



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:16 AM GMT

PDB ID : 3E04
Title : Crystal structure of human fumarate hydratase
Authors : Kavanagh, K.L.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2008-07-30
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

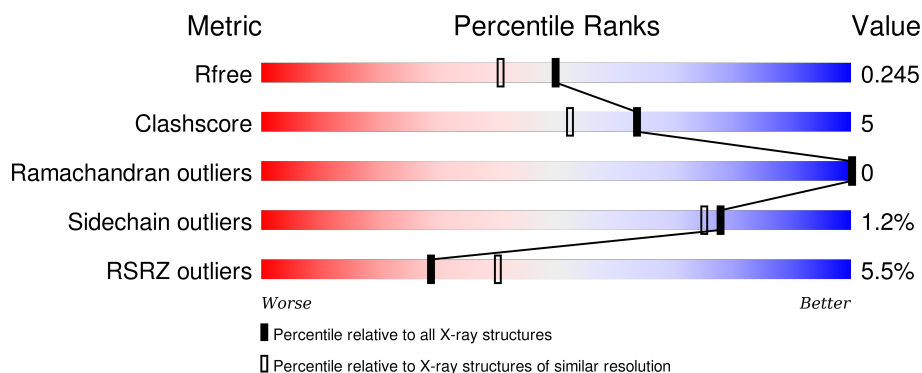
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 ≥ 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	490	<div> <div>5%</div> <div>80% 12% 7%</div> </div>
1	B	490	<div> <div>6%</div> <div>82% 11% 7%</div> </div>
1	C	490	<div> <div>4%</div> <div>78% 7% 15%</div> </div>
1	D	490	<div> <div>6%</div> <div>84% 9% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	1	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13827 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 Fumarate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	1	0
			3380	2133	587	639	21			
1	B	454	Total	C	N	O	S	0	1	0
			3350	2108	586	634	22			
1	C	415	Total	C	N	O	S	0	0	0
			3063	1929	533	579	22			
1	D	459	Total	C	N	O	S	0	1	1
			3367	2121	582	642	22			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	EXPRESSION TAG	UNP P07954
A	22	HIS	-	EXPRESSION TAG	UNP P07954
A	23	HIS	-	EXPRESSION TAG	UNP P07954
A	24	HIS	-	EXPRESSION TAG	UNP P07954
A	25	HIS	-	EXPRESSION TAG	UNP P07954
A	26	HIS	-	EXPRESSION TAG	UNP P07954
A	27	HIS	-	EXPRESSION TAG	UNP P07954
A	28	SER	-	EXPRESSION TAG	UNP P07954
A	29	SER	-	EXPRESSION TAG	UNP P07954
A	30	GLY	-	EXPRESSION TAG	UNP P07954
A	31	VAL	-	EXPRESSION TAG	UNP P07954
A	32	ASP	-	EXPRESSION TAG	UNP P07954
A	33	LEU	-	EXPRESSION TAG	UNP P07954
A	34	GLY	-	EXPRESSION TAG	UNP P07954
A	35	THR	-	EXPRESSION TAG	UNP P07954
A	36	GLU	-	EXPRESSION TAG	UNP P07954
A	37	ASN	-	EXPRESSION TAG	UNP P07954
A	38	LEU	-	EXPRESSION TAG	UNP P07954
A	39	TYR	-	EXPRESSION TAG	UNP P07954
A	40	PHE	-	EXPRESSION TAG	UNP P07954
A	41	GLN	-	EXPRESSION TAG	UNP P07954

