2	A	401	Y8R	C02-C03-C04	-3.05	109.32	112.48
2	A	401	Y8R	C09-C05-C04	-3.00	112.56	119.67
2	D	401	Y8R	C10-C09-C05	-2.85	114.35	120.43
2	B	401	Y8R	C10-C09-C05	-2.83	114.39	120.43
2	C	401	Y8R	O11-C04-C05	-2.74	116.24	121.91
4	B	403	AKG	C3-C4-C5	-2.57	108.06	113.60
4	C	403	AKG	C4-C3-C2	-2.51	108.31	113.03
2	C	401	Y8R	C09-C05-C04	-2.50	113.74	119.67
4	A	403	AKG	O2-C1-C2	2.31	120.28	113.97
4	D	403	AKG	C3-C4-C5	-2.31	108.64	113.60
4	A	403	AKG	C3-C2-C1	2.27	120.18	115.97
4	C	403	AKG	C3-C2-C1	2.22	120.09	115.97
4	C	403	AKG	C3-C4-C5	-2.18	108.92	113.60
4	D	403	AKG	O4-C5-C4	2.10	120.79	114.03
4	B	403	AKG	O2-C1-C2	2.04	119.54	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	403	AKG	C3-C2-C1	2.02	119.72	115.97
4	D	403	AKG	O2-C1-C2	2.02	119.49	113.97
4	B	403	AKG	C3-C2-C1	2.00	119.69	115.97
4	A	403	AKG	C4-C3-C2	-2.00	109.26	113.03

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Y8R	C04-C05-C09-C10
2	C	401	Y8R	C04-C05-C09-C10
4	A	403	AKG	O2-C1-C2-C3
4	A	403	AKG	C2-C3-C4-C5
2	B	401	Y8R	C04-C05-C09-C10
2	D	401	Y8R	C04-C05-C09-C10
2	A	401	Y8R	C06-C05-C09-C10
2	A	401	Y8R	C06-C05-C09-O12
2	B	401	Y8R	C06-C05-C09-O12
2	C	401	Y8R	C06-C05-C09-C10
2	D	401	Y8R	C06-C05-C09-O12
2	C	401	Y8R	C04-C05-C09-O12
2	B	401	Y8R	C06-C05-C09-C10
2	C	401	Y8R	C06-C05-C09-O12
2	D	401	Y8R	C06-C05-C09-C10
4	C	403	AKG	C3-C4-C5-O3
2	A	401	Y8R	C04-C05-C09-O12
2	B	401	Y8R	C04-C05-C09-O12
2	D	401	Y8R	C04-C05-C09-O12
4	C	403	AKG	C3-C4-C5-O4
4	A	403	AKG	C3-C4-C5-O3
4	A	403	AKG	C3-C4-C5-O4

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	AKG	1	0
2	D	401	Y8R	1	0
4	A	403	AKG	1	0
4	C	403	AKG	1	0
2	C	401	Y8R	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^{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	347/348 (99%)	-1.06	0	100	100	19, 33, 53, 86	0
1	B	348/348 (100%)	-1.08	0	100	100	17, 29, 52, 84	0
1	C	346/348 (99%)	-1.08	0	100	100	19, 32, 53, 96	0
1	D	348/348 (100%)	-1.11	0	100	100	15, 30, 50, 94	0
All	All	1389/1392 (99%)	-1.08	0	100	100	15, 31, 53, 96	0

There are no RSRZ outliers to report.

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
2	Y8R	D	401	11/11	0.97	0.06	29,32,38,39	0
4	AKG	A	403	10/10	0.97	0.12	20,24,25,26	0
2	Y8R	C	401	11/11	0.98	0.05	29,32,38,39	0
2	Y8R	A	401	11/11	0.98	0.06	37,38,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	Y8R	B	401	11/11	0.98	0.06	29,32,38,39	0
4	AKG	B	403	10/10	0.98	0.06	17,19,26,28	0
4	AKG	C	403	10/10	0.98	0.05	19,21,24,25	0
4	AKG	D	403	10/10	0.99	0.04	19,21,24,24	0
3	CO	A	402	1/1	1.00	0.02	36,36,36,36	0
3	CO	B	402	1/1	1.00	0.03	16,16,16,16	0
3	CO	C	402	1/1	1.00	0.01	24,24,24,24	0
3	CO	D	402	1/1	1.00	0.03	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.