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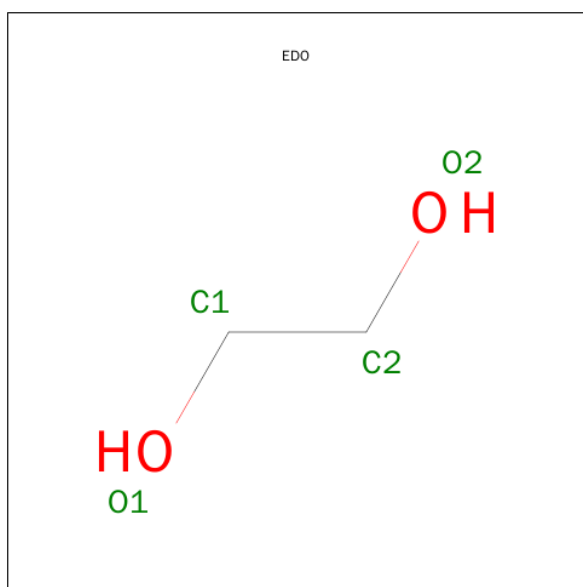
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	-	EXPRESSION TAG	UNP P07954
A	43	MET	-	EXPRESSION TAG	UNP P07954
B	21	MET	-	EXPRESSION TAG	UNP P07954
B	22	HIS	-	EXPRESSION TAG	UNP P07954
B	23	HIS	-	EXPRESSION TAG	UNP P07954
B	24	HIS	-	EXPRESSION TAG	UNP P07954
B	25	HIS	-	EXPRESSION TAG	UNP P07954
B	26	HIS	-	EXPRESSION TAG	UNP P07954
B	27	HIS	-	EXPRESSION TAG	UNP P07954
B	28	SER	-	EXPRESSION TAG	UNP P07954
B	29	SER	-	EXPRESSION TAG	UNP P07954
B	30	GLY	-	EXPRESSION TAG	UNP P07954
B	31	VAL	-	EXPRESSION TAG	UNP P07954
B	32	ASP	-	EXPRESSION TAG	UNP P07954
B	33	LEU	-	EXPRESSION TAG	UNP P07954
B	34	GLY	-	EXPRESSION TAG	UNP P07954
B	35	THR	-	EXPRESSION TAG	UNP P07954
B	36	GLU	-	EXPRESSION TAG	UNP P07954
B	37	ASN	-	EXPRESSION TAG	UNP P07954
B	38	LEU	-	EXPRESSION TAG	UNP P07954
B	39	TYR	-	EXPRESSION TAG	UNP P07954
B	40	PHE	-	EXPRESSION TAG	UNP P07954
B	41	GLN	-	EXPRESSION TAG	UNP P07954
B	42	SER	-	EXPRESSION TAG	UNP P07954
B	43	MET	-	EXPRESSION TAG	UNP P07954
C	21	MET	-	EXPRESSION TAG	UNP P07954
C	22	HIS	-	EXPRESSION TAG	UNP P07954
C	23	HIS	-	EXPRESSION TAG	UNP P07954
C	24	HIS	-	EXPRESSION TAG	UNP P07954
C	25	HIS	-	EXPRESSION TAG	UNP P07954
C	26	HIS	-	EXPRESSION TAG	UNP P07954
C	27	HIS	-	EXPRESSION TAG	UNP P07954
C	28	SER	-	EXPRESSION TAG	UNP P07954
C	29	SER	-	EXPRESSION TAG	UNP P07954
C	30	GLY	-	EXPRESSION TAG	UNP P07954
C	31	VAL	-	EXPRESSION TAG	UNP P07954
C	32	ASP	-	EXPRESSION TAG	UNP P07954
C	33	LEU	-	EXPRESSION TAG	UNP P07954
C	34	GLY	-	EXPRESSION TAG	UNP P07954
C	35	THR	-	EXPRESSION TAG	UNP P07954
C	36	GLU	-	EXPRESSION TAG	UNP P07954
C	37	ASN	-	EXPRESSION TAG	UNP P07954

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Chain	Residue	Modelled	Actual	Comment	Reference
C	38	LEU	-	EXPRESSION TAG	UNP P07954
C	39	TYR	-	EXPRESSION TAG	UNP P07954
C	40	PHE	-	EXPRESSION TAG	UNP P07954
C	41	GLN	-	EXPRESSION TAG	UNP P07954
C	42	SER	-	EXPRESSION TAG	UNP P07954
C	43	MET	-	EXPRESSION TAG	UNP P07954
D	21	MET	-	EXPRESSION TAG	UNP P07954
D	22	HIS	-	EXPRESSION TAG	UNP P07954
D	23	HIS	-	EXPRESSION TAG	UNP P07954
D	24	HIS	-	EXPRESSION TAG	UNP P07954
D	25	HIS	-	EXPRESSION TAG	UNP P07954
D	26	HIS	-	EXPRESSION TAG	UNP P07954
D	27	HIS	-	EXPRESSION TAG	UNP P07954
D	28	SER	-	EXPRESSION TAG	UNP P07954
D	29	SER	-	EXPRESSION TAG	UNP P07954
D	30	GLY	-	EXPRESSION TAG	UNP P07954
D	31	VAL	-	EXPRESSION TAG	UNP P07954
D	32	ASP	-	EXPRESSION TAG	UNP P07954
D	33	LEU	-	EXPRESSION TAG	UNP P07954
D	34	GLY	-	EXPRESSION TAG	UNP P07954
D	35	THR	-	EXPRESSION TAG	UNP P07954
D	36	GLU	-	EXPRESSION TAG	UNP P07954
D	37	ASN	-	EXPRESSION TAG	UNP P07954
D	38	LEU	-	EXPRESSION TAG	UNP P07954
D	39	TYR	-	EXPRESSION TAG	UNP P07954
D	40	PHE	-	EXPRESSION TAG	UNP P07954
D	41	GLN	-	EXPRESSION TAG	UNP P07954
D	42	SER	-	EXPRESSION TAG	UNP P07954
D	43	MET	-	EXPRESSION TAG	UNP P07954

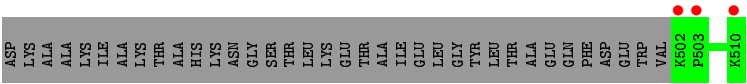
- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



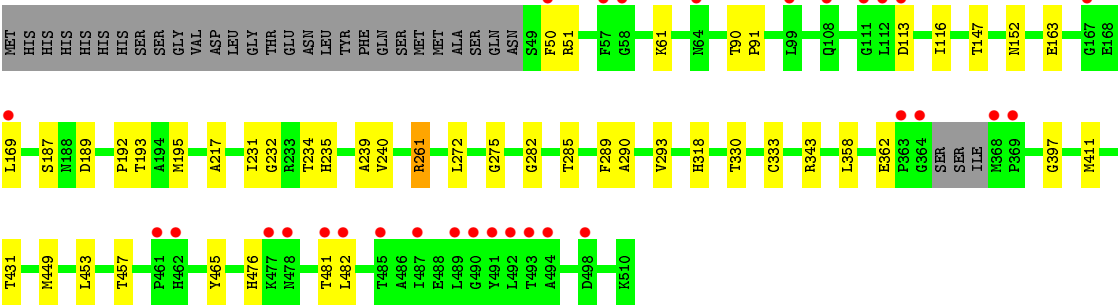
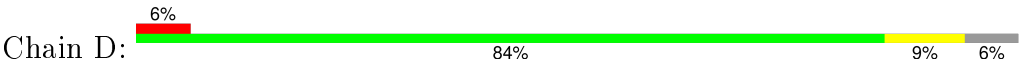
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	174	Total	O	0	0
			174	174		
3	C	161	Total	O	0	0
			161	161		
3	D	168	Total	O	0	0
			168	168		



● Molecule 1: Fumarate hydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.48Å 188.48Å 114.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.95 24.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-1.95) 99.3 (24.89-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.244 0.200 , 0.245	Depositor DCC
R_{free} test set	1995 reflections (1.20%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
Estimated twinning fraction	0.245 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 168620 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13827	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/3443	0.70	0/4672
1	B	0.70	0/3409	0.72	0/4623
1	C	0.68	0/3116	0.71	3/4226 (0.1%)
1	D	0.69	0/3429	0.70	5/4656 (0.1%)
All	All	0.69	0/13397	0.71	8/18177 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	189	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	51	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	261	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	411	MET	CG-SD-CE	-5.12	92.02	100.20
1	D	189	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	51	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	425	ASP	CB-CG-OD1	5.08	122.87	118.30

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	3380	0	3347	54	0
1	B	3350	0	3323	35	0
1	C	3063	0	3041	26	0
1	D	3367	0	3305	35	0
2	A	8	0	12	0	0
2	B	4	0	6	7	0
3	A	152	0	0	1	0
3	B	174	0	0	1	0
3	C	161	0	0	0	0
3	D	168	0	0	2	0
All	All	13827	0	13034	137	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 5.

All (137) 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:231:ILE:HG12	1:A:454:MET:HE2	1.37	1.04
1:A:231:ILE:HG12	1:A:454:MET:CE	1.98	0.94
1:A:277:THR:HG21	1:A:285:THR:HG23	1.56	0.87
1:A:497:PHE:CE2	1:A:501:VAL:HG11	2.13	0.83
1:A:231:ILE:HD11	1:A:452:SER:HB3	1.61	0.82
1:A:360:GLU:OE2	1:A:372:VAL:HG21	1.80	0.81
1:D:147:THR:HG23	1:D:187:SER:CB	2.14	0.77
1:C:289:PHE:O	1:C:293:VAL:HG23	1.88	0.74
1:B:368:MET:HE3	2:B:1:EDO:H11	1.70	0.73
1:A:231:ILE:CG1	1:A:454:MET:HE2	2.18	0.72
1:B:186:SER:O	1:B:190:THR:HG23	1.92	0.69
1:A:501:VAL:O	1:A:501:VAL:HG13	1.92	0.69
1:A:360:GLU:OE2	1:A:372:VAL:CG2	2.43	0.67
1:C:231:ILE:HD11	1:C:239:ALA:O	1.96	0.66
1:A:497:PHE:O	1:A:501:VAL:HG12	1.96	0.65
1:B:486:ALA:HB1	1:B:492:LEU:HD11	1.78	0.65
1:C:446:ASN:O	1:C:449:MET:HB3	1.97	0.64
1:A:240:VAL:HG13	1:C:368:MET:CE	2.28	0.63
1:A:360:GLU:HG3	1:A:372:VAL:HG21	1.80	0.63
1:A:231:ILE:CD1	1:A:452:SER:HB3	2.29	0.62
1:D:289:PHE:O	1:D:293:VAL:HG23	2.00	0.61
1:A:277:THR:CG2	1:A:285:THR:HG23	2.29	0.61
1:D:192:PRO:HA	1:D:195:MET:CE	2.32	0.60
1:C:397:GLY:HA3	1:C:411:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLU:HB2	1:D:169:LEU:HD11	1.82	0.59
1:A:231:ILE:HD12	1:C:351:SER:OG	2.04	0.58
1:D:282:GLY:O	1:D:285:THR:HG22	2.03	0.58
1:B:72:THR:O	1:B:76:THR:HG23	2.04	0.57
1:B:147:THR:HG23	1:B:187:SER:CB	2.34	0.56
1:A:225:PHE:HB3	1:A:244:LEU:HB3	1.87	0.56
1:C:282:GLY:O	1:C:285:THR:HG22	2.06	0.56
1:B:368:MET:CE	2:B:1:EDO:H11	2.36	0.55
1:A:241:PRO:HG3	1:A:454:MET:HE3	1.88	0.55
1:B:486:ALA:CB	1:B:492:LEU:HD11	2.37	0.55
1:C:143:THR:HG23	1:C:148:GLN:OE1	2.07	0.54
1:B:367:ILE:HG22	1:D:457:THR:HG23	1.88	0.54
1:B:282:GLY:O	1:B:285:THR:HG22	2.07	0.54
1:A:474:THR:HB	1:A:485:THR:HG21	1.90	0.54
1:A:240:VAL:HG13	1:C:368:MET:HE2	1.89	0.53
1:A:239:ALA:C	1:C:368:MET:HE2	2.28	0.53
1:D:192:PRO:HA	1:D:195:MET:HE2	1.90	0.53
1:A:188:ASN:HD21	2:B:1:EDO:C1	2.22	0.52
1:D:397:GLY:HA3	1:D:411:MET:HE1	1.91	0.52
1:D:231:ILE:HD11	1:D:239:ALA:O	2.10	0.52
1:C:409:LYS:HB2	1:C:410:PRO:HD3	1.92	0.52
1:A:277:THR:CG2	1:A:285:THR:CG2	2.88	0.51
1:D:289:PHE:CZ	1:D:293:VAL:HG21	2.45	0.51
1:A:192:PRO:HA	1:A:195:MET:CE	2.40	0.51
1:D:195:MET:HE1	1:D:318:HIS:CE1	2.46	0.51
1:A:240:VAL:HG13	1:C:368:MET:HE3	1.91	0.51
1:D:217:ALA:CB	1:D:431:THR:HG23	2.42	0.50
1:B:217:ALA:HB2	1:B:431:THR:HG23	1.93	0.49
1:D:453:LEU:HD11	1:D:476:HIS:HB2	1.93	0.49
1:D:453:LEU:CD1	1:D:476:HIS:HB2	2.41	0.49
1:A:82:GLY:HA3	1:A:86:GLU:HG3	1.93	0.49
1:A:308:ALA:O	1:A:311:LYS:NZ	2.41	0.48
3:A:566:HOH:O	2:B:1:EDO:H22	2.12	0.48
1:A:501:VAL:O	1:A:501:VAL:CG1	2.60	0.48
1:B:367:ILE:HG22	1:D:457:THR:CG2	2.43	0.48
1:A:383:VAL:HG13	1:A:422:LEU:HB3	1.96	0.48
1:B:261:ARG:HD3	1:B:330:THR:HG21	1.95	0.48
1:C:266:MET:N	1:C:267:PRO:CD	2.76	0.48
1:A:361:ASN:HB2	1:A:362:GLU:OE2	2.15	0.47
1:A:72:THR:HG23	1:A:138:LEU:HD21	1.96	0.47
1:A:395:THR:HG23	1:D:333:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:PHE:CD1	1:D:61:LYS:HB3	2.50	0.47
1:A:192:PRO:HA	1:A:195:MET:HE2	1.97	0.47
1:B:217:ALA:CB	1:B:431:THR:HG23	2.45	0.47
1:D:261:ARG:HD3	1:D:330:THR:HG21	1.96	0.47
1:A:492:LEU:HD12	1:A:492:LEU:C	2.34	0.47
1:B:204:HIS:HE2	1:B:270:TYR:HH	1.59	0.46
1:D:192:PRO:HA	1:D:195:MET:HE3	1.96	0.46
1:C:397:GLY:HA3	1:C:411:MET:CE	2.44	0.46
1:C:266:MET:N	1:C:267:PRO:HD3	2.31	0.46
1:D:358:LEU:HD12	3:D:555:HOH:O	2.15	0.46
1:A:266:MET:N	1:A:267:PRO:CD	2.79	0.46
1:B:486:ALA:HB1	1:B:492:LEU:CD1	2.45	0.46
1:A:283:LEU:CD2	1:D:240:VAL:HG11	2.46	0.46
1:B:248:PHE:HA	1:B:251:TYR:CD2	2.51	0.46
1:A:473:LYS:O	1:A:477:LYS:HG2	2.16	0.46
1:D:217:ALA:HB2	1:D:431:THR:HG23	1.97	0.45
1:D:90:THR:N	1:D:91:PRO:CD	2.79	0.45
1:A:113:ASP:HB3	1:A:116:ILE:HD12	1.98	0.45
1:A:237:GLN:HB3	1:C:371:LYS:HG3	1.97	0.45
1:B:449:MET:HE3	1:B:455:LEU:HD11	1.98	0.45
1:A:231:ILE:HG22	1:A:232:GLY:O	2.16	0.45
1:B:397:GLY:HA3	1:B:411:MET:HE1	1.98	0.45
1:A:297:VAL:HG12	1:A:305:PHE:CD2	2.50	0.45
1:B:191:PHE:N	1:B:192:PRO:HD2	2.32	0.45
1:A:351:SER:CB	1:C:231:ILE:HG21	2.47	0.45
1:D:481:THR:HG22	1:D:482:LEU:N	2.32	0.45
1:B:62:VAL:HG22	1:B:73:VAL:HG21	1.98	0.45
1:B:483:LYS:NZ	1:B:498:ASP:OD1	2.50	0.44
1:A:360:GLU:CG	1:A:372:VAL:HG21	2.46	0.44
1:B:203:VAL:HA	1:B:207:LEU:HB3	1.99	0.44
1:A:217:ALA:CB	1:A:431:THR:HG23	2.47	0.44
1:C:239:ALA:O	1:C:454:MET:HG3	2.18	0.44
1:D:232:GLY:O	1:D:239:ALA:HB3	2.17	0.44
1:B:186:SER:O	1:B:190:THR:CG2	2.62	0.44
1:D:113:ASP:HB3	1:D:116:ILE:HG12	2.00	0.44
1:C:212:GLN:HB2	1:C:259:MET:HE3	1.99	0.44
1:B:191:PHE:O	1:B:195:MET:HG3	2.18	0.44
1:B:374:PRO:HD2	1:D:235:HIS:HB3	1.99	0.44
1:C:143:THR:HG21	1:D:362:GLU:OE2	2.19	0.43
1:A:123:ALA:HB3	1:A:157:ILE:HG23	2.01	0.43
1:B:200:ALA:HA	1:B:266:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:THR:HG21	3:D:631:HOH:O	2.19	0.43
1:A:397:GLY:HA3	1:A:411:MET:HE1	2.01	0.42
1:B:409:LYS:HB2	1:B:410:PRO:HD3	2.01	0.42
1:B:369:PRO:HA	1:D:465:TYR:CZ	2.53	0.42
1:A:231:ILE:CG1	1:A:454:MET:CE	2.83	0.42
1:A:456:VAL:HG11	1:A:472:ALA:HB2	2.02	0.42
1:B:368:MET:CE	2:B:1:EDO:C1	2.98	0.42
1:B:114:PRO:O	1:B:118:ASN:ND2	2.52	0.42
1:B:401:GLY:HA3	3:B:518:HOH:O	2.19	0.42
1:D:343:ARG:HH11	1:D:343:ARG:HD3	1.73	0.42
1:D:193:THR:HG23	1:D:272:LEU:HD22	2.01	0.42
1:B:160:ARG:NH1	1:B:164:MET:HG3	2.35	0.42
1:C:371:LYS:NZ	1:C:373:ASN:OD1	2.45	0.42
1:C:277:THR:HG21	1:C:285:THR:HB	2.01	0.41
1:D:231:ILE:HB	1:D:449:MET:HA	2.02	0.41
1:A:411:MET:HE3	1:A:412:MET:HG3	2.01	0.41
1:C:96:PHE:CG	1:C:153:VAL:HG21	2.55	0.41
1:C:196:HIS:HB3	1:C:269:ILE:O	2.20	0.41
2:B:1:EDO:HO1	1:D:234:THR:CB	2.34	0.41
1:D:275:GLY:HA3	1:D:290:ALA:HB2	2.03	0.41
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.88	0.41
1:A:191:PHE:O	1:A:195:MET:HG3	2.21	0.41
1:A:154:ASN:HA	1:A:181:VAL:HG11	2.01	0.41
1:A:362:GLU:O	1:A:372:VAL:HG22	2.21	0.41
1:B:266:MET:N	1:B:267:PRO:CD	2.84	0.41
1:B:368:MET:HE3	2:B:1:EDO:C1	2.44	0.40
1:C:191:PHE:O	1:C:195:MET:HG3	2.20	0.40
1:A:90:THR:N	1:A:91:PRO:CD	2.84	0.40
1:C:231:ILE:CD1	1:C:239:ALA:O	2.67	0.40
1:A:359:PRO:HG3	1:A:437:GLY:HA3	2.02	0.40
1:A:75:SER:HB2	1:A:138:LEU:HD22	2.03	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	453/490 (92%)	441 (97%)	12 (3%)	0	100	100
1	B	449/490 (92%)	434 (97%)	15 (3%)	0	100	100
1	C	411/490 (84%)	397 (97%)	14 (3%)	0	100	100
1	D	456/490 (93%)	443 (97%)	13 (3%)	0	100	100
All	All	1769/1960 (90%)	1715 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/396 (87%)	343 (99%)	3 (1%)	84	83
1	B	345/396 (87%)	335 (97%)	10 (3%)	50	38
1	C	317/396 (80%)	315 (99%)	2 (1%)	90	89
1	D	342/396 (86%)	341 (100%)	1 (0%)	94	94
All	All	1350/1584 (85%)	1334 (99%)	16 (1%)	78	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	184	SER
1	A	362	GLU
1	B	85	THR
1	B	115	LYS
1	B	116	ILE
1	B	152	ASN
1	B	186	SER
1	B	230	LYS
1	B	286	ARG

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Mol	Chain	Res	Type
1	B	307	THR
1	B	404	GLU
1	B	411	MET
1	C	152	ASN
1	C	411	MET
1	D	152	ASN

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	1	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	A	511	-	3,3,3	0.53	0	2,2,2	0.06	0
2	EDO	B	1	-	3,3,3	0.17	0	2,2,2	1.18	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
2	EDO	A	1	-	-	0/1/1/1	0/0/0/0
2	EDO	A	511	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1	-	-	0/1/1/1	0/0/0/0

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.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	EDO	7	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, 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	456/490 (93%)	0.24	24 (5%) 30 41	18, 24, 34, 46	0
1	B	454/490 (92%)	0.14	27 (5%) 26 36	17, 22, 39, 48	0
1	C	415/490 (84%)	0.08	18 (4%) 39 50	18, 23, 38, 53	0
1	D	459/490 (93%)	0.24	30 (6%) 22 32	18, 24, 44, 51	0
All	All	1784/1960 (91%)	0.18	99 (5%) 29 40	17, 23, 38, 53	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	PHE	6.4
1	B	52	ILE	6.3
1	B	461	PRO	5.8
1	B	50	PHE	5.6
1	B	489	LEU	5.5
1	A	372	VAL	5.3
1	D	492	LEU	5.1
1	D	461	PRO	4.8
1	A	364	GLY	4.8
1	C	450	ASN	4.8
1	C	453	LEU	4.5
1	D	487	ILE	4.5
1	A	370	GLY	4.4
1	D	490	GLY	4.3
1	C	365	SER	4.3
1	D	462	HIS	4.2
1	D	493	THR	4.1
1	D	363	PRO	4.0
1	D	478	ASN	4.0
1	A	114	PRO	3.9
1	C	451	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	487	ILE	3.8
1	A	500	TRP	3.7
1	D	477	LYS	3.6
1	D	481	THR	3.5
1	C	366	SER	3.5
1	A	166	GLY	3.4
1	C	364	GLY	3.4
1	A	52	ILE	3.3
1	A	461	PRO	3.3
1	C	52	ILE	3.3
1	A	371	LYS	3.2
1	B	157	ILE	3.1
1	C	287	ILE	3.1
1	C	50	PHE	3.0
1	C	454	MET	3.0
1	C	447	LYS	3.0
1	D	57	PHE	3.0
1	C	58	GLY	3.0
1	D	111	GLY	3.0
1	B	495	GLU	2.9
1	B	478	ASN	2.8
1	C	503	PRO	2.8
1	A	477	LYS	2.8
1	D	489	LEU	2.8
1	B	463	ILE	2.8
1	B	510	LYS	2.8
1	D	491	TYR	2.7
1	B	479	GLY	2.7
1	A	363	PRO	2.7
1	A	227	GLN	2.7
1	B	497	PHE	2.6
1	A	489	LEU	2.6
1	A	495	GLU	2.6
1	D	169	LEU	2.6
1	B	49	SER	2.6
1	A	57	PHE	2.5
1	D	494	ALA	2.5
1	D	482	LEU	2.5
1	D	99	LEU	2.5
1	B	153	VAL	2.5
1	B	491	TYR	2.5
1	A	496	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	498	ASP	2.4
1	C	502	LYS	2.4
1	B	472	ALA	2.4
1	B	486	ALA	2.4
1	D	167	GLY	2.3
1	B	493	THR	2.3
1	A	476	HIS	2.3
1	A	482	LEU	2.2
1	B	498	ASP	2.2
1	A	478	ASN	2.2
1	B	464	GLY	2.2
1	C	448	LEU	2.2
1	D	112	LEU	2.2
1	D	108	GLN	2.2
1	D	64	ASN	2.2
1	A	465	TYR	2.2
1	D	369	PRO	2.1
1	D	58	GLY	2.1
1	A	49	SER	2.1
1	A	490	GLY	2.1
1	A	494	ALA	2.1
1	B	156	VAL	2.1
1	D	113	ASP	2.1
1	C	166	GLY	2.1
1	D	364	GLY	2.1
1	B	471	ILE	2.1
1	B	84	VAL	2.1
1	B	166	GLY	2.1
1	B	115	LYS	2.0
1	C	510	LYS	2.0
1	B	113	ASP	2.0
1	D	368	MET	2.0
1	B	494	ALA	2.0
1	A	60	LEU	2.0
1	C	111	GLY	2.0
1	D	485	THR	2.0

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

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

6.3 Carbohydrates [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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	B	1	4/4	0.83	0.23	10.63	32,32,32,35	0
2	EDO	A	1	4/4	0.89	0.25	1.74	40,42,42,44	0
2	EDO	A	511	4/4	0.92	0.16	1.39	43,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.